Modeling of electron emission : its physics and novel applications

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**NANYANG
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UNIVERSITY**

**MODELING OF ELECTRON EMISSION: ITS PHYSICS
AND NOVEL APPLICATIONS**

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SCHOOL OF ELECTRICAL & ELECTRONIC ENGINEERING

2009

MODELING OF ELECTRON EMISSION: ITS PHYSICS AND NOVEL APPLICATIONS

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SUMMARY

Electrons emitted from the surface of a material subjected to heat, electromagnetic radiation and electric field, are respectively known as thermionic emission, photoemission and field emission. In many applications based on electron emission such as vacuum tubes, thermionic energy conversion systems, field emission displays and electron microscopes, the performance of the device strongly depends on the characteristics of the emitted electrons. This research is aimed at providing an understanding of electron emission physics that is absent from prior studies. Some novel applications are also explored by modeling free-electron based devices. The contributions of the thesis are as follows.

Ultrafast electron microscopy, diffraction and crystallography are able to provide ultrafast time-resolved information of the underlying dynamics in physics, chemistry and biology, with their temporal resolution limited by the duration of the electron pulse. A recent promising method to generate ultrashort electron pulses is to use a low-power femtosecond laser to trigger free electron pulses with duration of 10s femtosecond to attosecond to be emitted from a biased metallic field emitter. Understanding the time-dependent emission process is important to realize the sub-cycle electron pulse which is shorter than laser pulse duration. A consistent

SUMMARY

nonequilibrium model has been developed to clarify the electron emission process of an ultrafast laser excitation on a metallic surface.

For all envisioned novel applications of electron emission, the noise generated by the electron emission process is of scientific interest. In particular for high frequency high power microwave applications using field emitters as electron sources, the characteristics of shot noise for high current space-charge-limited field emission could be important. Our studies on shot noise of field emission consider the effects of both quantum partitioning and Coulomb correlation of the emitted electrons, over a wide range of applied voltages, gap spacings and electron pulse lengths in classical, quantum and relativistic regimes.

For traditional thermionic energy conversion systems (refrigerators), it is difficult to achieve significant commercial success because of the unattainable requirement of low work function (0.3 eV) at room temperature. This research proposes an improved low-temperature refrigeration method based on thermal-field electron emission in a crossed-field gap. Two kinds of geometric designs, planar diode with sharp field emitters and coaxial cylindrical diode, have been investigated. A versatile cooling capability is predicted using arbitrary work function emitters, with local cooling power density of about 600 kW/cm² at 300 K and 20 W/cm² at 10 K, respectively.

In some systems, it is important to avoid unnecessary electron emission. One such example occurs in a high-gradient dielectric-loaded accelerator, with applications ranging from medical accelerators to high-energy physics. During high-power operation of such structures, the avalanche of electrons called multipactor discharge, which is due to secondary electron emission, can absorb a significant fraction (up to 50%) of the incident power. A Monte-Carlo model is used to determine the conditions for multipacting and to explain the experimental observations, as well as to propose methods to suppress the multipactor discharge in the system.

SUMMARY

In short, this thesis provides a deeper understanding of the physics behind the process of various electron emission mechanisms and explores its novel applications. The significance and contribution are summarized as follows:

- A nonequilibrium model is formulated to clarify the electron photo-field emission mechanism for an ultrafast laser excitation on a metallic surface under a dc biased voltage.
- The reduction of shot noise for field emission is studied including the effects of quantum partitioning, Coulomb repulsion and quantum correlation effects.
- A statistical model is used to explain the occurrence of multipactor discharge due to secondary electron emission, and its high power absorption in a dielectric-loaded accelerating structure.
- For applications, a new technique for low-temperature refrigeration is proposed based on thermal-field electron emission in a crossed-field gap.

LIST OF SYMBOLS

Symbol	Unit	Physical Quantity
T	kelvin (K)	temperature
V_g	volt (V)	electric potential difference between electrodes
D	meter (m)	gap spacing between electrodes
F	volt per metre (V/m)	electric field strength in the vacuum gap
E	electronvolt (eV)	total energy of an electron
E_x	electronvolt (eV)	x -direction energy of an electron
$N(E_x)$	$\text{m}^{-2} \text{sec}^{-1}$	number of electrons per unit area and time
$\mathcal{T}(E_x)$	nil	transmission coefficient
ϕ_B	electronvolt (eV)	work function
U_{im}	joule (J)	image charge potential energy
U_{xc}	joule (J)	exchange-correlation potential energy
U_B	joule (J)	potential energy from magnetic field
V_v, U_v	volt (V), joule (J)	external applied potential, potential energy
V_{sc}, U_{sc}	volt (V), joule (J)	space charge potential, potential energy

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CHAPTER 1

INTRODUCTION

1.1 Background and Motivation

Electron emission from solids is a fundamental process in electrical transmission in vacuum. It was among the earliest phenomena to be observed. Much of electronics, including vacuum tubes, cathode ray tubes, and electron microscopes, depend on the emission of electrons from metals, and the manipulation of these electrons to perform various tasks.

The classical example of thermionic emission is the emission of electrons from a hot metal cathode into a vacuum, which is archaically known as the Edison effect. It formed the basis of vacuum tube circuit elements and thermionic energy conversion systems for power generation or refrigeration. In 1904 and 1907, vacuum tube diodes and triodes were invented, which were the basic building blocks of tube-based electronic devices. The relatively large size, cost and complexity had led to their replacement by solid-state semiconductor devices such as transistors and solid-state diodes in many applications after 1960. However, vacuum tubes still reign supreme in specialized applications, namely, high power coherent radiation sources

1.1 Background and Motivation

from millimeter-wave to terahertz frequency [1, 2]; modern audio amplification for their aesthetic appeal; the cathode ray tubes for display devices; the magnetron as the source of microwave energy in all microwave ovens; and the x-ray tubes used in radiography, computed axial tomography (CAT) scanners, airport luggage scanners, x-ray crystallography and industrial inspection.

A thermionic converter consists of a hot electrode that thermionically emits electrons over a potential energy barrier to a cooler electrode, producing a useful electric power output. If one takes the configuration for generation of electricity and drives the current in reverse, it operates as a refrigerator [3]. After the first demonstration of the practical arc-mode caesium vapor thermionic converter by Wilson in 1957, several applications were demonstrated in the following decades, including its use with solar, combustion, radioisotope and nuclear reactor heat sources. A serious application was the integration of thermionic nuclear fuel elements directly into the core of nuclear reactors for production of electrical power in space [4, 5]. The exceptionally high operating temperature of thermionic converters gives the thermionic reactor decisive advantages over other competing energy conversion technologies in the space power application where radiant heat rejection is required.

Photoemission – electron emission from matter after the absorption of energetic photons, forms the basis for photomultiplier and iconoscope, i.e. the early version of the television and video cameras. A television camera for recording electronic moving images is a device for converting photons into electrical signals which operates on the principle of photoemission. A photomultiplier is an extremely sensitive detector of light in the ultraviolet, visible and near infrared range. It can multiply the signal produced by incident light by as much as 10^8 , from which single photons can be resolved. The combination of high gain, low noise, high frequency response and large area of collection meant that these devices are capable of finding applications

1.1 Background and Motivation

in nuclear and particle physics, astronomy, medical imaging and motion picture film scanning (telecine).

Field emission (FE) is the emission of electrons from the surface of a solid into vacuum due to the presence of high electric fields. In this phenomenon, electrons with energies below the Fermi level tunnel through the potential barrier at the surface, which is narrowed sufficiently by the high electric field for the electrons to have a non-negligible tunneling probability. Field emission, sometimes called cold emission or Fowler-Nordheim tunneling, is unique in comparison with thermionic emission or photoemission in which only electrons with sufficient energy to surmount the surface potential barrier are able to escape the solid. Nowadays field emission is the principal means of generating an electron beam for use in displays that are based on field emitter arrays, transmitting and scanning electron microscopes, particle accelerators, and other vacuum microelectronic devices including FE triodes, amplifiers and microwave frequency devices.

The traditional cathode ray tube (CRT) equipped with a phosphorescent screen, has been the basic device for translating electronic signals into visual displays, initially in scientific instrumentation (e.g. oscilloscopes) and later in television and computer screens. The modern flat-panel field emission displays generally replace the thermal cathodes of conventional CRT displays with field emitter arrays, which provide greater life, brightness and focusing ability than the thermionic or photoemission sources. Transmission and scanning electron microscopes employ the optical properties of electrons, notably at shorter wavelength, to produce images of very high resolution. These electron microscopes require an electron beam of maximum brilliance, minimum divergence and high focusing ability, and they continue to place demands on the development of increasingly sophisticated electron beam technology.

1.1 Background and Motivation

Transmission electron microscopy (TEM) with its wide-ranging arsenal of tools has long been a powerful method in many areas of research, allowing for sub-nanometer spatial resolution, but currently it lacks the time-resolved capability. For many applications according to Zewail [6], one must be able to not only resolve the three-dimensional (3D) physical structures but also determine the temporal behavior of the dynamics. To develop a time-resolved electron microscopy, an ultrafast electron source is required, which attracts extensive research interests presently [7, 8, 9, 10, 11, 12, 13, 14]. The combined atomic-scale resolutions in space and time constitute the basis for a new field of study, i.e. four-dimensional (4D) ultrafast electron diffraction, crystallography and microscopy. The joint atomic-scale resolutions in space and time, plus the sensitivity reached, make it possible to determine complex transient structures and assemblies in different phases. Future applications of these methods are foreseen across areas of physics, chemistry and biology.

In addition to the applications of FE as an excellent electron source, field emission microscopy (FEM) and field ion microscopy (FIM) [15] employ field emission to directly investigate the molecular surface structure of an emitter and its electronic properties. In field emission microscopy, the anode incorporates a phosphorous screen, which converts variations in the radiation cone into visible patterns. The field ion microscope, which is capable of a considerably higher level of resolution, also relies on field emission but produces an image from a gas ionized near the surface by emitted electrons, rather than from the electrons themselves. Consequently the FIM is useful for studying spatial relationships at the surface of metallic solids with atomic resolution, and it is a valuable tool for designing more effective emitters. Furthermore, one modern application of FEM is the real-time observation of the vibration of a single adsorbed atom or molecule [16, 17, 18]. The time dependence of electron field emission through an atom or a molecule adsorbed on a metal tip was measured by focusing

1.2 Issues Investigated in this Research

the electrons into a beam, which was swept across a detector screen. In many of the individual recordings, the field emission was found to oscillate with a frequency between 5×10^{10} and 20×10^{10} hertz [16]. The oscillations, which were not observed from a bare tip, are believed to arise from the vibration of a single atom or molecule with respect to the surface [16].

Given the importance of electron emission to numerous critical applications, the motivation of this research work is to acquire an understanding of the physics of electron emission in some unexplored areas.

1.2 Issues Investigated in this Research

This dissertation concerns modeling of electron emission, which bridges the gap between theory of electron emission and its various modern applications. In particular, this thesis will analyze four issues of electron emission, where three of them are closely related to novel applications, and the last one is on an unexpected and undesirable phenomenon. Before any detailed discussions, the theory of electron emission and its recent development will be reviewed briefly in Section 1.3.

It is known that the temporal resolution of the ultrafast electron diffraction, ultrafast electron microscopy and ultrafast crystallography is limited by the duration of the electron pulse [6, 7]. One promising and experimentally realized ultrafast electron source has been recently introduced, which is to use a low-power femtosecond laser oscillator to trigger free electron pulses from sharp field emission sources [11, 12, 13, 14]. Therefore a comprehensive nonequilibrium model [19] is proposed in Chapter 2 to demonstrate the microscopic physics of this new electron emission process, which is a combination of field emission and photoemission.

For high-frequency, high-power microwave applications [20] or the novel femtosecond field emission camera for continuous observation of the motion of individual

1.2 Issues Investigated in this Research

adsorbed atoms and molecules [16, 17, 18], the characteristics of shot noise for a high current electron beam (by field emission) is important, which will be studied in Chapter 3. Shot noise is an electronic noise due to the discreteness of electron charges. Its spectral power density is linearly proportional to the current and independent of the frequency. Our studies on shot noise of high current field emission will consider the effects of both quantum partitioning [21] and Coulomb correlation [22] of the emitted electrons, over a wide range of applied voltages, gap spacings and electron pulse lengths, in classical, quantum and relativistic regimes.

The thermionic energy conversion systems (refrigerator) have never achieved significant commercial success, due to the unattainable requirement of low work function cathode (0.3 eV) at room temperature. In Chapter 4, we present an improved low temperature refrigeration proposal, which is based on thermal-field electron emission in a crossed-field gap. Two kinds of geometric designs, planar diode with sharp field emitters [23] and coaxial cylindrical diode with smooth surface [24], have been investigated. Analytical models and numerical calculations are systematically performed to obtain optimal cooling performance, as a function of the emitter's work function, gap spacing, external bias voltage, and external magnetic field.

Besides all the beneficial applications of electron emission listed above, electron emission needs to be prevented in some systems. One such example is a high-gradient dielectric-loaded accelerator (DLA), with applications ranging from medical accelerators to high-energy physics. During the high-power operation of such structures, an unforeseen avalanche of electrons called multipactor discharge (due to secondary electron emission) was observed [25], which can absorb a significant fraction (up to 50%) of the incident power. In Chapter 5, a Monte-Carlo model is used to explain this multipactor discharge and its large power absorption in the DLA structure [26], which aims to minimize or eliminate its detrimental effects.

1.3 Brief Review on Electron Emission Theory

Finally, Chapter 6 will conclude the current research work by summarizing the four topics studied in this thesis. Further and more in-depth studies from both experimental and theoretical aspects are thereafter suggested for future works.

1.3 Brief Review on Electron Emission Theory

Electron emission from a solid into a vacuum can be divided into four types: (1) thermionic emission, (2) photoelectric emission, (3) secondary emission, and (4) field emission. In all cases, emission occurs as a result of free electrons in the solid acquiring enough energy to overcome the potential energy barriers existing on the surface of the solid. The different forms of emission differ in the source of the energy. When the energy is supplied thermally by heating the solid, it is known as *thermionic* emission. When the energy is received as radiant energy, it is *photoelectric* emission. When the liberating energy is received as the kinetic energy of a bombarding particle, it is called *secondary* emission, as distinguished from (primary) thermionic emission. When the potential energy barrier is lowered by a strong electric field, large electron emission may occur due to tunneling process, and it is called *field* emission.

1.3.1 The Free-Electron Theory of Metals

The free-electron theory of metals [27] proposed by Sommerfeld (1928) [28] has provided the basis for practically all quantum-mechanical theories of electron emission from metals. The theory is based on the assumption that the conduction band electrons behave, effectively and for many practical purposes, as if they were free particles. In this model the electron states (in the conduction band) are described by plane waves ψ_k with wave vector $\vec{k}$, and the energy of the electron is $E = \frac{\hbar^2 k^2}{2m}$. The number of electron states per unit volume with energy between E and $E + dE$

1.3 Brief Review on Electron Emission Theory

is given by [29]

$$\rho(E) dE \equiv \frac{2}{(2\pi)^3} \iiint_E d^3k = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E^{1/2} dE, \quad (1.1)$$

where $\hbar = h/2\pi$ is reduced Planck's constant and m is electron rest mass. The probability of an electron state with energy E being occupied (at equilibrium) is given by the Fermi-Dirac distribution function

$$f(E) = \frac{1}{1 + \exp[(E - E_F)/k_B T]}, \quad (1.2)$$

where k_B is Boltzmann's constant, T is the absolute temperature, and E_F is the Fermi energy level (referring to the energy of the highest occupied quantum state at absolute zero temperature).

For the subsequent development of the theory of electron emission from metal surfaces, the number of electrons (under equilibrium conditions) across a unit area (parallel to the yz plane) from left to right, per unit time, with total energy between E and $E + dE$ and normal energy $E_x = \frac{\hbar^2 k_x^2}{2m}$ between E_x and $E_x + dE_x$ is given by

$$N(E, E_x) dE dE_x \equiv \frac{2f(E)}{(2\pi)^3} \iiint_{E, E_x} v_x d^3k = \frac{m}{2\pi^2 \hbar^3} f(E) dE dE_x, \quad (1.3)$$

where v_x is the velocity of the electron normal to the unit area under consideration, and $[E, E_x]$ indicates that only states with total energy between E and $E + dE$ and normal energy between E_x and $E_x + dE_x$ are to be included in the integration. Therefore the total number of electrons with normal energy between E_x and $E_x + dE_x$ at equilibrium condition is

$$\begin{aligned} N(E_x) dE_x &= \frac{m dE_x}{2\pi^2 \hbar^3} \int_{E_x}^{\infty} f(E) dE \\ &= \frac{mk_B T}{2\pi^2 \hbar^3} \ln \left[1 + \exp \left(- \frac{E_x - E_F}{k_B T} \right) \right] dE_x. \end{aligned} \quad (1.4)$$

Here for electrons with normal energy E_x far above or below the Fermi energy level E_F , the expression can be simplified

$$\ln \left[1 + \exp \left(- \frac{E_x - E_F}{k_B T} \right) \right] \simeq \begin{cases} \exp \left[- (E_x - E_F)/k_B T \right] & \text{if } E_x \gg E_F \\ -(E_x - E_F)/k_B T & \text{if } E_x \ll E_F \end{cases} \quad (1.5)$$

1.3 Brief Review on Electron Emission Theory

In Fig. 1.1 [left], the term $N(E_x, T)$ is plotted as function of the electron normal energy E_x for three different temperatures $T = 300, 1000$ and 2000 K. It shows that $N(E_x, T)$ changes slowly (i.e. linearly) with E_x for small E_x , with similar values for different temperatures; while it drops drastically (i.e. exponentially) as E_x increases to above E_F , and varies with temperature prominently.

1.3.2 Electron Emission from a Metal Surface

Consider a semi-infinite metal occupying the half-space from $x = -\infty$ to $x \approx 0$. According to the free-electron theory of metals, an electron inside the metal sees a constant (zero) potential. At zero temperature, a certain minimum energy equal to the work function ϕ_B , must be supplied to the metal before an electron can escape from it. From the classical electrostatics, an electron situated at a finite distance from the plane surface of a perfect conductor is attracted to it, by the well-known “image” potential: $-e^2/16\pi\epsilon_0 x$, where the minus sign arises because we have assumed that the x axis points outwards from the metal. Hence the potential energy of the electron on the vacuum side of the metal-vacuum interface is asymptotically given by

$$U(x) \simeq E_F + \phi_B - \frac{e^2}{16\pi\epsilon_0 x}, \quad (1.6)$$

which is graphically shown in Fig. 1.1 [right] using the dashed line. In 1970s, a lot of effort were put into microscopic studies of the potential barrier at a metal-vacuum interface [30, 31, 32, 33, 34], which confirmed that Eq. (1.6) is valid for $x > 3 \text{ \AA}$. The detailed profile of the barrier for $x < 3 \text{ \AA}$ depends on the properties of metal surface under consideration. In the traditional (free-electron) theories of electron emission, it is assumed that Eq. (1.6) remains valid right up to a point x_c such that $U(x_c) = 0$.

1.3 Brief Review on Electron Emission Theory

Figure 1.1: [Left] The number of electrons $N(E_x)$ with normal energy between E_x and $E_x + dE_x$ impinging on the surface barrier at $T = 300, 1000$, and 2000 K. [Right] The surface potential energy barrier seen by an electron in a field emission experiment (solid line), which is the summation of the image charge potential energy (dashed line) and applied electric field ($F = 5$ V/nm) potential energy (dash-dotted line).

1.3 Brief Review on Electron Emission Theory

When an external electric field $F > 0$ is applied to the surface, an electrostatic term of $-eFx$ is added on the right of Eq. (1.6), which becomes

$$\begin{aligned} U(x) &\simeq E_F + \phi_B - \frac{e^2}{16\pi\epsilon_0 x} - eFx & \text{for } x > x_c \\ &\simeq 0 & \text{for } x < x_c \end{aligned} \quad (1.7)$$

where x_c is determined by $U(x_c) = 0$. In Fig. 1.1 [right] we show this potential energy barrier (solid line) for a typical value of $E_F = 5.782$ eV, $\phi_B = 4.40$ eV and the applied field $F = 5.0$ V/nm. The resultant energy barrier having a maximum at a distance x_m from the cathode shows a reduction in magnitude by an amount of $\Delta\phi_B$. This may be considered as work function reduction by the presence of the external field. Note in this large electric field case, the potential energy barrier through which the tunneling occurs could be located very close to the cathode-vacuum interface ($x < 3$ Å), where the charge density is quite high due to the “spillover” effects [35]. To elaborate, the conduction electrons of a real metal spill over, via quantum-mechanical behavior penetration, into the vacuum for a very short distance (< 5 Å). In this immediate vicinity of the surface the density of “spillover” electrons is far higher than that of “tunneling” electrons, and thus the “spillover” electrons must have the dominant electrostatic effect. But the classical concept of image charge force in Eq. (1.7) assumes that the electrode is an electrostatically-ideal metal with an infinite screening capacity, which imposes an artificial separation of electrons and leads image-force theory to overemphasize the electrostatic effect of the tunneling electron. It needs to be improved by a density-gradient analysis [35] or the Green function method [36].

As the electric field is negligible inside the metal, it is assumed that the number of electrons with normal energy between E_x and $E_x + dE_x$ impinging on the surface barrier from within the metal is practically identical with its equilibrium value given

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in Eq. (1.4). Each of these electrons has a probability $\mathcal{T}(E_x)$ to be transmitted through the surface potential barrier that is given by either Eq. (1.6) or Eq. (1.7).

For a general analysis of electron emission phenomena, a useful method leading to an analytic expression for the transmission coefficient was developed by Miller and Good (1953) [37], which has been extensively used in the study of electron emission. Their method is a generalization of the ordinary WKB (Wentzel, Kramers and Brillouin) method (1926) and it leads to the WKB results under certain limiting conditions. Their theory applies to the case of a slowly varying potential barrier, with only two classical turning points. This means that there are only two real roots of the equation $E_x - U(x) = 0$, when E_x lies below the top of the barrier. We denote them by x_1 and x_2 with $x_1 < x_2$. It is assumed that when E_x goes above the top of the barrier, the two real roots go unambiguously into two complex roots. When conditions for the applicability of their method are satisfied, for example, in the case of the barrier shown in Fig. 1.1, the transmission coefficient is given to a good approximation by the following formula

$$\mathcal{T}(E_x) = \left\{ 1 + \exp [\Lambda(E_x)] \right\}^{-1},$$

where $\Lambda(E_x) = -2i \int_{x_1}^{x_2} \Theta(x) dx$ and $\Theta(x) = \sqrt{\frac{2m}{\hbar^2} [E_x - U(x)]}$, (1.8)

and the normal energy E_x may lie above or below the top of the barrier. In performing the integration of x , one must remember that x_1 and x_2 hence x are complex when E_x lies above the top of the barrier. One can easily show that $\Lambda(E_x)$ is always real and that it is negative for energies above the top of the barrier, and positive for energies below the top of the barrier. It is also obvious that when the energy E_x lies well below the barrier top, we have $\exp [\Lambda(E_x)] \gg 1$ and Eq. (1.8) reduces to

$$\mathcal{T}(E_x) \simeq \exp \left[-2 \int_{x_1}^{x_2} |\Theta(x)| dx \right], \quad (1.9)$$

which can be obtained by the ordinary WKB method [38]. Recently, an even more convenient approach to estimate $\mathcal{T}(E_x)$ was suggested by Jensen [39, 40], using a

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linear expansion of $\Lambda(E_x)$ through the barrier maximum. It performs rather well for a typical potential energy barrier profile as shown in Eq. (1.7) [39].

Hence, the emitted current density, i.e., the number of electrons emitted per unit area per unit time, multiplied by the magnitude of the electronic charge, is given by

$$J(F, T) = e \int_0^\infty N(E_x, T) \mathcal{T}(E_x) dE_x, \quad (1.10)$$

where T and F denote the temperature and the applied field, respectively. Murphy and Good (1956) [41] have shown that if one assumes the validity of the surface barrier given by Eq. (1.7), and uses Eq. (1.8) for the calculation of the transmission coefficient for this barrier, one obtains, starting from Eq. (1.10), an expression for $J(F, T)$ valid for any values of F and T . The Murphy and Good theory leads in a systematic way to the Fowler-Nordheim formula for field emission, i.e. emission at very low temperatures with a strong applied field, and to the Richardson and Schottky formulas for thermionic emission, i.e. emission at high temperatures with a weak or zero applied field.

1.3.3 Thermionic and Field Emission

The physical picture of thermionic emission is simply that, as the temperature of the emitter is raised (usually by electrical heating), some of the electrons in the conduction band acquire a greater energy than others. The high-energy electrons may have velocities of sufficient magnitude and of suitable direction to permit them to surmount the surface potential energy barrier.

It has already been indicated in Fig. 1.1 that the distribution of x -direction energies among electrons in the conduction band of metals is a function of temperature, and there is a potential energy barrier (dashed line) that electrons must overcome before they can escape. At zero temperature the function $N(E_x)$ is a straight line from a finite number of electrons at zero energy to zero electrons at the Fermi level.

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For higher temperatures ($T = 300, 1000$ and 2000 K) the curve extends its toe above the Fermi energy level as shown. At high temperatures and weak applied fields most of the contribution to the $J(F, T)$ comes from a very narrow region of energy at the top of the surface potential barrier. By considering $E_x \gg E_F$ for the electrons with enough energy to escape, a theoretical analysis of the Eq. (1.4) [42] gives a universal equation for electron emission current density as a function of temperature T and work function ϕ_B , of the form

$$J_{\text{RLD}} = A_e T^2 \exp \left[- \frac{\phi_B}{k_B T} \right], \quad (1.11)$$

where J_{RLD} is current density of emitted current (A cm^{-2}), A_e is a constant of theoretical value $120 \text{ A cm}^{-2} \text{ K}^{-2}$, k_B is Boltzmann's constant, $1.38 \times 10^{-23} \text{ J K}^{-1}$, ϕ_B is work function (eV) and T is temperature (K). This is known as the Richardson-Laue-Dushman equation for thermionic emission [43]. The value of the current density is influenced by the exponential term and is accordingly a sensitive function of the work function and the temperature. For years, in the field of thermionic emission, a great deal of efforts have been devoted to search for low work function materials with a high melting temperature [44].

It was shown in Section 1.3.2 that, if there is an electric field at an emitter surface, the emission is increased giving the effect of a reduced work function. This can be considered as equivalent to an increased temperature as implied in Eq. (1.11). Accordingly, it is expected that, if the field is made strong enough, there may be found emission of electrons at room temperature. This is indeed the case and such emission is called field emission.

For field emission, the height of the potential energy barrier will be reduced to nearly the Fermi level within the emitter, and the width of the barrier above this level will be very narrow. Since at room temperature the electrons in the emitter will not have enough excess energy to climb even a low barrier, emission will occur by tunneling

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through the barrier. From Fig. 1.1 [left] that for sufficiently low temperatures, the supply function $N(E_x, T)$ diminishes rapidly for $E_x > E_F$. And for a typical surface barrier ($\phi_B = 4.4$ eV, $F = 5$ V/nm), $\mathcal{T}(E_x, F)$ diminishes rapidly for $E_x < E_F$. Therefore most of the contribution to the integral Eq. (1.10) comes from the immediate neighborhood of the Fermi level. Based on this concept, a theoretical formula similar to the thermionic emission equation has been developed by Fowler and Nordheim [45]

$$J_{\text{FN}} = A' F^2 \exp \left[- B' \phi_B^{3/2} / F \right], \quad (1.12)$$

where $A' \equiv e^3 / [16\pi^2 \hbar \phi_B t^2(y)]$ and $B' \equiv \frac{4}{3e} \left(\frac{2m}{\hbar^2} \right)^{1/2} v(y)$

and numerical values of $t(y)$ and $v(y)$ with $y = \sqrt{e^3 F} / \phi_B$ are listed in the literature by Burgess, Kroemer and Houston [46]. This well-known Fowler-Nordheim equation is one of the most important equations in electron emission theory and has found many applications [29].

In contrast to the thermionic emission, the main research interests in field emission involve (i) theory of field emission from nonplanar cathodes [47, 48, 49, 50], e.g. atomically sharp aluminum tips [51], carbon nanotubes [52, 53], and knife-edge field emitters [54], which is complicated by geometric field enhancement and changes in the image force; (ii) space-charge effects of an intense electron beam in high current field emission [55, 56, 57, 58, 59, 60]; (iii) development of field emitter arrays and the various applications [61, 62, 63, 64, 65, 20]; (iv) the stabilization of the emission current, i.e. to reduce the flicker noise and minimize the local temporal change of the work function [44] by means of reducing the number of migrating atoms on surface; (v) simulation of field emission through an oscillating barrier [66, 67, 68, 69].

Electron emission at intermediate temperatures and applied fields which do not belong either to the thermionic emission region or the field emission region is referred to as thermal-field emission. For this thermal-field emission (TF emission) region,

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Christov [70] was able to derive an analytic expression for the emitted current density with sufficient accuracy for any values of temperature and field. The expressions contain factors with a complicated dependence on F and T , and a computer program is usually required for a calculation of the current density using his formula. In a recent work [71], Jensen *et al.* derived an unrestricted analytic thermal-field emission equation for which the Fowler-Nordheim (FN) and Richardson-Laue-Dushman (RLD) equations are asymptotic limits. The methodology can analytically address *warm* field emission, *cool* thermionic emission, and electron transport between interfaces. Thanks to the power of modern desktop computing, further they developed a more generalized analytical-numerical methodology [40] to simplify the evaluation of the current density, and applied it to general potentials, particularly when both tunneling and thermal emission are non-negligible. Their model revealed the connection between the FN and RLD equations, and exposed a subtle beauty in the transition from the thermal-dominated regime to the field-dominated regime.

1.3.4 Photoemission

The photoemissive effect refers to the emission of electrons in a vacuum from metal and semiconductor surfaces, caused by absorption of electromagnetic energy from visible and near-visible radiation. It was discovered early (1887) and has given rise to a whole group of phototubes. Two principal effects of photoemission have been known for a long time: (1) the maximum velocity of emission of the photoelectrons is independent of the intensity of the illumination; (2) a progressively lower velocity of emission is observed as the frequency of the incident radiation is decreased. If the maximum emission energy of electrons is plotted against the frequency of incident radiation, a straight-line relation is obtained. This shows that the maximum emission

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energy is related to frequency of excitation by

$$\frac{1}{2}mv_m^2 = k_1\nu - k_2, \quad (1.13)$$

where m is electron mass, v_m is maximum emission velocity and ν is frequency. The constants k_1 and k_2 have a definite significance given by the Einstein theory.

The wave theory of light meets with considerable difficulty in explaining the various aspects of the photoelectric effect. The proportionality between the photoelectric current and the intensity of illumination is consistent with the wave theory, but the fact that the maximum velocity of emission is independent of the intensity of the illumination cannot be explained on the basis of the wave theory. Einstein applied the quantum theory to explain photoelectric emission. He suggested that radiation energy was transmitted by *photons*, which are hypothetical particles of zero mass, each with an energy $h\nu$ and localized in space so that each is capable of reacting with an electron. The photons are capable of transferring their entire energy to electrons, after which they disappear. Of the energy $h\nu$ transferred from the photon to an electron, a certain amount w may be used up overcoming the potential barrier at the surface of the material. This amount, w , will be recognized as the work function of the material. The maximum kinetic energy that any electron may have after emission is then

$$\frac{1}{2}mv_m^2 = h\nu - w, \quad (1.14)$$

which is known as the Einstein photoelectric equation. The work function w is seen to be proportional to the threshold (minimum) frequency, $w = h\nu_0$, where h is Planck's constant. This relation offers an experimental means of determining the work function. The work function so determined is known as the photoelectric work function to distinguish it from the thermionic work function, which is determined by observations on thermionic emission. Values of the photoelectric and thermionic work functions are in good agreement for pure metals.

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In addition to the fundamental Einstein photoelectric equation, Spicer’s three-step model of photoemission [72] has been widely used to predict the quantum efficiency and the energy spectrum of emitted electrons for a photocathode as a function of the photoenergy of the incident light [73]. This model treats photoemission as a sequence of three independent processes: photon absorption or electron excitation, electron migration to the surface, and electron escape from the surface. Each process has an associated probability. The first step calculates the probability of absorption of a photon and excitation of an electron to an energy E . The second step calculates the probability that an electron of energy E will reach the surface without scattering. The third step calculates the probability that the electron of energy E will have sufficient momentum perpendicular to the surface to escape. The product of these probabilities represents the probability that an electron will be emitted from the surface. This information is useful, as it provides the energy spectrum of the emitted electrons, i.e. the energy distribution curve. The quantum efficiency is then the area under the energy distribution curve.

Furthermore a modified Fowler-Dubridge (MFD) model mirrors the well-known Spicer’s three-step model, where the designation “MFD” refers to a sequence of modifications acting as coefficients to the Fowler-Dubridge (FD) function [74, 75]. The MFD model differs from Spicer’s three-step model in its usage of different scattering factors, emission probability estimates and an explicit focus on temperature-related modifications. With the rapid development of photoinjectors in recent years, there is a great need for an empirically validated photocathode model. Hence a series of time-dependent models for field-enhanced photoemission based on the modified Fowler-Dubridge functions were developed [76, 77, 78] to analyze current distribution and quantum efficiency of metal or dispenser photocathode. The impact of geometrical field enhancement, contribution of tunneling to the photocurrent from a tungsten needle, time-dependent thermal effects due to absorption of laser energy, and impact

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of temperature rise on thermal conductivity and scattering rate, are all taken into account. Generally these modifications accounting for practical complications will bring the predictions of the theory into substantially closer agreement with experimental measurements. More noticeably, a general electron emission equation accounting for thermal, field and photoemission has been developed [79], in which the three canonical equations (FN, RLD, FD) are shown to be the limiting cases. The formula is able to explicitly deal with transition regions where each of the processes is comparable. This treatment of transition regions is significant especially when an assessment of their relative importance is required, for example, field assisted photoemission.

1.3.5 Secondary Electron Emission

Another form of electron emission is secondary electron emission [80, 81]. The term “secondary” is used to distinguish it from primary emission. Secondary electron emission refers to the emission of electrons as a result of other electrons (or ions) striking a solid. It may occur for conductors, semiconductors or insulators. The most striking aspect of secondary emission is that the number of secondary electrons can be several times greater than the number of primary electrons. It is equally significant that it may occur at low impact energies of the primary electrons down to a few electron volts. As a result, secondary electron emission is virtually always present in an electron tube.

The first characteristic of secondary emission is the yield, i.e., the ratio of the number of secondary electrons to the number of primary electrons. When the ratio (indicated by the symbol δ) is measured, it is found that δ first increases very rapidly with primary impact energy, reaches a maximum, and then decreases very slowly with further increase of impact energy. In fact, this action seems to be universal. However, different materials will have different maximum values of δ at different energies. This

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universal characteristics of secondary electron emission can be explained qualitatively as follows. At low impact energies, it is expected that the number of secondary electrons will increase with the impact energy on the basis that a high-energy particle can knock more electrons out of a material than one with low energy. However, as the energy of the primary electron increases, it will bore deeper into the metal. The energy transferred to surface electrons of the material from the primary electron will be small; and the electrons of the material at greater depth that acquire more energy will have little probability getting out the metal. Accordingly, beyond a certain point the secondary-emission yield is expected to decrease with impact energy. Another secondary-emission property of interest is that the emission ratio increases by factors as much as 2 or 3 for glancing incidence of the primaries. The smaller the angle between the primary beam and the surface, the greater the ratio. The secondary emission is best described by Vaughan's empirical formula [82] that will be discussed in Chapter 5.

Secondary emission is often undesirable, as was the case with the screen-grid tetrode, where it necessitated the addition of another grid to give the pentode. A triode is an electronic amplification device having three active electrodes (the cathode, the grid, and the anode), and a tetrode is an electronic device having four active electrodes. It has the three electrodes of a triode and an additional screen grid to isolate the control grid from the anode. This helps to suppress unwanted oscillation, and to reduce an undesirable effect in triode called the "Miller effect", where the gain of the tube causes a feedback effect which increases the apparent capacitance of the tube's grid, limiting the tube's high-frequency gain. A pentode is an electronic device having five active electrodes. A tetrode could supply sufficient power to a speaker or transmitter, and offered a larger amplification factor than the earlier triode. However, the positively charged screen grid can collect the secondary electrons emitted from the anode, which can cause increased current toward the screen grid, and cause the anode

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current to decrease with increasing anode voltage over part of the I_a/V_a characteristic. Tellegen [83] introduced an additional electrode, called the suppressor grid, which solved the problem of secondary emission. It does this by being held at a low potential, usually either grounded or connected to the cathode. The secondary emission still occurs, but the electrons can no longer reach the screen grid, since they have less energy than the primary electrons and hence cannot pass the grounded suppressor grid. Therefore these secondary electrons are recollected by the anode.

The other example is the multipactor discharge – an avalanche of secondary electrons, which is frequently observed in microwave systems such as radio frequency (rf) windows, accelerator structures, microwave tubes, coupling structures and mode converters, antennae or transmission lines, and rf satellite payloads [84]. The secondary electrons are accelerated by an alternating rf electric field and periodically strike some nearby surface releasing further secondary electrons. It is found that the multipactor will transfer energy from the rf electric field to the surface of the structure [84, 85, 86, 87, 88]. This may lead to damage of the metallic structure at or near the point of impact of the multipacting electrons due to extreme local heating. It can also lead to the mechanical failure of vacuum rf windows. The multipactor may also be thought of as a current being driven by the rf field, and as such may load a resonant cavity changing the amount of electromagnetic energy it can store, as well as changing the resonant frequency. Multipactor may also lead to outgassing and be the initiator for catastrophic failure of components [89].

CHAPTER 2

FEMTOSECOND-LASER INDUCED ULTRAFAST ELECTRON EMISSION

2.1 Introduction

Ultrashort electron pulses are able to provide ultrafast time-resolved characterization of the underlying processes in physics, chemistry and biology [8, 90, 91, 92], by using techniques such as ultrafast electron diffraction, microscopy, and crystallography [6]. To probe the microscopic structural dynamics of molecular and solid state systems, complete control over the spatiotemporal characteristics of the ultrafast electron pulse is required to realize the time-resolved atomic-scale images. A recent promising method is to use a low-power femtosecond (fs) laser to trigger free electron pulses with duration of 10s femtosecond to 100s attosecond to be emitted from a biased metallic field emitter [11, 12, 13, 14, 93].

On the other hand, operating at a higher charge (100s pC or more) and longer time regime i.e. picosecond (ps), short electron bunches with low emittance and high brightness have been produced by the laser-photofield emission cathode [94], and the

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radio frequency (rf) photoinjector [95], which is critical for the fourth generation light sources such as x-ray free electron lasers (FEL).

There have been some debates on the emission process of ultrafast laser excited electron emission, which include various mechanisms such as optical field emission [12], multiphoton field emission [13], and multiphoton absorption followed by over-the-barrier emission [14]. Understanding the detailed emission process is important to realize the sub-cycle electron pulse which is shorter than laser pulse duration. All the models proposed so far to explain the experimental results [11, 12, 13, 14, 93] have been restricted to equilibrium models, which may not be valid at ultrashort time scales. In this work, a consistent nonequilibrium model will be presented to clarify the electron emission process of an ultrafast laser excitation on a metallic surface.

2.2 Theoretical Model

Consider a laser pulse of moderate fluence focused on the surface of a metallic target is absorbed by the electrons in the conduction band, leaving the lattice unperturbed due to its heat capacity, which generates a nonequilibrium condition. Transition to equilibrium state is governed by electron-electron (e-e) and electron-phonon (e-p) collisions. The e-e collisions will lead to an energy relaxation within the electron gas at a time scale of < 100 fs, which is called “internal thermalization”. The excess of electron energy due to laser energy absorption is transferred to the lattice through the e-p collisions to provide the local equilibrium condition, which is known as “external thermalization” at a time scale from 100s fs to a few picoseconds. The time scales of the internal and external thermalization are compared in Fig. 2.1.

For a picosecond laser (red bar in Fig. 2.1), the electron gas quickly achieves the internal thermalization through the electron-electron collisions on a femtosecond scale, but the electron-lattice system is still far from equilibrium at the end of laser pulse.

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Figure 2.1: In a metal, first, free electrons absorb energy from the laser while the lattice remains cold. On a femtosecond time scale the energy is distributed among the free electrons by electron-electron collisions leading to the thermalization of the electron gas. The energy transfer from the hot electrons to the lattice (electron-phonon collisions) will last much longer than the thermalization of the electron gas, typically a few tens of picoseconds.

At this condition, the classical two-temperature model (TTM) is normally used by assuming that electron distributions and phonon distributions can be characterized in terms of electron temperature (T_e) and lattice temperature (T_i), whose energy exchange is governed by the electron-phonon collisions. One good example of TTM is the time dependent field-assisted photoemission model proposed by Jensen and coauthors [78], which have been used to explain picosecond laser-excited ZrC field emission [94] and photoemission [77].

For a femtosecond laser (green bar in Fig. 2.1), the electron-electron collisions are however not fast enough to reach the internal thermalization during the laser pulse. Thus the TTM is inadequate and microscopic kinetic approach should be used [96, 97, 98]. The femtosecond laser excitation of the metallic tip (gold or tungsten) will generate a nonequilibrium electron distribution $f(E, t)$ with a pronounced population above the Fermi energy E_F , which are emitted from the surface under the influence of both laser and applied dc electric fields on the tip (F_L and F_{dc}). It is assumed that the assigned arbitrary values of F_L and F_{dc} in all calculations have included the geometrical enhancement factor of both laser field and dc field on the sharp tip. For

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simplicity, our model is based on a simplified metal description with a parabolic and isotropic conduction band, and the phonon dispersion relation is described by the Debye model.

2.2.1 Nonequilibrium Electron Distribution

Without using any relaxation-time approximation, the photon absorption, electron-electron interaction, and electron-phonon interaction are included in a system of Boltzmann equations to obtain the time-dependent distribution function of the electron gas $f(k)$ and the phonon gas $g(q)$

$$\begin{aligned}\frac{\partial f(k)}{\partial t} &= \left. \frac{\partial f(k)}{\partial t} \right|_{\text{e-e}} + \left. \frac{\partial f(k)}{\partial t} \right|_{\text{e-p}} + \left. \frac{\partial f(k)}{\partial t} \right|_{\text{absorb}}, \\ \frac{\partial g(q)}{\partial t} &= \left. \frac{\partial g(q)}{\partial t} \right|_{\text{p-e}}.\end{aligned}\tag{2.1}$$

Here, $f(k)$ and $g(q)$ depend on the modulus of the momenta $\mathbf{k}$ and $\mathbf{q}$. Before laser irradiation, $f_0(k)$ and $g_0(q)$, respectively, is assumed to be Fermi-Dirac and Bose-Einstein distribution at room temperature. The phonon gas is assumed to be affected only by the electron gas due to the phonon-electron collisions, while the direct absorption of the laser energy by the lattice and the phonon-phonon collisions are neglected (due to its heat capacity) [97, 98]. Typically, the order of magnitude of various relaxation time scales is femtosecond for electron-electron collisions, 100s femtoseconds to picoseconds for electron-phonon collisions, and a few tens of picoseconds for phonon-phonon collisions.

In the following the considered interaction processes and their collision terms in Eq. (2.1) will be individually specified. Subsequently we give an overview of how the equation system with the introduced collision terms is numerically solved, to follow the time evolution of the distribution function $f(E(k), t)$ and $g(E_{\text{ph}}(q), t)$ and observe their changes due to the excitation of the electron gas by the laser beam, thermalization of the electron gas by electron-electron collisions, and energy exchange

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between the electron gas and phonon gas due to electron-phonon collisions. Note the $E(k)$ or $E_{\text{ph}}(q)$ is the energy of an electron or phonon with the modulus of the wave vector k or q .

A. Electron-Electron Collisions

Electron-electron collisions lead to an energy relaxation within the electron gas, through which the absorbed energy is distributed among the free electrons so that the electron gas tends towards a thermal equilibrium (a Fermi distribution). In the first order perturbation theory framework, using the Fermi's golden rule, the probability that two electrons with states $\mathbf{k}, \mathbf{k}_1$ scatter into $\mathbf{k}_2, \mathbf{k}_3$ can be written as [99, 100]

$$\begin{aligned} S(\mathbf{k}, \mathbf{k}_1; \mathbf{k}_2, \mathbf{k}_3) &= \frac{2\pi}{\hbar} |M_{\text{ee}}|^2 f(\mathbf{k})f(\mathbf{k}_1)[1 - f(\mathbf{k}_2)][1 - f(\mathbf{k}_3)] \\ &\times \delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \\ &\times \delta[E(k) + E(k_1) - E(k_2) - E(k_3)], \end{aligned} \quad (2.2)$$

where the momentum and energy conservation conditions appear, together with the Pauli exclusion principle, $f(\mathbf{k})f(\mathbf{k}_1)[1 - f(\mathbf{k}_2)][1 - f(\mathbf{k}_3)]$, which takes into account the probability that the $\mathbf{k}$ and $\mathbf{k}_1$ states are occupied while the $\mathbf{k}_2$ and $\mathbf{k}_3$ states are empty. The term M_{ee} represents the interaction matrix element.

The collision term that describes the electron-electron interaction, i.e. the sum over all possible two-body scattering events in three dimensions which populate and depopulate the state $\mathbf{k}$, is thus given by [97, 98]

$$\begin{aligned} \left. \frac{\partial f(k)}{\partial t} \right|_{\text{e-e}} &= \frac{2\pi}{\hbar} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} |M_{\text{ee}}|^2 F(\mathbf{k}, \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \\ &\times \delta(\mathbf{k} + \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \delta[E(k) + E(k_1) - E(k_2) - E(k_3)], \end{aligned} \quad (2.3)$$

where

$$\begin{aligned} F(\mathbf{k}, \mathbf{k}_1; \mathbf{k}_2, \mathbf{k}_3) &= - f(\mathbf{k})f(\mathbf{k}_1)[1 - f(\mathbf{k}_2)][1 - f(\mathbf{k}_3)] \\ &+ f(\mathbf{k}_2)f(\mathbf{k}_3)[1 - f(\mathbf{k})][1 - f(\mathbf{k}_1)], \end{aligned} \quad (2.4)$$

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The wave vector $\mathbf{k}_3$ results from momentum reservation, and the $\Delta\mathbf{k} = \mathbf{k}_1 - \mathbf{k}_2 = \mathbf{k}_3 - \mathbf{k}$ is the scattering transferred momentum. The e-e matrix element M_{ee} is derived from a screened Coulomb potential, and it depends on the scattering transferred momentum Δk and the static screening length κ_{sc} [97]:

$$|M_{ee}|^2 = \left[\frac{e^2}{\epsilon_0 V} \frac{1}{\Delta k^2 + \kappa_{sc}^2} \right]^2, \quad \text{where } \kappa_{sc}^2 = \frac{e^2 m_e}{\pi^2 \hbar^2 \epsilon_0} \int_0^\infty f(k) dk. \quad (2.5)$$

Here, V is the volume. The screening length κ_{sc} represents an important parameter for the electron-electron interaction, and is calculated at each time step for the updated distribution function $f(k)$, while m_e is the effective mass of a free electron in the conduction band.

B. Electron-Phonon Collisions

The main effect of electron-phonon collisions is to transfer energy from the laser-heated electron gas to the cold lattice. The electron-phonon interaction consists of phonon emission and absorption process by the electron gas. The phonon emission and absorption scattering rates can be calculated through Fermi's golden rule, in the framework of the first order perturbation theory. The probability that an electron in state $\mathbf{k}$ emits a phonon with wave number $\mathbf{q}$ and energy E_{ph} scattering into the state $\mathbf{k}^- = \mathbf{k} - \mathbf{q}$ is given by

$$\begin{aligned} S(\mathbf{k}; \mathbf{k}^-, \mathbf{q}) &= \frac{2\pi}{\hbar} |M_{ep}|^2 f(\mathbf{k}) [1 - f(\mathbf{k}^-)] [1 + g(\mathbf{q})] \\ &\times \delta[E(\mathbf{k}) - E(\mathbf{k}^-) - E_{ph}(\mathbf{q})], \end{aligned} \quad (2.6)$$

where M_{ep} represents the electron-phonon matrix element, and the factor $f(\mathbf{k})[1 - f(\mathbf{k}^-)][1 + g(\mathbf{q})]$ takes into account the Pauli exclusion principle, as electron can scatter only into unoccupied states $[1 - f(\mathbf{k}^-)]$. The proportionality of the phonon emission processes on the factor $[1 + g(\mathbf{q})]$ is due to both the spontaneous and stimulated emission. On the other hand, the phonon absorption probability should be

2.2 Theoretical Model

proportional to $g(\mathbf{q})$ instead of $[1 + g(\mathbf{q})]$. Finally the term $\delta[E(k) - E(k^-) - E_{\text{ph}}(q)]$ represents the total energy conservation condition.

Therefore the electron distribution change in the state $\mathbf{k}$ due to the electron-phonon collisions is given by the sum of two terms, representing the total scattering rate of both phonon emission and absorption processes, involving transition towards all the states $\mathbf{k}^+ = \mathbf{k} + \mathbf{q}$ and $\mathbf{k}^- = \mathbf{k} - \mathbf{q}$. The collision terms for the electron-phonon interaction read [97, 98]

$$\left. \frac{\partial f(k)}{\partial t} \right|_{\text{e-p}} = \frac{2\pi}{\hbar} \sum_{\mathbf{q}} |M_{\text{ep}}|^2 \left\{ \begin{aligned} & F^-(\mathbf{k}, \mathbf{q}) \delta[E(k) - E(k^-) - E_{\text{ph}}(q)] \\ & + F^+(\mathbf{k}, \mathbf{q}) \delta[E(k) - E(k^+) + E_{\text{ph}}(q)] \end{aligned} \right\}, \quad (2.7)$$

where

$$\begin{aligned} F^-(\mathbf{k}, \mathbf{q}) &= f(\mathbf{k}^-)[1 - f(\mathbf{k})]g(\mathbf{q}) - f(\mathbf{k})[1 - f(\mathbf{k}^-)][1 + g(\mathbf{q})], \\ F^+(\mathbf{k}, \mathbf{q}) &= f(\mathbf{k}^+)[1 - f(\mathbf{k})][1 + g(\mathbf{q})] - f(\mathbf{k})[1 - f(\mathbf{k}^+)]g(\mathbf{q}). \end{aligned} \quad (2.8)$$

The e-p matrix element M_{ep} can be calculated taking into account the e-p interaction screening due to the electron gas, and written as

$$|M_{\text{ep}}|^2 = \frac{1}{2\epsilon_0 V} \frac{e^2}{q^2 + \kappa_{\text{sc}}^2} E_{\text{ph}}(q), \quad (2.9)$$

where $E_{\text{ph}}(q) = \hbar v_s q$ is the energy of a phonon with the modulus of wave vector q and v_s is the sound speed of longitudinal phonon [97].

The phonon distribution function is assumed to change only due to the phonon-electron collisions. Direct absorption of the laser energy is neglected. For simplicity we consider only one phonon mode and do not take umklapp processes into account. Thus phonon-phonon collisions are neglected as well. In this case phonon-electron interaction leads to heating of the phonon gas, analogously to the cooling of the electron gas. The corresponding phonon distribution change, i.e. the phonon-electron

2.2 Theoretical Model

collision term is given by

$$\left. \frac{\partial g(q)}{\partial t} \right|_{\text{p-e}} = 2 \times \frac{2\pi}{\hbar} |M_{\text{pe}}|^2 \sum_{\mathbf{k}} F^+(\mathbf{k}, \mathbf{q}) \delta[E(k) - E(k^+) + E_{\text{ph}}(q)]. \quad (2.10)$$

The matrix element M_{pe} is the same as the matrix element M_{ep} in Eq. (2.9). Similar to M_{ee} , they both take into account the electron-phonon interaction screening due to the electron gas, which would reduce the e-p interactions. Physically, in metals, not only the interaction of one electron with lattice deformation has to be considered but also the screening of the lattice deformation by free electrons and the interaction of that electron with the screening electrons [97]. The electron screening length κ_{sc} is given above by Eq. (2.5).

C. Laser Perturbation and Energy Absorption

Free electrons oscillating in the laser field can absorb energy only when they are perturbed [96]. With laser light of frequency ω and amplitude of electric field F_{L} , the photon absorption (mediated by electron-phonon collisions) term reads

$$\begin{aligned} \left. \frac{\partial f(k)}{\partial t} \right|_{\text{absorb}} &= \frac{2\pi}{\hbar} \sum_{\mathbf{q}} |M_{\text{ep}}|^2 \sum_l J_l^2 \left(\frac{e\mathbf{F}_{\text{L}} \cdot \mathbf{q}}{m_e \omega^2} \right) \\ &\times \left\{ \begin{aligned} &F^-(\mathbf{k}, \mathbf{q}) \delta[E(k) - E(k^-) - E_{\text{ph}}(q) + l\hbar\omega] \\ &+ F^+(\mathbf{k}, \mathbf{q}) \delta[E(k) - E(k^+) + E_{\text{ph}}(q) + l\hbar\omega] \end{aligned} \right\}, \quad (2.11) \end{aligned}$$

where the perturbation occurs when an oscillating electron collides with a phonon absorbing or emitting its momentum. The probability of absorption (or emission) of l photons is given by the square of the Bessel function. The product $\mathbf{F}_{\text{L}} \cdot \mathbf{q}$ in the argument of the Bessel function indicates that, the absorption of the photon is allowed only if the change of the electron wave vector $\mathbf{q}$ has a component parallel to the laser field $\mathbf{F}_{\text{L}}$. Since we do not consider a definite polarization of laser light, an average is made over all directions of the laser field.

2.2 Theoretical Model

D. Numerical Solutions

To solve the equation system Eq. (2.1) numerically, the collision sums in Eqs. (2.3), (2.7), (2.10) and (2.11) need to be transformed into collision integrals and analytically reduced (i.e. sixfold to twofold and threefold to onefold) due to the assumed isotropy [99, 100]. Then the system of nonlinear integrodifferential equations and the collision integrals can be rewritten in terms of time and energy, using the dispersion relation of electrons $E = \hbar^2 k^2 / 2m_e$ and phonons $E_{\text{ph}} = \hbar v_s q$. By considering discrete E and E_{ph} , we have a system of fully coupled, nonlinear ordinary differential equations. The integration over time is done by applying the Euler's algorithm with adaptive time steps. With this procedure, for given values of laser wavelength (λ) [i.e. frequency (ν) and angular frequency (ω)], amplitude of laser field strength (F_L), laser pulse duration (τ), we are able to calculate the time evolution of the distribution functions of the electron gas $f(E, t)$ and the phonon gas $g(E_{\text{ph}}, t)$. From the time-dependent electron energy distribution function $f(E, t)$, the emission of electrons or current density $J(t)$ can be obtained. Note the temporal profile of the laser pulse is simplified as a step function from $t = 0$ to τ in all calculations.

Consider a tungsten tip subjected to a laser excitation ($F_L = 0.5$ V/nm) of $\lambda = 800$ or 1000 nm with a pulse duration up to $\tau = 1$ ps. Figure 2.2 shows the temporal evolution of $f(E, t)$ versus electron energy with respect to the Fermi level E_F . Before the excitation $t = 0$, the tungsten (at equilibrium) is described by a Fermi-Dirac distribution function at 300 K. The laser excitation creates a strong nonequilibrium distribution, characterized by a step-like profile with the step-size in $E - E_F$ equal to the photon energy (a) $h\nu = 1.553$ eV and (b) $h\nu = 1.240$ eV. For example, the first step goes from the Fermi level E_F to $E_F + h\nu$, which is due to one-photon absorption process by electrons between $E_F - h\nu$ and E_F . Excited electrons can subsequently absorb a further photon, leading to an occupation number increase for electron energies up to $2h\nu$ above E_F , and so on for $nh\nu$ above E_F .

2.2 Theoretical Model

Figure 2.2: Temporal evolution of electron energy distribution function $f(E)$ of a tungsten tip under a laser excitation (a) $\lambda = 800$ nm or $h\nu = 1.553$ eV (b) $\lambda = 1000$ nm or $h\nu = 1.240$ eV with pulse duration up to $\tau = 1$ ps.

2.2 Theoretical Model

In Fig. 2.2, the step-like characteristic is dominant till about $t = 100$ fs, and the smoothing effect (due to electron-electron and electron-phonon collisions) starts to occur at a longer time scale $t > 100$ fs. At about 1 ps or more, the electron energy redistribution will modify $f(E)$ towards a new equilibrium Fermi-Dirac distribution at a higher temperature. Thus the two temperature model is justified for picosecond laser excitation on metals, but not for femtosecond laser pulse ($\tau < 100$ fs) where the step-like profile remains present at end of laser pulse.

2.2.2 Tunneling in Time-Independent Barrier

From the free electron theory of metals introduced in Chapter 1, the number of electrons per unit area and time, with total energy between E and $E + dE$, and normal energy (with respect to barrier surface) between E_x and $E_x + dE_x$ is

$$N(E, E_x, t) dE dE_x = \frac{m}{2\pi^2 \hbar^3} f(E, t) dE dE_x, \quad (2.12)$$

which is similar to Eq. (1.3). For the electron emission from ultrafast laser excited metal surfaces, the time-dependent emitted current density is calculated by

$$J(t) = e \int_0^\infty N(E_x, t) \mathcal{T}(E_x) dE_x, \quad \text{where } N(E_x, t) dE_x = \frac{m dE_x}{2\pi^2 \hbar^3} \int_{E_x}^\infty f(E, t) dE. \quad (2.13)$$

Here, $N(E_x, t) dE_x$ is the instantaneous number of electrons with normal energy between E_x and $E_x + dE_x$ impinging on the surface barrier per unit area and time. This supply function of electrons incident on the metal-vacuum interface is plotted in Fig. 2.3(a) at the end of a 10 fs laser pulse of photon energy 1.553 eV for two different laser power $F_L = 0.1$ and 0.5 V/nm. Depending on their respective x -direction energy E_x , these excited electrons (under nonequilibrium condition) will transmit through a surface barrier with finite probability $\mathcal{T}(E_x)$, giving the instantaneous emitted current density $J(t)$.

2.2 Theoretical Model

Figure 2.3: For a tungsten tip ($\phi_B = 4.4$ eV) under a 10 fs laser excitation of $F_L = 0.1$ V/nm (solid lines) and 0.5 V/nm (dashed lines): (a) the number of electrons ($\text{eV}^{-1}\text{m}^{-2}\text{s}^{-1}$) with normal energy between E_x and $E_x + dE_x$ impinging on the surface barrier, and the spectrum of transmitted electrons ($\text{eV}^{-1}\text{m}^{-2}\text{s}^{-1}$) at various $F_{dc} =$ (b) 0.001, (c) 0.1 and (d) 1 V/nm.

2.3 Comparison to Experiments

The electron tunneling probability $\mathcal{T}(E_x)$ is calculated through a simplified potential barrier of

$$U(x) = E_F + \phi_B - \frac{e^2}{16\pi\epsilon_0 x} - eF_{\text{dc}}x, \quad (2.14)$$

using a modified Miller-Good method introduced by Jensen [39, 40]. Specifically, we calculate $\Lambda(E_x) = 2 \int_{x_1}^{x_2} \sqrt{\frac{2m}{\hbar^2} [U(x) - E_x]} dx$ and $\mathcal{T}(E_x) = \left\{ 1 + \exp [\Lambda(E_x)] \right\}^{-1}$ using traditional Miller-Good method for E_x below the barrier top, and estimate the $\mathcal{T}(E_x)$ by a linear extension of $\Lambda(E_x)$ above the barrier, so that for $E_x \geq E_0$, we have

$$\Lambda(E_x) = \Lambda_0 + \left. \frac{\partial \Lambda(E_x)}{\partial E_x} \right|_{E_0} \times (E_x - E_0), \quad (2.15)$$

where E_0 represents a computationally convenient choice to begin the linear extension of $\Lambda(E_x)$. The value of E_0 should be close to but avoid the barrier maximum, at which $\Lambda(E_x)$ does not behave as a polynomial in E_x .

In Fig. 2.3 (b) - (d), the calculated results of $N(E_x)\mathcal{T}(E_x)$ are plotted as a function of $E_x - E_F$ at various dc bias $F_{\text{dc}} = 0.001$ to 1 V/nm. It is evident that at small dc field F_{dc} , only electrons with $E_x \geq E_F + \phi_B$ are able to emit over the barrier as pure photoemission as shown in Fig. 2.3(b). At larger $F_{\text{dc}} = 1$ V/nm, significant amount of electrons of energy range from $E_x - E_F = 0$ to 6 eV are emitted through the photo-field emission as shown in Fig. 2.3(d).

2.3 Comparison to Experiments

In order to obtain a direct comparison with experimental measurement to validate the proposed nonequilibrium model, we will study the electron flux as function of laser power P and tip bias voltage V_g , i.e. the laser field $F_L \propto P^{1/2}$ and dc electric field $F_{\text{dc}} \propto V_g$ in our model. It is assumed that the assigned arbitrary values of F_L and F_{dc} in all calculations have included the geometrical enhancement factor of both laser field and dc field on the sharp tip.

2.3 Comparison to Experiments

Figure 2.4: The dependence of (a) J and (b) n_{eff} on various F_L and F_{dc} for a 10 fs laser ($h\nu = 1.553 \text{ eV}$) excitation on a tungsten tip ($\phi_B = 4.4 \text{ eV}$). The dashed lines in (a) are fitted by a power law $y \propto x^{2n}$. The solid line in (b) is the base-line calculation at $F_L = 0.5 \text{ V/nm}$.

2.3 Comparison to Experiments

In Fig. 2.4(a), for a 10 fs laser ($h\nu = 1.553$ eV) excitation on a tungsten tip ($\phi_B = 4.4$ eV), the calculated J at $t = 10$ fs are plotted in symbols as function of laser field F_L for three different dc electric fields F_{dc} , which can be fitted by a power law $J \propto (F_L)^{2n}$ (dashed lines), i.e. $J \propto P^n$ with $n = 2.91, 2.12, 1.16$ for $F_{dc} = 0.001, 1, 3$ V/nm, respectively. This finding indicates a reduced power dependence of J (or electron counts) on F_L (or P) for increased F_{dc} (or V_g), which have also been generally observed in recent experiments [13, 14, 93]. From our model, at small F_{dc} , it is the pure multiphoton electron emission, satisfying $n \cdot h\nu \geq \phi_B$. As F_{dc} increases, significant amount of electrons are emitted through tunneling process (field emission), which are responsible for small values of fitted n .

However from the experimental observations [13, 14], it is difficult to fit $J \propto (F_L)^{2n} \propto P^n$ with a constant n for large F_{dc} (> 1 V/nm). To solve this problem, we define an effective number of photon absorption as

$$n_{\text{eff}} = \frac{\bar{E}_x - E_F}{h\nu}, \quad \text{where } \bar{E}_x(t) = \frac{\int_0^\infty E_x N(E_x, t) \mathcal{T}(E_x) dE_x}{\int_0^\infty N(E_x, t) \mathcal{T}(E_x) dE_x}. \quad (2.16)$$

Here $\bar{E}_x(t)$ is the average emission energy. In Fig. 2.4(b), the calculated n_{eff} is plotted as a function of F_{dc} for various $F_L = 0.5$ V/nm (solid line) and 0.1, 0.2, 1, 2, 5 V/nm (symbols). It is observed that $n_{\text{eff}} \approx 2.87$ to 2.93 is approximately independent of F_L at small $F_{dc} < 0.1$ V/nm, which agrees well with the fitted $n = 2.91$ at $F_{dc} = 0.001$ V/nm as shown in Fig. 2.4(a). The discrepancy among the n_{eff} for different F_L is significant at large F_{dc} , which explains why fitting $J \propto (F_L)^{2n}$ is difficult at $F_{dc} > 1$ V/nm. For instance, at $F_{dc} = 3$ V/nm, the fitted n is 1.16 but the n_{eff} ranges from 0.2 to 1.5 for $F_L = 0.1$ to 5 V/nm. The decreased n_{eff} with smaller F_L could be understood by taking a closer look at Fig. 2.3(d). The difference between $F_L = 0.1$ (solid) and 0.5 V/nm (dashed) increases with E_x , and the two cases overlap with each other for $E_x \leq E_F$. Therefore those excited electrons with $E_x > E_F$ will be more dominant in the emitted electron spectrum for 0.5 V/nm case, and the average emission energy and n_{eff} are both larger.

2.3 Comparison to Experiments

It is not a trivial matter to measure the exact time evolution of ultrafast electron emission or duration in femtosecond or attosecond time scales [101]. Here, we attempt to compare our calculated n integrated over the laser pulse duration (32 fs) with an experimental measurement in the published range of F_L and F_{dc} for a 32 fs and 810 nm laser excitation on a metal surface of $\phi_B = 6$ eV [14]. Figure 2.5 shows rather good agreement between the calculation (bold solid line) and the measurement (symbols) over a wide range of F_{dc} . For comparison, the time dependence of the calculated $n(t)$ for a laser pulse duration of 1 fs to 1 ps are also plotted in thin solid lines. It is clear that the nonequilibrium model proposed in this work shows better agreement as compared to the TTM-based calculations (dashed lines) at various arbitrary temperatures 1000, 2000 and 5000 K.

While the model is able to explain the experimental observation as shown in Fig. 2.4 and Fig. 2.5, it is important to clarify the assumptions used in the model for further improvements. First, it is a one-dimensional model, for which we assume the assigned arbitrary values of F_L and F_{dc} have included the geometrical enhancement factor of both laser field and dc field on the sharp tip. An improvement of calculating the enhancement factor will be useful to have a direct relation to the experimental parameters such as applied dc voltage (V_g) and laser power (P). Second, the polarization of the laser field is important to both the laser energy absorption and the geometrical enhancement factor on emitting tip. For simplicity, the current model does not consider a definite polarization of laser light, an average study (over all directions of the laser field) is performed for the laser perturbation term, and also a mean geometrical enhancement factor is used. The effects of laser polarization can be included when the geometrical shape of emitter is taken into account. Third, the model also assumes that the power of the laser is low enough that effects such as optical field emission [12] and the electron space charge field [102] can be ignored. Finally, we ignore the effects of finite tunneling time, which should be valid when the

2.3 Comparison to Experiments

Figure 2.5: The comparison of nonequilibrium calculated time-integrated n (bold solid line) at $h\nu = 1.553$ eV and $\phi_B = 6$ eV with the the measured (symbols) values of n [14]. The time-dependence of $n(t)$ for a laser pulse of 1, 10, 100 fs and 1 ps (thin solid lines), and TTM calculations (dashed lines) are also plotted.

2.4 Summary

time-varying laser field does not modulate the potential barrier significantly. This limitation will require revision when the effect of optical tunneling is included in future works.

2.4 Summary

To summarize, a nonequilibrium model [19] has been proposed to explain the electron emission process from a metallic surface under the excitation of a low-power femtosecond laser pulse and a dc electric field [11, 12, 13, 14]. The model has successfully confirmed the gradual decrease of the power dependence from a high-order nonlinearity at low bias to linear order emission at high bias voltages observed in the experiments. Good agreement with a direct comparison with an experimental measurement [14] has been obtained.

CHAPTER 3

SHOT NOISE OF HIGH CURRENT

SPACE CHARGE LIMITED FIELD EMISSION

3.1 Introduction

Vacuum-tube and transistor amplifiers are capable of giving extremely high amplification of power and voltage, which seems to imply that arbitrarily small signals could be detected. However, there is always a limit determined by the noise generated by the random motion of electrons at the input of the amplifier, as any signal smaller than this electronic noise will be masked by it. Accordingly, the sensitivity of amplifiers and receivers depends upon how noisy the input circuit is rather than upon how much amplification it has [42]. Similarly for all envisioned novel applications of electron emission, the noise generated by the electron emission process could be the limiting factor in the ultimate sensitivity of electron devices.

Two basic types of noise in electron emission are the *inherent* shot noise and *excess* flicker noise [103]. The frequency independent (or “white”) shot noise is caused by the fact that the current is carried by discrete charges, i.e. electrons. The

3.1 Introduction

independently and randomly emitted electrons arrive at the anode like hail or the lead particles from a shotgun [104]. The grouping of electrons (rather than individual electrons alone) gives rise to detectable statistical fluctuations in a measurement. Flicker noise, also known as $1/f$ noise, is a signal or process with a frequency spectrum that falls off steadily into the higher frequencies. In 1926, the noise from coated filaments was explained by the appearance of foreign atoms on the surface [105]. The adsorbed particle opens or shuts a channel for an increased emission. The superposition of the statistically appearing adsorbed particle controlled emission currents, is one of the causes of the flicker noise in electron emission [103].

Knowing the fundamentals of the shot and flicker noise, for high frequency applications of electron emission such as microwave power tubes, the shot noise is the considerable issue because of the very low-frequency nature of the flicker noise power. For example, broadening of a 10 GHz carrier signal would be expected and may interfere with those practical voice-communication or radar applications. Moreover in a new instrument i.e. the femtosecond field emission camera [16, 17, 18] that has been developed to continuously record the motion of single adsorbed atoms or molecules, the electron emission rate needs to be measured at the picosecond and subpicosecond time scale. Correspondingly in frequency domain, mainly the “white” shot noise remains significant at high frequency range and possibly affects the instrument’s performance. It is therefore of great scientific interest to study the shot noise in the electron emission process.

The early emission fluctuation theories given by Schottky were meant for thermionic emission without mutual electron correlation [104], and the model was later extended to include the space charge effects [106]. For new generation electron emitters under strong applied electric fields, the shot noise has been shown theoretically to be much smaller than the Schottky noise in thermionic emission [21], where the analysis had neglected the Coulomb correlation of the tunneling electrons.

3.2 Historical Review on Shot Noise Study

Hence it is the aim of this research to study the shot noise properties of electron field emission, especially for the case of space charge limited currents.

3.2 Historical Review on Shot Noise Study

Shot noise is a type of electronic noise that occurs due to the discreteness of electron charges. Its spectral power density is linearly proportional to the current and independent of the frequency. By considering the electron emission from a thermionic cathode in a vacuum tube as a Poisson process, Schottky [104] first proposed that the spectral power density of shot noise at low frequency (small compared to the inverse transit time through the vacuum gap but larger than the regime where the effects of Flicker noise dominate) is $S = 2eI$, where e is electron charge and I is the mean value of the transmitted current. Recent studies of shot noise have been focused on mesoscopic devices [107], which can provide crucial information that is not available in the time-averaged value such as the particle-wave duality of electron transport.

The deviation from the uncorrelated shot noise is commonly termed as the Fano factor $\gamma = S/2eI$, where $\gamma < 1$ indicates the suppression of shot noise due to the correlations among the electrons. It was first found that the shot noise could be smoothed out by the space charge effects (or Coulomb repulsion among the electrons) for thermionic emission operating at space charge limited (SCL) condition [106, 108]. This phenomenon is usually called space-charge smoothing, which simply means some noise suppression by space charge effect. For mesoscopic devices, the main source of correlation is the Pauli exclusion principle, which provides the effect of quantum partitioning for shot noise suppression observed in many systems, such as ballistic quantum point contact [109, 110], nondegenerate diffusive conductors [111, 112], chaotic systems [113] and avalanche photodiodes [114]. Suppression of shot noise due to Coulomb correlation was also studied in ballistic conductors [115, 116, 117].

3.2 Historical Review on Shot Noise Study

In a recent paper [21], the shot noise from electron field emission was analyzed as a quantum scattering problem within the Landauer-Büttiker framework. The transverse and longitudinal motion of electrons are assumed to be separable, so that one can specify the quantum channels associated with transverse mode and define the scattering states. The current-noise power for a two-terminal quantum conductor (i.e. a vacuum gap) for a unidirectional charge injection is given by

$$\begin{aligned} S &= 2 G_0 \sum_n \int dE [f (1 - f) \mathcal{T}_n^2 + f \mathcal{T}_n (1 - \mathcal{T}_n)] \\ &\equiv S_{\text{em}} + S_{\text{part}}, \end{aligned} \quad (3.1)$$

where $G_0 = q^2/\pi\hbar$ is the unit of conductance, $\mathcal{T}_n$ is the transmission probability associated with n quantum channels at energy E , and $f(E)$ is the energy distribution function at the emitter. This formula describes the spectral density of current fluctuations of an electron emitter. It unifies two sources of randomness: (i) the probabilistic occupation of states in the emitter through the function f , and (ii) the probabilistic reflection and transmission at the interface barrier through the probability $\mathcal{T}_n$. The first source of randomness is intimately related to intrinsic thermal agitations of the emitter and can be associated to the first term in Eq. (3.1). It dominates in the absence of partitioning when all transmission coefficients $\mathcal{T}_n$ are either 0 or 1, which is interpreted as the *emission shot noise*. The second source of randomness associated with the last term in Eq. (3.1) is caused by quantum partitioning, and the fact that charge is carried by discrete portions (shot effect). It only contributes for transmission probabilities $\mathcal{T}_n \neq 0, 1$ and can be called the *partition shot noise*.

Equation (3.1) can be used to calculate the noise power of the emitter with an arbitrary number of quantum channels. The problem can be simplified by assuming that the interface of the emitter is plane and its transversal area is large compared with wavelength (a large number of channels). The summation over the transverse

3.2 Historical Review on Shot Noise Study

channels can be replaced by integration over the transverse energy $E_\perp$. Then for wide multichannel emitters with equilibrium Fermi-Dirac electrons, Eq. (3.1) is reduced to

$$S = 2 G_S \frac{k_B T}{E_F} \left\{ \int_0^\infty \frac{\mathcal{T}^2(E_x)}{1 + e^{(E_x - E_F)/k_B T}} dE_x + \int_0^\infty \mathcal{T}(E_x) [1 - \mathcal{T}(E_x)] \ln \left[1 + e^{(E_F - E_x)/k_B T} \right] dE_x \right\}, \quad (3.2)$$

where $G_S = (k_F^2 A / 4\pi) G_0$ is the Sharvin conductance, $E_F = \hbar^2 k_F^2 / (2m)$ is the Fermi energy, A is the cross sectional area and $\mathcal{T}(E_x)$ is the transmission probability at the longitudinal energy $E_x = E - E_\perp$. On the other hand according to the Landauer-Büttiker formulism, the steady-state anode current is given by (see Chapter 1)

$$I = AJ = A \times \frac{emk_B T}{2\pi^2 \hbar^3} \int_0^\infty \mathcal{T}(E_x) \ln \left[1 + e^{(E_F - E_x)/k_B T} \right] dE_x. \quad (3.3)$$

Summarizing the Eq. (3.2) and Eq. (3.3), the shot noise power spectrum of the emission current can be rewritten as $S = 2eI\gamma$ with the Fano factor expression

$$\gamma = 1 - \frac{\int_{-\infty}^{+\infty} \mathcal{T}^2(E_x) g(-\beta E_x) dE_x}{\int_{-\infty}^{+\infty} \mathcal{T}(E_x) h(-\beta E_x) dE_x}, \quad (3.4)$$

where $\beta = 1/k_B T$, k_B is Boltzmann's constant, T is temperature, E_x is the longitudinal energy with respect to the Fermi level E_F , $h(z)$ and $g(z)$ are defined as $h(z) = \ln(1 + e^z)$ and $g(z) = h(z) - dh(z)/dz$. The integral appearing in the numerator in the expression of γ in Eq. (3.4) is smaller than the integral in the denominator, leading to a Fano factor less than unity. This shot noise reduction has been attributed to the quantum partitioning between the transmitted electrons through and the reflected electrons from the potential barrier near the cathode-vacuum interface [21]. The original model on a simplified triangular potential barrier [21] was later extended to a more realistic potential barrier profile with image force potential, using quantum-mechanical wave impedance approach; and analytical expressions for the Fano factor were derived for both pure field emission (Fowler-Nordheim law) and pure thermionic emission (Richardson law) [118, 119].

3.3 Shot Noise of SCL Field Emission

However, all of these treatments have completely ignored the space charge effects (or Coulomb correlation) of the tunneling electrons, which would become important for high current field emission. Such high current field emission are relevant in the fabrication of large area SCL carbon nanotube field emitters [120], the applications for high frequency high power microwave sources [20], and short-pulse field emission using ultrafast laser excitation [11, 12]. Therefore in this context, several interesting questions will be answered [22]: What is the suppression of shot noise for space charge limited field emission operating over a wide range of parameters? What is the role of Coulomb correlation in the presence of quantum partitioning? Can we have the effect of space charge smoothing in field emission similar to thermionic emission? How does the electron emission pulse length affect the shot noise suppression for space charge limited field emission?

3.3 Shot Noise of SCL Field Emission

The high current electron field emission is limited by space charge because the space charge in the diode presents a potential barrier to the incident electrons. A steady state is defined when the whole diode gap is filled with charges (see Fig. 3.6(a) below). Depending on the gap spacing and applied voltage, the Coulomb interaction and the dynamics of electrons have to be treated quantum mechanically when the electron de Broglie wavelength is comparable to the characteristic length scales [55, 58, 121] or relativistically at high voltages [102].

3.3.1 Formulation

Following the Landauer-Büttiker framework, the Fano factor of the field emission from a metallic surface is expressed in Eq. (3.4). And the transmitted electron current

3.3 Shot Noise of SCL Field Emission

density J is obtained by solving (refer to Chapter 1)

$$J = e \int_{-\infty}^{\infty} N(E_x) \mathcal{T}(E_x) dE_x, \quad (3.5)$$

where $N(E_x)$ is the density of incident electrons and the transmission coefficient $\mathcal{T}(E_x)$ is calculated using the modified Miller-Good approximation as introduced in Chapter 2. To calculate $\mathcal{T}(E_x)$ for both γ and J , we consider that the electrons are emitted from the cathode at $x = 0$ with an applied anode voltage V_g at $x = D$. The electrical potential energy profile across the vacuum gap is

$$U_{tot}(x) = \phi_B + U_{im}(x) + U_v(x) + U_{sc}(x) + U_{xc}(x), \quad (3.6)$$

where ϕ_B is the work function of the field emitter, $U_{im}(x)$ is the image charge potential energy including the effect of anode screening that is significant in a sub-10 nm gap [36],

$$U_{im}(x) = - \left[\frac{e^2}{16\pi\epsilon_0 x} + \frac{e^2}{8\pi\epsilon_0} \sum_{n=1}^{\infty} \left(\frac{nD}{n^2 D^2 - x^2} - \frac{1}{nD} \right) \right]. \quad (3.7)$$

The term $U_v(x) = -eV_v(x) = -eFx$ is the external applied electric field potential energy with $F = V_g/D$. The last two terms $U_{xc}(x)$ and $U_{sc}(x) = -eV_{sc}(x)$ are, respectively, the exchange-correlation and the space charge potential energy due to transmitted electrons in the gap, which are calculated self-consistently.

To calculate the profile $V_{sc}(x)$ and $U_{xc}(x)$ for an emitting current density J , we use the Schrödinger-Poisson approach and the relativistic formulation of the Poisson equation, respectively, to account for the quantum dynamics (for a nanogap) and relativistic effects (for large gap voltage). The detailed formulation and derivation are shown in Appendix A. In the quantum regime, the normalized time-independent Schrödinger and Poisson equations in a quantum mean field model (see Appendix A.2) are [55]

$$q'' + \lambda^2 \left[\phi_{sc} + \bar{x} - \phi_{xc} - \frac{4}{9} \frac{\mu^2}{q^4} \right] q = 0, \quad (3.8)$$

$$\phi_{sc}'' = \frac{2}{3} q^2, \quad (3.9)$$

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where q is the normalized wave amplitude, $\phi_{sc} = V_{sc}/V_g$ is the normalized space charge potential, $\phi_{xc} = U_{xc}/eV_g$ is the normalized exchange-correlation potential energy based on the local density functional theory [122], q'' (and ϕ_{sc}'') denote the second derivative of q (and ϕ_{sc}) with respect to $\bar{x} = x/D$, $\lambda = D/\lambda_0$ is the normalized gap spacing with respect to the electron de Broglie wavelength at V_g : $\lambda_0 = \hbar/\sqrt{2emV_g}$, and $\mu = J/J_{CL}$ is the normalized electron current density with respect to the classical Child-Langmuir (CL) current density [123, 124]:

$$J_{CL} = \frac{4\epsilon_0}{9} \sqrt{\frac{2e}{m}} \frac{V_g^{3/2}}{D^2}. \quad (3.10)$$

The Poisson equation in the relativistic regime (see Appendix A.3) is [102, 125]

$$\Gamma'' = \mu \frac{4\sqrt{2}}{9} U_0^{3/2} \frac{\Gamma}{\sqrt{(\Gamma^2 - 1)}}, \quad (3.11)$$

where $\Gamma = 1 + e(V_{sc} + V_v)/(mc^2)$ and $U_0 = eV_g/(mc^2)$. At $\lambda \gg 1$ or $U_0 \ll 1$, ϕ_{xc} is negligible, and the space charge field ϕ_{sc} will recover the classical limit by solving (see Appendix A.1)

$$\phi_{sc}'' = \frac{4}{9} \frac{\mu}{\sqrt{\phi_{sc} + \bar{x}}}. \quad (3.12)$$

3.3.2 Results and Discussions

For a given work function ϕ_B and temperature T , we can calculate the Fano factor γ and normalized current density μ by solving the above equations numerically, over a wide range of gap spacings and voltages. In particular, we will study three systems with different D and V_g in a range of electric field strength from $F = 1$ to 100 V/nm: quantum gap at $D = 1$ nm, classical gap at $D = 1$ μm and relativistic gap at $D = 0.1$ mm. Unless it is specified elsewhere, we set $\phi_B = 2.48$ eV (Ba material) and $T = 300$ K in all our calculations. Note that for a relativistic gap of $D = 0.1$ mm, the value of V_g will be as large as 0.1 to 10 MV, where arcing is inevitable in practise. Then our study in relativistic regime is to provide a theoretical prediction on how the relativistic effect will change the properties of shot noise.

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A. Coulomb Correlation

In Fig. 3.1, the calculated (a) γ and (b) μ are plotted as a function of electric field strength F in a quantum gap $D = 1$ nm. For comparison, the results without including the Coulomb correlation [$U_{sc}(x) = 0$ and $U_{xc}(x) = 0$] are plotted in dotted lines, similar to the previous calculations [21, 118, 119]. It is clear that the Coulomb correlation among the tunneling electrons will further reduce the shot noise. However, this further suppression of the shot noise is due to the *combination* of Coulomb correlation by the space charge field (Coulomb repulsion) and the exchange-correlation effects of the tunneling electrons.

To illustrate this argument, we calculate a case with only the space charge field by ignoring the exchange-correlation effects [$U_{xc}(x) = 0$] and plot it using dashed lines. In Fig. 3.1(a), it shows a larger γ as compared to pure field emission (dotted lines). The finding suggests that pure space charge field or Coulomb repulsion of the emitted electrons will decrease the effect of quantum partitioning by creating a larger potential barrier. This leads to smaller quantum suppression and larger γ . On the other hand the exchange-correlation effects of transmitted electrons will result in a smaller potential barrier, which enhances the electron tunneling (larger current) as shown in Fig. 3.1(b), and the suppression of shot noise (smaller γ) as shown in Fig. 3.1(a). Note this quantum Coulomb correlation is due to the quantum dynamics of high current electron flows in a nanogap, as the SCL current density (in quantum regime) has exceeded the classical CL law ($\mu > 1$) [55].

Similarly we show in Fig. 3.2 the calculated results of (a) γ and (b) μ in a classical gap $D = 1$ μm for electric field strength $F = 1$ to 100 V/nm ($V_g = 1$ to 100 kV) at $T = 300$ K. In the classical regime of large gap spacing, the exchange-correlation effect of the emitting electrons inside the gap is negligible on the dynamics of the electron transport. The Coulomb correlation is mainly due to the classical Coulomb repulsion

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Figure 3.1: (a) The Fano factor γ and (b) the normalized current density μ at $T = 300$ K and $\phi_B = 2.48$ eV in a quantum gap ($D = 1$ nm) due to the Coulomb correlation as a function of F (solid lines). The dashed lines are the calculations without the exchange-correlation potential energy [$U_{xc}(x) = 0$]. The dotted lines are the calculations without the Coulomb correlation [$U_{xc}(x) = U_{sc}(x) = 0$].

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Figure 3.2: (a) The Fano factor γ and (b) the normalized current density μ at $T = 300$ K and $\phi_B = 2.48$ eV in a classical gap ($D = 1 \mu\text{m}$) due to the Coulomb correlation of the space charge field $[U_{sc}(x) \neq 0]$ (dashed lines). The dotted lines are the calculations of pure field emission $[U_{sc}(x) = 0]$.

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of the space charge field, which will reduce the shot noise suppression (dashed lines) and thus produce a large γ as compared to pure field emission (dotted lines), as shown in Fig. 3.2(a). This finding implies that there is no space charge smoothing for space charge limited field emission operating in a classical gap at high F .

B. Various Gap Spacings, Work Functions and Temperatures

The degree of quantum suppression of SCL field emission including the effects of both $U_{xc}(x)$ and $U_{sc}(x)$ will depend on the gap spacing, work function and temperature. Figure 3.3 shows the Fano factor γ (solid) and SCL current density μ (dashed) as a function of electric field strength F for (a) $D = 1, 10$ and 1000 nm, (b) $\phi_B = 2.14, 2.48, 3.76$ and 4.4 eV and (c) $T = 300, 1000$ and 2000 K.

For a fixed electric field strength, γ decreases with a smaller gap spacing D because of the manifestation of quantum Coulomb correlation at smaller D as shown in Fig. 3.3(a). Similarly γ will decrease with smaller work function in Fig. 3.3(b), as the effects of quantum partitioning become more significant with a smaller potential barrier. This noise suppression effect originates from Fermi statistical correlations under the conditions of current partitioning since the noise power is determined by the relative position of the Fermi level with respect to the barrier height. At high current density, it is expected that the resistive heating on the field emitter will increase the temperature of the tip. For this practical issue, we study the effects of high temperature (up to 2000 K) as shown in Fig. 3.3(c). From the figure we see that γ will increase with temperature at high electric field ($F > 3$ V/nm), for which the regime of SCL field emission has been reached (same μ at different T). At a relatively low $F = 1$ V/nm and $T = 2000$ K, the emission behaves like a thermionic enhanced field emission, which shows a slight suppression of shot noise with $\gamma = 0.92$. This suppression is due to the space charge smoothing as expected in the thermionic-like emission, which is dominant at low field and high temperature.

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Figure 3.3: The Fano factor γ (solid) and the normalized current density μ (dashed) in a quantum gap due to the Coulomb correlation for (a) $D = 1, 10$ and 1000 nm, (b) $\phi_B = 2.14, 2.48, 3.76$ and 4.4 eV and (c) $T = 300, 1000$ and 2000 K. The arrows in each figure indicate the direction of increasing D , ϕ_B and T .

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C. Image Charge Potential

It is clear that the classical image charge potential shown in Eq. (3.7) is not valid to account for the spillover effects of the electrons into the vacuum region near the electrodes, especially for a gap less than 10 nm. To improve on this limitation such as removing the singularities near the electrodes, we solve a Thomas-Fermi approximated (TFA) model to obtain the ground state and zero field image charge potential energy $U_{im}(x)$, which is due to Coulomb repulsion of the charges in the cathode, vacuum and anode. The TFA-based image charge potential energy is [126]

$$U_{im}(x) = -e^2 \int_0^\infty p \, dp \left[D_{\text{vac}}(p, x) + \frac{1}{2p} \right], \quad (3.13)$$

where the $D_{\text{vac}}(p, x)$ term is the longitudinal self-consistent field describing the screened Coulomb interaction between two charges at position x and x' , and p is the wave vector along the x -direction. The formulation is basically by solving the screened Poisson equation in its Green's function form using the TFA method [36]. Note that this TFA approach can be considered as a type of density-gradient theory, which has been used to describe field emission from metals [35].

In Fig. 3.4(a), it is shown that the (ii) TFA image charge potential energy is continuous at both metal-vacuum interfaces for Barium (Ba) electrodes at $D = 1$ nm. For the (i) classical image charge potential with the effect of anode screening given by Eq. (3.7), the singularity of $U_{im}(x)$ at the metal-vacuum interfaces may cause an underestimation of the barrier width. In Fig. 3.4(b) and (c), we compare, respectively, the calculated γ and μ for $F = 1$ to 10 V/nm for the two different forms of image charge potentials. By comparing the solid lines of (i) and (ii) in Fig. 3.4(b), we see that the influence of the image charge potential on the Fano factor is more significant at low field $F < 3$ V/nm. At relatively high field $F > 5$ V/nm, the Fano factor varies between $\gamma = 0.37$ to 0.42, and the field emission current saturates at

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Figure 3.4: (a) The image charge potential profile $U_{im}(x)$ for (i) the classical Ba-vacuum-Ba system in Eq. (3.7) and (ii) the TFA quantum Ba-vacuum-Ba system for a quantum gap ($D = 1$ nm) of Barium electrodes ($E_F = 2.317$ eV and $\phi_B = 2.48$ eV). (b) The Fano factor γ and (c) the normalized current density μ at $T = 300$ K due to the Coulomb correlation as a function of F (solid lines) for the two different forms of image charge potential energy. The dashed lines are the calculations without the exchange-correlation potential energy [$U_{xc}(x) = 0$]. The dotted lines are the calculations without the Coulomb correlation [$U_{xc}(x) = U_{sc}(x) = 0$].

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space charge limited condition in the quantum regime with a value of $\mu = 2$ to 3 as shown in Fig. 3.4(c).

For completeness, the calculations without including the Coulomb correlation [$U_{sc}(x) = 0$ and $U_{xc}(x) = 0$] are plotted in dotted lines, and the calculations with only the space charge field but no exchange-correlation effects [$U_{xc}(x) = 0$] are plotted using dashed lines. The finding on using the TFA approach is similar to the one using the classical image charge potential as shown in Fig. 3.1, where the *combination* of Coulomb repulsion by the space charge field and the exchange-correlation effects of the tunneling electrons inside the nanogap will reduce the shot noise to a smaller Fano factor γ . The Coulomb repulsion (dash lines) alone will increase the Fano factor as compared with pure field emission (dotted lines).

D. Relativistic Effects

In a classical gap such as 0.1 mm, same magnitude of electric field strength $F = 1$ to 100 V/nm requires the bias voltage as large as several megavolt. The velocity of electrons inside the gap exceeds half the speed of light. Consequently, a complete description of electron transportation necessitates a relativistic treatment, where the detailed formulation is shown in Appendix A.3. Basically a term named Lorentz factor Γ is adopted to relate the potential energy of electrons with its rest energy mc^2 , and the Poisson equation is rewritten in terms of Γ in Eq. (3.11).

In Fig. 3.5, we compare the results with (solid) and without (dashed) including the relativistic effects at $D = 0.1$ mm for $F = 1$ to 100 V/nm ($V_g = 0.1$ to 10 MV), where both cases include the space charge field, i.e. Coulomb repulsion. It is found that the relativistic effect will produce less shot noise suppression, but the difference is not significant: $\gamma = 0.91$ (relativistic) and 0.86 (classical) even at $F = 100$ V/nm. The difference of γ is negligible at low $F < 10$ V/nm or $V_g < 1$ MV. Thus although

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Figure 3.5: (a) The Fano factor γ and (b) the normalized current density μ at $T = 300$ K and $\phi_B = 2.48$ eV in a relativistic gap ($D = 0.1$ mm) due to the Coulomb correlation of the space charge field i.e., Coulomb repulsion, with (solid) or without (dashed) including the relativistic effects.

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the electrons could attain half speed of light at lower $V_g = 64$ kV, the relativistic effect is not important to shot noise in weak relativistic regime.

E. Possible Experiments

To the best of our knowledge, there is no experimental measurement of shot noise reduction for field emission even at low current regime (negligible space charge effects). Most studies of the electron emission noise have been concentrated on the flicker noise at very low frequency [127, 128, 129] with a spectrum proportional to $1/f^b$, where $b = 1$ for carbon nanotube (CNT) cathode [127, 128] and $b = 3/2$ for ZnO cathode [129]. The main difficulty in measuring shot noise is the requirement of high frequency and dedicated setup in order to avoid the significance of flicker noise at low frequency and to distinguish the relatively small shot noise spectrum from the background noise.

IBM had introduced one possible means for high frequency measurement to record the varying emission rate at the picosecond and subpicosecond time scale [18]. It is to focus the emitted electrons into a narrow beam, which is electrostatically deflected across a sensitive detector screen. The spatial density of the detected electrons as a function of position at the screen records the field emission rate as a function of time. It is claimed that by using small optics, sharp focusing and high sweep rates, 10^{-14} -s resolution is achievable [18].

Based on the flicker noise data (up to 25 Hz) from a recent field emission experiment on a single carbon nanotube (CNT) operating at a local field of about 6 V/nm and 600 K, with an emitting current of 2.4 nA [128], we can estimate the frequency range to reach the shot noise regime. The experiment gives a normalized flicker noise spectrum of $S_{\text{flicker}}/I^2 = a/f$, where $a = 4.5 \times 10^{-9}$ and f is the frequency in Hz. The CNT has a work function of 5 eV according to their experimental Fowler-Nordheim plot. At this operating condition, our calculation (ignoring space charge effect) shows no shot noise suppression and the calculated Fano factor is about 1 (γ

3.3 Shot Noise of SCL Field Emission

$= 0.9999$). By setting the flicker noise equal to the classical full shot noise $S_{\text{shot}}/I^2 = 2e/I = 1.3 \times 10^{-10} \text{ Hz}^{-1}$, the minimum frequency that the shot noise will become dominant is at $f > 35 \text{ Hz}$. From the results at its maximum measurable frequency of 25 Hz , the measured normalized noise spectrum has a large variation from 0.8 to $3 \times 10^{-10} \text{ Hz}^{-1}$ due to the uncertainty in the measurement system.

Thus, it is required to have a low work function emitter ($< 3 \text{ eV}$) operating at a reasonable electric field of $< 10 \text{ V/nm}$ in order to observe the significant shot noise suppression. By using the same conditions mentioned above but with a smaller work function of 3 eV , the Fano factor is about 0.88 according to our calculation with no space charge effects. To observe the shot noise of space charge limited field emission studied in this work, the work function has to be even smaller, such as lanthanum sulfide (LaS) material, which has a work function of about 1.14 eV at 300 K [119].

F. Remarks on the Model

It is important to note that the model proposed here is an equilibrium model, where the electronic properties of the metal surfaces are assumed to be at equilibrium. To include the nonequilibrium behavior of the electrons, nonequilibrium Kohn-Sham theory or Green's function approaches are required. Here, we would like to make some comments on the consistency of our model. First, our equilibrium model is able to show a reduction of shot noise for thermionic enhanced field emission, as shown in Fig. 3.3(c) at $F = 1 \text{ V/nm}$ and $T = 2000 \text{ K}$. This finding is consistent with the known effect of space charge smoothing for thermionic emission. Second, using TFA based model including the effects of Coulomb repulsion and exchange-correlation effects of the tunneling electrons, the model gives a better estimation on the emission area of an experimental IV curve in a nanogap [130]. Our model [126] estimates an area of about 1.2 nm^2 for $D = 0.8 \text{ nm}$, which is more consistent than the value of 0.004 nm^2 calculated based on a classical model [131]. Finally, our model is able to show

3.3 Shot Noise of SCL Field Emission

a smooth transition to the classical SCL current (or classical CL law) of $\mu = 1$ at a large gap spacing for which quantum effects are expected to be insignificant [55, 132].

There are some doubts that the boundary conditions on the potential (grounded at cathode and at voltage V_g at anode) automatically include the image charge potential when one solves the Poisson equation. It is possible that we have double counted the image charge potential by including it in Eq. (3.6). This puzzle is a question about the origin of the image charge potential (what is it and how to solve it). It still remains as an active research area [35, 36, 133, 134].

The origin of the image charge potential can be attributed by two mechanisms. The first one is the regular classical image charge potential in the form of k/x term. This classical image charge potential is to account for the classical electrostatic field in a region close to a grounded perfect conducting metal (cathode) due to a point charge (the electron tunneling through the barrier). In this consideration, solving Poisson equation with same boundary condition should give the same classical image charge potential of k/x .

However, it has been recognized that this classical image correction represents a rather severe idealization. It has assumed that the electrode is an electrostatically ideal metal with an infinite screening capacity, which causes the classical image potential to have a singularity at the cathode surface. The assumption of ideal metal also imposes an artificial separation of electrons, which overestimate the electrostatic effect of the tunneling electron. In reality, the conduction electrons of a metal spill over (via quantum-mechanical barrier penetration) into the vacuum for a very short distance. In the immediate vicinity of the surface the density of “spillover” electrons is far higher than that of “tunneling” electrons, and thus the “spillover” electrons must have the dominant electrostatic effect. In general, one needs to incorporate this effect by some quantum approach, such as density gradient theory [35], the Thomas-Fermi approximation [36] which modifies the k/x to $k/(x + x_0)$ where x_0

3.4 Shot Noise of Short Pulse SCL Field Emission

depends on the electronic structure of the cathode. It was also recently found that k/x term is approximately similar to the Kohn-Sham exchange potential at large x [134]. Therefore solving Poisson equation in the gap alone will not be able to give the image charge potential (including the spillover effect).

The recognition that image-force-corrected FN theory is flawed in assuming an ideal metal has fostered many efforts to provide a more fundamental theory of field emission. However the classical image force is still in wide use, because it is simple and corresponds fairly well to experiment. The more-exact theories tend not to improve agreement much and they rapidly become much more complex. Hence in our model, we still make use of the classical image charge potential as shown in Eq. (3.7).

3.4 Shot Noise of Short Pulse SCL Field Emission

Due to the advances in femtosecond lasers, it is now possible to have electron emission with very short pulse length through the laser-induced field emission as reviewed in Chapter 2. When the pulse length of the electron beam (τ_e) is less than the gap transit time at SCL condition: $T_{CL} = 3D\sqrt{m/2eV_g}$, the previous investigations in Section 3.3 on a steady state solution where the space charge extends between the cathode and anode are no longer valid. The classical short pulse CL law has been derived [135], which shows that the classical value of the steady state (or long pulse) CL law in Eq. (3.10) is enhanced. Later a consistent quantum and relativistic model of short pulse Child-Langmuir law has also been developed [102]. Hence in this section, we turn our attention to the effects of electron pulse length (τ_e) on the shot noise suppression (Fano factor γ) in the classical regime by including the space charge field in an equivalent diode model [102, 135]

In the equivalent diode approximation, we treat the electron pulse as a pulse of finite length, so that a continuous injection of current (of density J) takes place over

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Figure 3.6: Schematic drawing of steady state (long pulse) SCL field emission and short pulse SCL field emission, with potential profile $V_v(x)$ (dashed lines) and $V(x) = V_v(x) + V_{sc}(x)$ (solid lines). For a pulse of electron emission of finite length τ_e , at the moment of $t = \tau_e$, the pulse extends a length $x = \xi < D$ into the cathode-anode classical gap.

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a time period $0 < t < \tau_e$. At the moment of $t = \tau_e$ the pulse extends a length $x = \xi$ into the cathode-anode gap (x being zero at cathode and equal to D at anode) as shown in Fig. 3.6(b). We denote the potential in the gap as $V(x) = V_v(x) + V_{sc}(x)$ and the electric field as $-V'(x)$, where the prime here denotes the derivative with respect to x . At the front of the beam, the potential and the electric field is $V(\xi)$ and $-V'(\xi)$, respectively. One can immediately obtain the following relation from the Gauss law, i.e. the total electric flux out of a closed surface is equal to the charge enclosed divided by the permittivity,

$$[-V'(0)] - [-V'(\xi)] = \frac{J\tau_e}{\epsilon_0}, \quad (3.14)$$

where the electric flux through an area is defined as the electric field multiplied by the area of the surface projected in a plane perpendicular to the field. In terms of normalized parameters: pulse length $X_{CL} = \tau_e/T_{CL}$, potential $\phi(\bar{x}) = V(x)/V_g = \bar{x} + \phi_{sc}(\bar{x})$, position $\bar{x} = x/D$ and $\bar{\xi} = \xi/D$, we have

$$\phi'(0) - \phi'(\bar{\xi}) = -\frac{4}{3} \mu X_{CL}, \quad (3.15)$$

where the prime here denotes the derivative with respect to $\bar{x}$.

It is interesting to see that at long pulse limit $X_{CL} = 1$ and $\bar{\xi} = 1$, under the classical space charge limited (Child-Langmuir) condition $\mu = 1$, the electric field at cathode goes to zero $\phi'(0) = 0$, thus the electric field at anode now is $-\phi'(1) = -4/3$ or $-V'(D) = -\frac{4}{3} \frac{V_g}{D}$, which is well-known in the literature [136]. However at short pulse length $X_{CL} < 1$ with some injected current μ , the position of beam front ξ needs to be found numerically, together with the space charge potential profile $V_{sc}(x)$ inside the beam region ($0 < x < \xi$), by consistently solving the Eqs. (3.12) and (3.15) with boundary conditions $\phi_{sc}(0) = 0$ and $\phi_{sc}(\bar{\xi}) = 0$.

In Fig. 3.7, we show the calculated Fano factor γ (solid) and normalized current density μ (dashed) as a function of normalized pulse length $X_{CL} = \tau_e/T_{CL}$ at fixed $F = 5$ V/nm for a classical gap of $D = 1$ μm ($V_g = 5$ kV). At short pulse length $X_{CL} <$

3.4 Shot Noise of Short Pulse SCL Field Emission

Figure 3.7: The Fano factor γ (solid) and the normalized current density μ (dashed) at $T = 300$ K, $\phi_B = 2.48$ eV, $D = 1$ μm and $F = 5$ V/nm (the classical regime) due to the space charge field, as a function of normalized pulse length X_{CL} in terms of the gap transit time $T_{\text{CL}} = 72$ femtosecond.

3.5 Summary

1, the SCL current density is high because it is inversely proportional to X_{CL} [102]. At ultrashort pulse length $X_{CL} < 0.01$, the field emission is basically source limited where the space charge effect is not important. The Fano factor is independent of X_{CL} , which is about $\gamma = 0.7$, similar to the pure field emission case calculated before [see the dotted line in Fig. 3.2(a) at $F = 5$ V/nm]. At large X_{CL} approaching the long pulse (steady-state) limit at $X_{CL} = 1$, the space charge effect is significant to increase the potential barrier, leading to smaller quantum partitioning and larger $\gamma = 0.98$ [see also the dashed line in Fig. 3.2(a) at $F = 5$ V/nm]. Thus, the Coulomb correlation can be ignored for the suppression of shot noise, if the pulse length is short enough for source limited electron emission, where space charge effect is negligible.

3.5 Summary

In conclusion, the influence of the Coulomb correlation on the degree of quantum partitioning has been studied, for the space charge limited field emission by including the space charge field and exchange-correlation potential of the tunneling electron inside a gap [22]. The Fano factor is calculated over a wide range of gap spacings, applied voltages and pulse lengths in classical, quantum and relativistic regimes. For field emission in a large gap, Coulomb correlation will increase the Fano factor (smaller suppression of shot noise) because the space charge field will increase the potential barrier (less quantum partitioning). Therefore there is no effect of space charge smoothing in SCL field emission, different from what is predicted in SCL thermionic emission. Nevertheless in a nanogap with low voltage, the combination of space charge field and exchange-correlation potential of the tunneling electrons will enhance the suppression of shot noise as compared to pure field emission. At short pulse limit (smaller than gap transit time), space charge effect could be ignored and thus a larger suppression of shot noise is predicted for short electron pulses.

CHAPTER 4

THERMAL-FIELD ELECTRON EMISSION FOR LOW TEMPERATURE REFRIGERATION

4.1 Introduction

Refrigeration describes the process of cooling an object by transferring its heat away at a certain temperature. Mechanical refrigeration systems are based on the absorption of heat by the refrigerant during its phase change from liquid to gas, which will lower the temperature of the object. Thermoelectric cooling occurs when a current is passed through two dissimilar metals or semiconductors (n-type and p-type) that are connected to each other at two junctions (also known as Peltier junctions), and the current drives a transfer of heat from one junction to the other. Compared with mechanical refrigerators, thermoelectric coolers have no moving parts; hence they are quiet and require little maintenance.

However, the Peltier coolers even using the best materials today cannot compete with traditional cooling devices in terms of efficiency. The primary research objective on Peltier coolers is to find new materials which could be used to make more efficient

4.1 Introduction

thermoelectric coolers [137, 138]. For optimal efficiency, it is required to maximize the dimensionless figure of merit defined as $ZT = \frac{\Pi^2}{\rho\kappa T}$, where $\Pi = Q/J$ is the Peltier coefficient, ρ is electrical resistivity, κ is thermal conductivity, Q is power density and J is current density. It is unlikely that ZT will ever exceed 4 in any solid material [139]. Another possibility of obtaining large ZT is to have a free space with low thermal conduction ($\kappa \rightarrow 0$) between the cold and hot sides. This is also known as thermal-field electron emission based vacuum cooling, which has attracted considerable interest [3, 140, 141, 142, 143, 144, 145, 146, 147, 23].

As introduced in Chapter 1, thermionic emission is the emission of electrons from a metal or metal oxide surface by using the thermal energy to overcome the potential barrier (work function). Thermionic emission across a vacuum gap promises to have a much higher figure of merit than a solid thermoelectrics, because there is no lattice thermal conductivity, no ohmic resistivity due to absence of electron scattering, and the Peltier coefficient is greater than that of thermoelectric materials. However as of today, there are no successful examples of refrigeration based on thermionic emission in vacuum, because as Mahan [3] pointed out, a work function of 0.3 to 0.4 eV is necessary to obtain sufficient high currents for practical thermionic refrigeration at room temperature. Thus thermionic refrigerators can be effective only at temperatures above 1000 K [3].

The principle of thermal-field emission refrigeration is based on the Nottingham effect [148]. The difference in the heat fluxes carried by the emitted electrons and the replacement electrons will determine if heating or cooling occurs on the emitted surface. To cool a cathode efficiently, a filtering mechanism is required to enable only the emission of high energy electrons (above the Fermi energy level E_F), such as by having a Schottky barrier of a semiconductor heterojunction [142, 143], resonant tunneling structures [144, 145], using field emission in a nanoscale gap [146], and sharp (nanoscale) diamond emitters [147].

4.2 Electron Emission in a Crossed-Field Gap

In this research, we propose an improved low-temperature refrigeration method [23, 24] based on thermal-field electron emission in a crossed-field vacuum gap, with an external magnetic field that is perpendicular to the applied electric field, which will be formulated in Section 4.2. By properly tuning the electric and the magnetic fields, the emission of the unfavorable low energy electrons that are responsible for the heating can be suppressed significantly. The concept of the proposed method is to suppress the potential barrier close to the cathode, in order to enhance the emission of high energy electrons; and concurrently to create a second barrier (due to Lorentz force) near the anode to prevent the transmission of the low energy electrons. The locally lowered barrier near cathode can be realized by two geometric designs, i.e. a planar diode with sharp field emitters (see Section 4.3) and a coaxial cylindrical diode with smooth emitting surface (see Section 4.4). Based on this concept, it is theoretically possible to achieve the refrigeration from room temperature down to 10 K, by using emitters with arbitrary work functions at some optimal conditions.

4.2 Electron Emission in a Crossed-Field Gap

Consider the electrons being emitted normally from a metallic cathode into a crossed-field vacuum gap with an external uniform magnetic field B parallel to the electrode surfaces. The anode is held at a dc voltage V_g with a spacing of D from the cathode. Once the electrons are emitted normally into the vacuum region, the Lorentz force will cause a lateral velocity. The momentum operator and the vector potential of the magnetic field commute, for which we may reduce the two-dimensional (2D) electron motion problem to a simple one-dimensional (1D) model [149, 150] with an additional potential term of $U_B(x)$.

The amount of the emitted current density and its associated heat flow are obtained by solving the one-dimensional (1D) time-independent Schrödinger equation

4.2 Electron Emission in a Crossed-Field Gap

using the following electrical potential energy $U_{tot}(x)$ with respect to E_F ,

$$U_{tot}(x) = \phi_B + U_{im}(x) + U_v(x) + U_{sc}(x) + U_B(x), \quad (4.1)$$

where ϕ_B is the work function of the field emitter, $U_{im}(x)$ represents the effect of image force potential, $U_v(x) = -eV_v(x)$ is the electric potential energy from the externally applied electric field and $U_{sc}(x) = -eV_{sc}(x)$ is from the space charge field. The last term $U_B(x)$ is the potential energy of the external magnetic field, where in the derivation we had ignored the effects of the magnetic field inside the cathode and also the interaction of intrinsic magnetic moment of the electrons with the magnetic field. The detailed expression of each term in Eq. (4.1) will be specified in their respective sections (see below).

The schematic drawing of a typical potential energy barrier profile $U_{tot}(x)$ in a crossed-field gap is shown in Fig. 4.1 (solid line). In addition to the traditional electrostatic potential barrier near the emitter ($x \rightarrow 0$) which depends on the localized large electric field, there exists another potential barrier at the anode ($x = D$) due to the applied magnetic field. When the magnetic field is tuned carefully to block only the low energy emitted electrons (responsible for heating), but to allow large transmission of high energy electrons (for cooling), it can provide a filtering mechanism for efficient cooling purpose. Define U_{max} and U_A as the peak of the potential barrier near cathode and anode respectively, and denote U_{m1} (U_{m2}) as the larger (the smaller) one among them. Using Eq. (4.1), the thermal-field emitted electrons lead to a local current density of J and a local cooling (or heating) power density of $Q > 0$ (or $Q < 0$), which are calculated by

$$J = e \int_{-\infty}^{\infty} N(E_x) \mathcal{T}(E_x) dE_x, \quad (4.2)$$

$$Q = \int_{-\infty}^{\infty} (k_B T + E_x) N(E_x) \mathcal{T}(E_x) dE_x. \quad (4.3)$$

Here, $N(E_x)$ is the density of incident electrons at cathode-vacuum interface with energy in the range of E_x and $E_x + dE_x$, and $\mathcal{T}(E_x)$ is the tunneling probability. The

4.2 Electron Emission in a Crossed-Field Gap

Figure 4.1: A typical potential barrier profile in a crossed-field gap $U_{tot}(x)$ (solid line), the dashed line is the image charge potential energy $U_{im}(x)$, the dash-dotted line is the external electric field potential energy $U_v(x)$, and the dotted line is the potential energy from the external magnetic field $U_B(x)$. The peak of the potential barrier near cathode and anode is, respectively, indicated as U_{max} and U_A .

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detailed expression and derivation of $\mathcal{T}(E_x)$ is shown in Appendix B. By defining $\Theta(x) = \sqrt{\frac{2m}{\hbar^2} [E_x - U_{tot}(x)]}$, $\alpha = \exp \left[\int_{x_1}^{x_2} |\Theta(x)| dx \right]$, $\beta = \exp \left[\int_{x_3}^{x_4} |\Theta(x)| dx \right]$, and $\gamma = \int_{x_2}^{x_3} |\Theta(x)| dx$, where x_1, x_2, x_3, x_4 are the roots of $U_{tot}(x) - E_x = 0$, the $\mathcal{T}(E_x)$ is calculated according to

$$\mathcal{T}(E_x) = \begin{cases} 1 & \text{if } E_x > U_{m1} \\ \exp \left[-2 \int_{x_1}^{x_2} |\Theta(x)| dx \right] & \text{if } U_{m2} < E_x < U_{m1} \\ 4 / \left[(4\alpha\beta + \frac{1}{4\alpha\beta})^2 \cos^2 \gamma + (\frac{\alpha}{\beta} + \frac{\beta}{\alpha})^2 \sin^2 \gamma \right] & \text{if } E_x < U_{m2} \end{cases}$$

For electrons with high energy of $E_x > U_{m1}$, we assume $\mathcal{T}(E_x) = 1$. Electrons with energy between U_{m2} and U_{m1} will tunnel through a single barrier of width $x_2 - x_1$. Below U_{m2} , low energy electrons have to tunnel through a dual barrier of width $x_2 - x_1$ and $x_4 - x_3$. For simplicity, a normalized cooling power density ($0 \leq \eta \leq 1$) is also defined as

$$\eta = \frac{Q}{Q_u}, \quad \text{where } Q_u = \int_{-k_B T}^{\infty} (k_B T + E_x) N(E_x) dE_x. \quad (4.4)$$

Here Q_u depends only on temperature and it accounts for the ultimate cooling power density that can be extracted by complete transmission of high energy electrons with $\mathcal{T}(E_x > -k_B T) = 1$, and blocking of low energy electrons with $\mathcal{T}(E_x < -k_B T) = 0$.

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For a planar diode geometry, the electrons are emitted *normally* from a single spherical point source at $x = 0$ of a blunt nanotip-based metallic cathode [147] into a crossed-field vacuum gap with an external uniform magnetic field B parallel to the electrode surfaces. The anode is held at a dc voltage V_g with a spacing of $x = D$ from the tips of the metallic nanoscale field emitters. Once the electrons are emitted normally into the vacuum region, the Lorentz force will cause a lateral velocity $v_y = -\Omega x$, which is linearly proportional to x due to the acceleration by the

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applied electric field, and $\Omega = eB/m$ is the electron cyclotron frequency. For such a planar diode geometry, the potential energy terms are specified as [147, 23]

$$U_{im}(x) = -\frac{e^2}{4\pi\epsilon_0} \frac{R}{(2R+x)2x}, \quad (4.5a)$$

$$U_v(x) = -e[F_0 \times \Gamma(x)]x \quad \text{and} \quad U_{sc}(x) = 0, \quad \text{where } \Gamma(x) = \frac{D+R}{x+R}, \quad (4.5b)$$

$$U_B(x) = \frac{1}{2}mv_y^2 = \frac{1}{2}m\Omega^2x^2. \quad (4.5c)$$

Here $R \ll D$ is the radius of the nanoscale emitter, $F_0 = V_g/D$ is the average electric field, $\Gamma(x)$ is the x -dependent electric field enhancement factor due to small $R \ll D$, ϵ_0 is free space permittivity, and e (m) is the electron charge (rest mass). At $R \gg D$ limit, i.e. a flat field emitter, the image charge term in Eq. (4.5a) will recover to its usual expression $U_{im}(x) = -e^2/16\pi\epsilon_0x$ as in Chapter 2, and the field enhancement factor $\Gamma(x) \rightarrow 1$ suggests a uniform electric field F_0 inside the vacuum gap for a flat field emitter.

4.3.1 Cooling Power Density Optimization

To suppress the low energy electrons below $-k_BT$, the potential barrier at the anode ($x = D$) is tuned to $U_A = \phi_B - eV_g + \frac{1}{2}m\Omega^2D^2 = -k_BT$ (negligible image force potential at anode) which gives an optimal setting of

$$eB_oD = \sqrt{2m(eV_g - \phi_B - k_BT)}. \quad (4.6)$$

For a given ϕ_B , D , V_g and T , this is the condition for the optimal value of magnetic field $B = B_o$. In Fig. 4.2, we confirm the optimal magnetic field B_o by finding the maximum η (for $V_g = 100$ V, $D = 100$ μm , $\phi_B = 4$ eV and $R = 10$ nm) at $T = 50$ and 300 K, which agrees very well with the analytical values of B_o shown in Eq. (4.6). When a smaller magnetic field $B < B_o$ is used, $U_A < -k_BT$, the second barrier does not block the heating electrons below $-k_BT$ effectively. But if large magnetic field

4.3 Planar Diode Geometry

$B > B_o$ is applied, $U_A > -k_B T$, the second barrier will block some cooling electrons above $-k_B T$, decreasing the cooling power density η .

In addition to suppressing low energy electrons by tuning $U_A = -k_B T$ at anode, η can be further optimized by simultaneously tuning both the electric and magnetic fields to ensure also the maximum transmission of high energy electrons from the cathode. In doing so, the potential barrier near the cathode is tuned to $U_{\max} = -k_B T$ at a critical voltage V_c and a critical magnetic field B_c , which are derived under the assumption of $D \gg R$,

$$eV_c = 4\pi\epsilon_0 R [\phi_B + k_B T/e]^2, \quad (4.7a)$$

$$eB_c D = \sqrt{2m(eV_c - \phi_B - k_B T)}. \quad (4.7b)$$

In Fig. 4.3, we present the dependence of η on V_g at $B = B_o(V_g)$ for low temperatures $T = 50, 20$ and 10 K (top to bottom), which shows that high $\eta = 0.94$ to 1 can be obtained with $V_c \approx 114$ V and $B_c \approx 0.35$ T. By applying $B = B_o(V_g)$ for each V_g , the U_A is always maintained at $-k_B T$ as shown in Fig. 4.3. For $V_g < V_c$, the barrier near cathode is higher than that of anode ($U_{\max} > U_A$), the transmission of high energy electrons for cooling purposes is limited ($\eta < 1$). For $V_g > V_c$, we have $U_{\max} < U_A$ and higher tunneling of low energy electrons between $U_{\max}$ and U_A , which leads to a saturated (and smaller) η . This saturation phenomenon will lower the cooling power density only at $T < 20$ K.

It is clear from Eq. (4.7b) that the critical magnetic field B_c required for maximum $\eta \approx 1$ is inversely proportional to D . This limits the possibility of using small D due to impracticably large B , which corresponds to $D > 20 \mu\text{m}$ for $B < 2$ T at $\phi_B = 4$ eV, $R = 10$ nm and $T = 300$ K. On the other hand, a large D will require a very fine tuning of magnetic field to obtain maximum η . At $D > 150 \mu\text{m}$, the full-width half maximum of the magnetic field is less than 1 gauss at room temperature. Thus, the practical range of D should be from 20 to 150 μm , which corresponds to $B = 0.23$ to 1.8 T. If a lower work function material (1 eV) is used, the value of

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Figure 4.2: Dependence of the normalized cooling power density η on the magnetic field B for $T = 300$ and 50 K, at $\phi_B = 4$ eV, $R = 10$ nm, $D = 100$ μ m, and $V_g = 100$ V.

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Figure 4.3: Dependence of the normalized cooling power density η on the external bias V_g for $T = 50$, 20 and 10 K, at $\phi_B = 4$ eV, $R = 10$ nm, $D = 100$ μ m, and $B = B_o(V_g)$.

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magnetic field may be further reduced to less than 0.1 T whereas the full-width half maximum of magnetic field can be increased to around 10 gauss.

4.3.2 Merits of Proposed Cooling Method

Besides the cooling power density Q or η , the capability of the cooling is also measured by the coefficient of performance ($\text{COP} = \Pi/V_g$), where $\Pi = Q/J$ is the Peltier coefficient. The Peltier coefficient indicates the average energy of emitted electrons, which also measures the effectiveness of the filtering mechanism. In Fig. 4.4(a), we show the calculated Π , Q and J as a function of V_g for $\phi_B = 1$ eV (solid) and 4 eV (dashed). At $\phi_B = 1$ eV, we have $Q = 1$ to 100 W/cm² at $V_g = 2.7$ to 3.6 V with $\Pi = 0.2$ to 0.4 V ($\text{COP} = 0.06$ to 0.15), which is comparable to previous methods [143, 146]. At higher voltage like $V_g > 8$ V, Q saturates at its maximum value about $Q_{\text{max}} = 600$ kW/cm² with lower $\Pi = 0.03$ V, for which other thermal-field emission based cooling methods will fail to produce a net cooling (i.e. Q or Π becomes negative at high field). If higher work function (4 eV) is used, same saturated values of Q and Π remain possible, but requiring higher $V_g > 115$ V.

The combined merits of using nanoscale emitters in a crossed-field gap is proved by comparing the maximum cooling power density Q_{max} and its corresponding Π at various temperatures, with two $B = 0$ cases using sharp ($R = 10$ nm) and flat emitter ($R \gg D = 100$ μm) as shown in Fig. 4.4(b). It is evident that the proposed method outperforms the other two cases by a large factor in terms of the maximum cooling power density, Peltier coefficient, and the range of minimum cooling temperature. Moreover, the proposed method is also relatively independent of R ($= 10$ to 100 nm) and ϕ_B ($= 1$ to 4 eV) for $T > 20$ K, and the variation at $T = 10$ K is about 17.3 to 20.6 W/cm². It is important to note that the cases with $B = 0$ cannot even provide cooling at $\phi_B = 4$ eV, where $\phi_B = 1$ eV have been used in the comparison. Therefore, compared to the other thermionic refrigeration methods, the proposed one

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Figure 4.4: (a) Dependence of Peltier coefficient Π , current density J and cooling power density Q on the applied bias V_g at $T = 300$ K, $R = 10$ nm, $D = 100$ μ m, $B = B_o(V_g)$, and $\phi_B = 1$ eV (solid) and 4 eV (dashed). (b) Optimal cooling power density $Q_{\max}$ (solid lines) and the corresponding Π (short dashed lines) for various temperatures T at $V_g = V_c$ and $B = B_c$ for $\phi_B = 1 - 4$ eV, as compared to $B = 0$ cases for flat ($R \gg D = 100$ μ m) and sharp ($R = 10$ nm) emitters of $\phi_B = 1$ eV.

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has the following advantages: (i) arbitrary high work function emitters can be used; (ii) cooling temperature can be as low as below 10 K; and (iii) higher cooling power density in the practical range of parameters with tuning capability.

4.4 Coaxial Cylindrical Diode Geometry

Other than making use of a nanoscale emitter in a planar diode geometry, the barrier near cathode can also be suppressed using a coaxial cylindrical diode geometry [151]. As shown in Fig. 4.5, the coaxial cylindrical diode has an inner cathode of radius r_c (in nanometer scale) and an outer anode of radius r_a (in sub-millimeter scale). The electrons are emitted from the cathode with a perfectly smooth surface, and the field enhancement is due to the large aspect ratio of r_a/r_c . The anode is held at a dc voltage V_g with a spacing of $D = r_a - r_c$ from the cathode. The electric field $F(r)$ and the corresponding electrical potential $V_v(r)$ are

$$F(r) = -\frac{V_g}{r \ln(r_a/r_c)} = -F_0 \times \Gamma(r), \quad \text{where } \Gamma(r) = \frac{1}{(r/D) \ln(r_a/r_c)}, \quad (4.8a)$$

$$V_v(r) = -\int_{r_c}^r F(r') \, dr' = V_g \frac{\ln(r/r_c)}{\ln(r_a/r_c)}. \quad (4.8b)$$

Compared to the constant electric field $F_0 = V_g/D$ for a planar diode with flat electrodes, the electric field near the cathode at $r \rightarrow r_c$ will be modified by the factor $\Gamma(r)$ for the same values of D and V_g . The electric field will be enhanced ($|\Gamma| > 1$) or suppressed ($|\Gamma| < 1$), which depends on whether the cathode or the anode is the inner electrode. Defining $w = r_a/r_c$, we have the field modification factor at cathode

$$|\Gamma(r_c)| = \frac{w-1}{\ln(w)}, \quad (4.9)$$

which is an increasing function of w and $\lim_{w \rightarrow 1} |\Gamma(r_c)| = 1$. Only if the cathode is the inner electrode ($w > 1$ and $r_a > r_c$), the electric field will be enhanced as $|\Gamma(r_c)| > 1$. If anode is the inner electrode ($w < 1$), $|\Gamma(r_c)| < 1$ suggests electric

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Figure 4.5: The schematic drawing of the coaxial cylindrical diodes with (a) zero magnetic field $B = 0$ and (b) uniform axial magnetic field $B = B_z$.

field suppression near the cathode, which is undesirable in the cooling application.

The image charge potential energy is [119]

$$U_{im}(r) = -\frac{e^2}{16\pi\epsilon_0(r - r_c + r_0)}, \quad (4.10)$$

where $r_0 = e^2/[16\pi\epsilon_0(E_F + \phi_B)]$ is used to ensure that the potential profile is continuous across the cathode-vacuum interface at $r = r_c$.

Once the electrons are emitted radially into the vacuum region between the cathode and anode, they will continue moving radially towards the anode [see Fig. 4.5(a)]. This case will be elaborated in Section 4.4.1. With an additional magnetic field B_z , the Lorentz force will cause a velocity in azimuthal direction [see Fig. 4.5(b)],

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where the expression of $U_B(r)$ and the resulting cooling performance will be shown in Section 4.4.2. For simplicity, the space charge effect is first ignored by assuming $U_{sc}(r) = 0$, and its consistent treatment will be included later in Section 4.4.3.

4.4.1 Zero Magnetic Field

Figure 4.5(a) shows a diagram of the zero magnetic field case. The emitted electrons will move radially from the cathode ($r = r_c$) to the anode ($r = r_a$) under the electric force. With zero magnetic field, i.e. $U_B(r) = 0$, there is only one potential peak near cathode $U_{\max}$ with an effective barrier height reduction of $\phi_B - U_{\max}$, dependent on the size of the coaxial cylindrical diode. By analyzing the electric field at the cathode, there is a field enhancement factor of (as compared to the planar flat diode F_0)

$$|\Gamma(r_c)| = \frac{1}{\bar{r}_c \ln(1 + 1/\bar{r}_c)}, \quad (4.11)$$

which increases with decreased $\bar{r}_c = r_c/D$. In Fig. 4.6(a), the dependence of potential barrier $U_{\max}$ on $\bar{r}_c$ is shown from $\bar{r}_c = 10$ to 10^{-4} at fixed voltage V_g and spacing D .

Using $D = 1$ mm as an example [see Fig. 4.6(b)], several cases of $r_c = 10$ nm or 100 nm with work function of $\phi_B = 1$ eV or 2 eV are selected, the applied voltage V_g is varied to show the normalized cooling power density η at room temperature $T = 300$ K. Here, η can achieve 0.012 by using $r_c = 10$ nm and $\phi_B = 1$ eV, which is about 7100 W/cm² at $V_g = 60$ volt. Larger $r_c = 100$ nm at same $D = 1$ mm (less field enhancement) will require a larger $V_g = 440$ volt to achieve its maximum cooling power density of about $\eta = 0.0068$ or $Q = 4040$ W/cm² at $T = 300$ K.

For metals with a higher work function (2 eV or more), η will diminish drastically to less than 10^{-9} . In this case, the wide barrier at small V_g will restrict most of the cooling (high-energy) electrons even though it is able to block heating (low-energy) electrons. At large V_g with smaller barrier, the undesirable heating (low-energy) electrons are however not suppressed sufficiently, which will lead to an abrupt

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Figure 4.6: (a) The potential barrier height $U_{\max}$ (solid line) and the amount of barrier height reduction (dashed line) as a function of normalized radius of cathode r_c in terms of spacing between electrodes D . (b) The normalized cooling power density η as a function of the applied voltage V_g for four different settings of $[\phi_B$ (eV), r_c (nm)] = [1, 10], [1, 100], [2, 10] and [2, 100] at $T = 300$ K and $B = 0$.

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termination of cooling (η becomes negative at high V_g). This finding agrees with Mahan's conclusion [3] and other recent works on thermal-field emission refrigeration [146, 147, 152], confirming that a low work function cathode is required for a practical cooling performance even at room temperature.

4.4.2 Uniform Axial Magnetic Field

To improve the cooling performance presented above, a uniform axial magnetic field B_z can be added, which will create a second potential barrier U_A at the anode. The strength of the magnetic field is properly tuned in order to block only the low-energy heating electrons, and concurrently to allow large transmission of high energy cooling electrons, which will provide an optimal filtering condition. In this case as shown in Fig. 4.5(b), electric field is radial and symmetrical about z axis, and the magnetic field is uniform and parallel to z axis.

To derive the expression of $U_B(r)$, we consider an electron emitted from a point at cathode $r = r_c$ with zero initial velocity. Under the influence of the constant magnetic field B_z and the symmetrical electric field $F(r)$, the equation of motion is [153]:

$$\frac{1}{r} \frac{d}{dt} \left(r^2 \frac{d\theta}{dt} \right) = B \frac{e}{m} \frac{dr}{dt}. \quad (4.12)$$

which has a solution of

$$\frac{d\theta}{dt} = \frac{eB}{2m} \left(1 - \frac{r_c^2}{r^2} \right). \quad (4.13)$$

By the conservation of kinetic and potential energy, the potential term $U_B(r)$ becomes

$$U_B(r) = \frac{1}{2} m \left(r \frac{d\theta}{dt} \right)^2 = \frac{1}{8} m \Omega^2 \left(r - \frac{r_c^2}{r} \right)^2, \quad (4.14)$$

where $\Omega = eB/m$ is electron cyclotron frequency. In the limit of large radius with both r_c and r_a much larger than D , Eq. (4.14) recovers to $U_B(x) = \frac{1}{2} m \Omega^2 x^2$ and $x = r - r_c$ in Eq. (4.5c), which behaves like a planar diode.

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To suppress the low energy heating electrons below $-k_B T$, the potential barrier at the anode should be tuned to $U_A = -k_B T$, which gives an optimal setting

$$eB_o r_a \left(1 - \frac{r_c^2}{r_a^2}\right) = 2\sqrt{2m(eV_g - \phi_B - k_B T)}. \quad (4.15)$$

For a given cylindrical diode (ϕ_B, r_c, r_a) working at some temperature T , Eq. (4.15) gives the optimal value of the magnetic field ($B_z = B_o$), which is a function of V_g . This indicates that for any applied voltage V_g at anode, the corresponding magnetic field B_o should be added to maximize the cooling power density at any low temperature T or high work function ϕ_B . The calculation results are shown in Fig. 4.7 for $\phi_B = 2$ eV, $r_c = 10$ nm, $D = 0.1$ mm and $T = 300$ K for three $V_g =$ (a) 250, (b) 300 or (c) 350 volt. For each V_g , the numerically calculated optimal magnetic field B_o at the maximal η agrees very well with the analytical condition given by Eq. (4.15).

In addition to suppressing the low-energy heating electrons by tuning $U_A = -k_B T$ at the anode, η can be further enlarged by simultaneously tuning both the voltage V_g and magnetic field B_z to ensure the maximum transmission of high energy electrons from the cathode, which provides the cooling effect. In doing so, the potential barrier near the cathode is tuned to $U_{\max} = -k_B T$ at a critical voltage of V_c . In Fig. 4.7(d), we present the dependence of η (solid line) on V_g at its corresponding $B_z = B_o(V_g)$ (dashed line) for $T = 300$ K. In this scenario, we keep the second barrier at anode $U_A = -k_B T$ to block the heating electrons at all values of V_g . At $V_g < V_c$, the barrier near cathode is higher than that of anode ($U_{\max} > U_A$), the transmission of high energy electrons for cooling purposes is thus limited ($\eta < 1$). With the heating electrons totally blocked by the second barrier U_A , the continuous increasing of V_g will decrease the cathode barrier $U_{\max}$ to allow more emission of cooling electrons and thus provide larger η . At $V_g > V_c$, the emission of heating (low energy) electrons is completely blocked by the combined effects of the dual barriers (near cathode and anode), and the complete transmission of high energy electrons for cooling purpose will give a saturated high value of $\eta \approx 1$. Figure 4.7(d) shows that high $\eta \rightarrow 1$

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Figure 4.7: The dependence of the normalized cooling power density η (solid lines) as a function of applied magnetic field B at different $V_g =$ (a) 250, (b) 300, (c) 350 volts, and as a function of (d) V_g at optimized value of $B = B_o(V_g)$ at $T = 300$ K. The dashed line in (d) is the value of B_o as a function of V_g . The tuning ranges ΔB are indicated in (a) to (c).

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or $Q = 5.94 \times 10^5 \text{ W/cm}^2$ can be obtained by applying $V_g > V_c \approx 360 \text{ volt}$ and $B_z > B_o(V_c) \approx 1.27678 \text{ T}$. At smaller $V_g = 300 \text{ volt}$ with $B_o = 1.16488 \text{ T}$, the cooling power density will be $\eta \approx 0.58$ or $Q = 3.44 \times 10^5 \text{ W/cm}^2$.

It is important to note that the effective tuning range of the magnetic field will become very strict at high V_g and η regime. For practical application, the tuning range should be larger than the geomagnetic field, which is from 0.3 gauss to 0.6 gauss. Here, we define the effective magnetic field tuning range ΔB as the full width at half maximum of η . In Fig. 4.7 (a) - (c), the tuning range is, respectively, $\Delta B = 2.0, 1.8$ and 1.5 gauss for $V_g = 250, 300$ and 350 volt . In our model, the value of ΔB is mainly determined by two parameters: r_c and D . In Fig. 4.8 and Fig. 4.9, we will vary the values of r_c and D , in order to increase the ΔB at a fixed cooling power density of $\eta \approx 0.6$ and $T = 300 \text{ K}$.

In Fig. 4.8, we consider that the ratio of r_c and D is fixed at 10^{-4} , and it is found that the tuning range ΔB and the optimal magnetic field strength B_o are increased by reducing the size from $D = 1 \text{ mm}$ to 0.01 mm and $r_c = 100 \text{ nm}$ to 1 nm , with an operating V_g reduced from 3000 to 34 volt. The tuning range can be as high as 55 gauss for the smallest diode ($D = 0.01 \text{ mm}$ and $r_c = 1 \text{ nm}$) with $B_o \approx 3.816 \text{ T}$ as shown in Fig. 4.8(a). For fixed $r_c = 10 \text{ nm}$, the tuning range ΔB is improved from 0.15 to 1.8 gauss, when D is varied from 1 mm to 0.1 mm , but at the expense of using higher magnetic field (about 1.1649 T) as shown in Fig. 4.9 (a) and (b). Compared to Fig. 4.9(b), further improvement can be made by decreasing r_c from 10 nm to 1 nm at fixed $D = 0.1 \text{ mm}$, and Fig. 4.9(c) shows a tuning range of about 5 gauss with smaller magnetic field (about 0.4295 T) and voltage (42.5 volt). In summary, there are three ways to improve the tuning range of magnetic field: (a) to decrease the spacing D for a nice improvement on ΔB but a larger B_o is required; (b) to decrease cathode radius r_c to obtain moderate improvement on ΔB and a desired reduced B_o ;

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Figure 4.8: For uniform $B = B_z$ case, the sensitivity of the tuning range ΔB for different r_c and D (with same ratio of $r_c/D = 10^{-4}$) at work function of $\phi_B = 2$ eV. The values of V_g are chosen to obtain $\eta \rightarrow 0.6$ at $T = 300$ K.

4.4 Coaxial Cylindrical Diode Geometry

Figure 4.9: For uniform $B = B_z$ case, the sensitivity of the tuning range ΔB for different $r_c = 1$ or 10 nm and $D = 0.1$ or 1 mm at work function of $\phi_B = 2 \text{ eV}$. The values of V_g are chosen to obtain $\eta \rightarrow 0.6$ at $T = 300 \text{ K}$.

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(c) to simultaneously decrease D and r_c to achieve a high improvement on ΔB and also an acceptable increment on B_o .

Similar to the planar diode case, the capability of the cooling is also measured by the coefficient of performance ($\text{COP} = \Pi/V_g$), where $\Pi = Q/J$ is the Peltier coefficient. In Fig. 4.10, we show the calculated (a) maximized cooling power density $Q_{\max}$ at its optimized voltage and (b) Π as a function of temperatures for cases with and without the external axial magnetic field B_z at different r_c , D and ϕ_B . The improvement with the applied magnetic field is clearly demonstrated by having much higher $Q_{\max}$ and Π over a broader range of temperatures (less than 100 K). For zero magnetic field $B = 0$ case, $Q_{\max}$ and Π will depend on r_c and D , which has been shown in Fig. 4.6. In this case, the performance ($Q_{\max} > 1 \text{ kW/cm}^2$) is better than the nanometer scale field emitter refrigeration (without crossed-field) [147], which has a cooling power density of 250 W/cm^2 or $< 100 \text{ W/cm}^2$ using a field emitter of $\phi_B = 1.7 \text{ eV}$ with a radius of $R = 5 \text{ nm}$ or 10 nm , respectively. For $B = B_z$ case, $Q_{\max}$ and Π are relatively independent on the structure's size or the cathode's work function, which has been shown in Fig. 4.8 and Fig. 4.9. The calculation (dashed-dotted lines) shown in the figure is general as the most optimized cooling power density can always be obtained by applying the proper values of V_g and B_z for any given r_c , D and ϕ_B .

4.4.3 Space Charge Effect

In the calculations above, the space charge field of the emitted electrons in the vacuum gap has been ignored by assuming $U_{sc}(r) = 0$ in Eq. (4.1), which may become important at high voltage. In this section, we will address this issue by including the space charge effect consistently. The space charge limiting (SCL) electron emission is defined as the maximum steady-state current density that can be transported across a vacuum gap of spacing D with a potential difference V_g without the formation of virtual cathode. For a planar diode, it is known as the Child-Langmuir (CL) law

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Figure 4.10: (a) The maximum cooling power density $Q_{\max}$ and (b) the corresponding Peltier coefficient Π as a function of temperatures for different cases of $B = 0$ and $B = B_z$, where B_z is assumed to be optimized at B_o , in which case the dashed-dot curve is insensitive to ϕ_B, r_c and D .

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[123, 124] given by

$$J_{\text{CL}} = \frac{4}{9}\epsilon_0\sqrt{\frac{2e}{m}}\frac{V_g^{3/2}}{D^2}. \quad (4.16)$$

The equivalent CL law for a coaxial cylindrical diode is also known as the Langmuir-Blodgett (LB) law [154] given by

$$J_{\text{LB}} = \frac{8\pi}{9}\epsilon_0\sqrt{\frac{2e}{m}}\frac{V_g^{3/2}}{r_a\beta_2^2} \approx \frac{8\pi}{9}\epsilon_0\sqrt{\frac{2e}{m}}\frac{V_g^{3/2}}{r_a}, \quad (4.17)$$

where J_{LB} (A/m) is the 1D electron current per unit length along the z axis, and $\beta_2 \approx 1$ for $r_a/r_c \rightarrow \infty$. For a planar crossed-field gap, the SCL electron flow has a smaller limiting value (due to the Lorentz force) as compared to the CL law [149].

To include the space charge effects in our cylindrical crossed-field gap, we use a similar and standard approach in solving the Poisson equation,

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{dV}{dr}\right) = \frac{\rho}{\epsilon_0}, \quad (4.18)$$

where $V(r) = V_v(r) + V_{sc}(r)$ is the potential at a distance $r - r_c$ from the cathode. The line current density (current per unit length) in the radial direction carried by the electrons is $i = 2\pi r\rho v_r$. Using the conservation of energy $\frac{1}{2}mv_r^2 + U_B(r) - eV(r) = 0$, Eq. (4.18) is rewritten as

$$r\frac{d^2V}{dr^2} + \frac{dV}{dr} = \frac{\sqrt{m}}{2\sqrt{2}\pi\epsilon_0}\frac{i}{\sqrt{eV(r) - U_B(r)}}, \quad (4.19)$$

which can be solved by using the boundary conditions of $V(r_c) = 0$ and $V(r_a) = V_g$ to calculate the space charge field for a given value of i . Here, the term $U_B(r)$ is either zero or based on Eq. (4.14) for the two specified configurations mentioned in Sections 4.4.1 and 4.4.2.

The maximum current i_{max} transported across the vacuum gap of a coaxial cylindrical diode can be calculated numerically, for which any value of $i > i_{\text{max}}$ will lead to no solution of Eq. (4.19). With respect to the analytical J_{LB} in Eq. (4.17), the calculated maximum normalized current $\mu_{\text{LB}} = i_{\text{max}}/J_{\text{LB}}$ are plotted in

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Figure 4.11: For $B = 0$ case, the normalized current density μ and cooling power density η as a function of V_g with (solid lines) and without (dashed lines) the space charge effect at $T = 300$ K. The normalized space charge limited current μ_{LB1} is shown in dotted lines.

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Fig. 4.11 and Fig. 4.12 (dotted lines), which are $\mu_{LB1} \approx 1$ for $B = 0$ and $\mu_{LB2} \approx 0.8$ for $B = B_z$. To include the space charge effect in our numerical calculation of the cooling power density for any given applied V_g and B , we first assume $V_{sc}(r) = 0$, and solve Eq. (4.2) to obtain a current line density of $i = J \times 2\pi r_c$, which is used to provide a new potential profile $V(r) = V_v(r) + V_{sc}(r)$ according to Eq. (4.19). Based on this updated $V(r)$, we will compute a new current density J and i , and the process repeats until the solutions of i_{SCL} and $V_{sc}(r) \neq 0$ satisfying Eqs. (4.1), (4.2) and (4.19) simultaneously are found.

Including the space charge effects, the normalized current density μ_{SCL} and normalized cooling power density η_{SCL} are plotted (solid lines) in Fig. 4.11 for $B = 0$ case and in Fig. 4.12 for $B = B_z$ case. The normalized constant for the current is J_{LB} given by Eq. (4.17). The results without the space charge effects are also plotted in dashed lines for comparison. For $B = 0$ case, the space charge effect will degrade the cooling power density at $V_g < 60$ volt, but a wider range of V_g from 50 to 150 volt may be used to provide a cooling of $Q = 250$ to 2100 W/cm² as shown in Fig. 4.11. In this case, the space charge effect will effectively make the refrigeration less sensitive to the applied bias. For case of $B = B_z = B_o$ in Fig. 4.12, the space charge effect will reduce the cooling power density. At $T = 300$ K in Fig. 4.12(a), the cooling power density is reduced from 5.94×10^5 to 3.57×10^4 W/cm² at 360 volt, and from 3.44×10^5 to 2.35×10^4 W/cm² at 300 volt. This degradation becomes less significant at low temperature. For example, μ_{FN} is always smaller than μ_{LB2} at $T = 50$ K as shown in Fig. 4.12(b), and the cooling power density is only reduced slightly from 2746 to 1658 W/cm² at 360 volt, and from 1357 to 814 W/cm² at 300 volt.

From the analysis and results shown above, it is clear that for room temperature refrigeration (around 200 K to 300 K), the method without using the external magnetic field shown in Fig. 4.5(a) would be a better choice, as it is much easier to implement over a broad range of applied voltages. In this case including space

4.4 Coaxial Cylindrical Diode Geometry

Figure 4.12: For uniform $B = B_z = B_o$ case, the normalized current density μ and cooling power density η as a function of V_g with (solid lines) and without (dashed lines) the space charge effect at $T =$ (a) 300 K and (b) 50 K. The normalized space charge limited current μ_{LB2} is shown in dotted lines.

4.5 Summary

charge effect, the room temperature cooling power density can still achieve about 2138 W/cm^2 at $V_g = 150$ volt for a design at $r_c = 10 \text{ nm}$, $D = 1 \text{ mm}$ and $\phi_B = 1 \text{ eV}$. The main challenge for this method is the requirement of using low work function cathode material, which is consistent with all other thermal-field emission based cooling methods reported before [146, 143, 147, 152]. For other applications that require a low temperature refrigeration below 200 K or high work function cathode, the proposed improvement with the axial magnetic field shown in Fig. 4.5(b) will be more promising. At $T = 50 \text{ K}$, the space charge limited cooling power density is about 1100 to 2300 W/cm^2 at $V_g = 320$ to 400 volt with a design of $r_c = 10 \text{ nm}$, $D = 0.1 \text{ mm}$ and $\phi_B = 2 \text{ eV}$. The main practical difficulty in this method will be the fine tuning and alignment of the magnetic field. The proposed setting of $r_c = 10 \text{ nm}$ and $D = 0.1 \text{ mm}$ would demand a magnetic field of about 1 T with tuning accuracy of 2 gauss, which is still higher the geomagnetic field. Note that the tuning range can be further improved by adjusting the size of the diode as shown in Fig. 4.8 and Fig. 4.9, which can have a much larger tuning range of about 50 gauss. Another practical issue will be the fabrication tolerance and the structure integrity of the nanowire at the applied electric field.

4.5 Summary

To summarize, we have proposed a novel cooling method by using thermal-field electron emission in a vacuum gap, either from nanoscale field emitters in a planar diode [23] or from an inner flat cathode in a coaxial cylindrical diode [24]. We have shown that it is possible to cool a low work function emitter of a diode significantly when only a dc bias is applied. Temperature down to 200 K can be achieved using well established work function around 1 eV.

4.5 Summary

To achieve lower cooling temperatures and to relax the low work function requirement, a constant magnetic field can be added. The purpose of the applied external magnetic field is to prevent the transmission of low energy electrons below the Fermi energy level, which will cause the heating on the emitting electrode. A set of optimal conditions is determined under which, all the cooling electrons can be extracted, while nearly all the heating electrons are blocked. By adding the external magnetic field, arbitrary work function emitters can be used to have a much higher cooling power density from room temperature down to 10 K.

The space charge effects of the emitted electrons have been included consistently in the cylindrical diode model. In general it shows a degraded cooling power density. But for case of zero magnetic field, the space charge effects will widen the range of applied voltages that can produce efficient cooling. For case of axial magnetic field, its effect of degrading cooling power density is only prominent for high temperatures. Therefore the configuration of $B = 0$ is suitable for room temperature refrigeration due to its simplicity. The configuration of $B = B_z$ is excellent for low temperature (< 100 K) refrigeration.

CHAPTER 5

MULTIPACTOR DISCHARGE IN DIELECTRIC LOADED ACCELERATOR

5.1 Introduction

Electron multipactor discharge presents a serious problem for the operation of modern microwave systems and accelerators. For example, to develop a new rf accelerating structure that is capable of producing electric field in excess of 100 MV/m, dielectric-loaded accelerating (DLA) structures look particularly promising. However, the undesirable multipactor phenomenon that occurs during high-power operation can absorb a significant fraction of the incident power [25, 155]. The underlying mechanism of multipactor discharge is the avalanche of electrons caused by secondary electron emission. Under some favorable conditions, primary electrons accelerated by electric fields can impact a surface and release a larger number of secondary electrons, which may be accelerated again to release more electrons at the subsequent impacts on the surface.

5.1 Introduction

In general, there are three types of multipactor discharge that have been studied prior to the studies of DLA structures. The first type [see Fig. 5.1(a)] is the multipactor discharge between two metal surfaces (or rf cavity) for which electrons released from one plate are accelerated by the electric field to reach the other plate, to emit more electrons [85, 86, 156, 157, 158]. In order to have multipactor discharge, the transit time of the emitted electrons is equal to $(n + 1/2)$ times of the rf cycles, where $n = 0, 1, 2, \dots$. The second type [see Fig. 5.1(b)] is a single-surface multipactor on a dielectric with an rf field parallel to the dielectric surface, such as a rf transmission window [86, 87, 88, 159, 160, 161, 162]. Due to the accumulated positive charges, there is a buildup of dc field on the dielectric surface, which attracts emitted electrons back to the surface. During the transit of the electrons, they gain energy from the rf field to emit more electrons at subsequent impacts. An early overview of the first two types of multipactor discharge can be found in a review paper [86]. By changing the orientation of the rf field to be perpendicular to the dielectric surface [see Fig. 5.1(c)], we have the third type of multipactor discharge, where both dc and rf electric fields will determine the transit time of electrons [163]. A. Valfells and his coauthors were the first one to analyze the effects of an oblique rf electric field on multipactor discharge on a dielectric [88].

In comparison, multipactor discharge in a DLA structure exposed to both the radial and axial rf electric fields of the propagating TM_{01} mode has not been studied theoretically in depth [25, 155]. In this research, a one and one-half dimensional ($1\frac{1}{2}D$) model [see Fig. 5.1(d)] is used to study the conditions of multipactor growth by constructing the susceptibility diagrams; and to predict the power absorbed by multipactor discharge at saturation [26]. In the model, a parallel plate geometry is substituted for the radial geometry, where the azimuthal coordinate (φ) is fixed at $\varphi = 0$ and $\varphi = \pi$, as compared to the radial geometry ($0 \leq \varphi \leq 2\pi$). This transformation also automatically ignores those particles emitted at an angle that will

5.1 Introduction

Figure 5.1: Multipactor discharge (a) between two metal plates with rf field in vertical direction; (b) at single dielectric surface with rf field in horizontal direction; (c) at single dielectric surface with rf field in vertical direction; (d) in a dielectric-loaded accelerating (DLA) structure with rf field in both horizontal (z) and radial (r) directions.

5.2 Theory of Multipactor Discharge

end up not going through the center, as they will see a different distance separating the two plates. The one and one-half dimension means that the actual position of the discharge in the z coordinate is ignored, but the emission and impact velocity in both r and z coordinates are included.

In particular, this research work will distinguish the difference between a maximum growth of secondary electrons under a *resonant* condition, and a steady-state multipactor discharge under a *saturated* condition, which were not interpreted clearly before [25]. The much higher power absorption in a DLA structure as compared to the simple dielectric windows will be clearly explained. Some suggestions on avoiding the power absorption using materials with suitable secondary electron emission (SEE) properties are provided. The occurrence of single-surface and two-surface multipactor discharge in the DLA structure is also demonstrated.

The rest of this chapter is organized as follows. Section 5.2 gives a short overview on the theory of multipactor discharge. Section 5.3 provides the information on how to construct a susceptibility diagram for the multipactor discharge in a DLA structure. Section 5.4 shows the dynamic calculations for the normalized power absorption by multipactor discharge at various conditions, and the comparison with previous experimental findings. It is concluded in Section 5.5.

5.2 Theory of Multipactor Discharge

Consider a cylindrical dielectric-loaded accelerating (DLA) structure of a uniform alumina-lined copper tube [see Fig. 5.1(d)] having a TM_{01} rf electric field with an axial (F_z) and a radial (F_r) component, which are (in vacuum region) [25, 164],

$$\begin{aligned} F_z &= F_{\text{rf}} I_0(k_r r) \cos(\omega t - k_z z + \theta), \\ F_r &= F_{\text{rf}} \left(\frac{k_z}{k_r} \right) I_1(k_r r) \sin(\omega t - k_z z + \theta). \end{aligned} \quad (5.1)$$

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Here, F_{rf} is the magnitude of the rf electric field, and the radii $r = a$ and $r = b$ are the inner and outer dielectric surface. The parameter $\omega = 2\pi f$ is the angular frequency, $k_z = \omega/v_p$ is the longitudinal wave number (the wave propagation constant) where v_p is the phase velocity, $k_r^2 = k_0^2 - k_z^2$ is the radial wave number where $k_0 = \omega/c$ and c is the speed of light, θ is the rf phase, and $I_0(x)$ and $I_1(x)$ are the modified Bessel functions of the first kind. From the dispersion curve (propagation constant versus frequency) for the TM_{01} mode propagating in a dielectric-lined circular waveguide with $a = 5$ mm, $b = 7.185$ mm and $\epsilon_r = 9.4$ (alumina), the designed synchronous frequency (at which the phase velocity equals the speed of light $v_p = c$) is $f = 11.424$ GHz [25, 164]. Operating at the synchronous frequency $f = 11.424$ GHz [25], we will have $k_z = k_0 = \omega/c$ and $k_r = 0$. At $k_r \rightarrow 0$, we have $I_0(k_r r) \approx 1$ and $I_1(k_r r) \approx k_r r/2$. Thus the TM_{01} rf fields within the central vacuum region ($0 \leq r < a$) can be simplified as

$$\begin{aligned} F_z &= F_{\text{rf}} \cos(\omega t - k_z z + \theta), \\ F_r &= F_{\text{rf}} \left(\frac{k_z r}{2} \right) \sin(\omega t - k_z z + \theta). \end{aligned} \quad (5.2)$$

It shows that at synchronous condition the longitudinal electric field F_z is independent of the radial coordinate, but the radial electric field F_r will vary as a function of r in the vacuum region.

For each secondary electron emitted from the surface of the dielectric, we assume that it has a random emission energy ($E_0 = \frac{1}{2}mv_0^2$) and emission angle (ϕ), which are determined by the following distribution functions:

$$\begin{aligned} f(E_0) &= \frac{E_0}{E_{0m}^2} e^{-E_0/E_{0m}}, \\ g(\phi) &= \frac{1}{2} \sin \phi, \end{aligned} \quad (5.3)$$

where E_{0m} is the peak of the distribution of emission energies. If the secondary emission has a yield larger than 1, a dc electric field F_{dc} in the radial direction can arise due to the accumulated positive charges on the dielectric surface.

5.2 Theory of Multipactor Discharge

For given values of F_{rf} and F_{dc} , the equations of motion are solved numerically to compute the trajectory of the emitted electrons,

$$\begin{aligned} m\ddot{z} &= -eF_{\text{rf}} \cos(\omega t - k_z z + \theta), \\ m\ddot{r} &= -eF_{\text{dc}} - eF_{\text{rf}} \left(\frac{k_z r}{2} \right) \sin(\omega t - k_z z + \theta). \end{aligned} \quad (5.4)$$

After some transit time τ , these emitted electrons will impact again at the dielectric surface (i.e. $r(\tau) = a$) to produce more secondary electrons. Thus multipactor discharge occurs if there is a growth in the number of electrons after several impacts. At each impact, the impact energy (E_i) and angle (ξ) with respect to the normal axis are calculated by

$$\begin{aligned} E_i &= \frac{1}{2}m(v_r^2 + v_z^2), \\ \xi &= \arctan\left(\frac{v_z}{v_r}\right). \end{aligned} \quad (5.5)$$

Using E_i and ξ , the secondary electron yield δ is calculated based on Vaughan's empirical formula [82],

$$\delta = \delta_{\text{max}}(we^{1-w})^k. \quad (5.6)$$

Here, we have $w = E_i/E_{\text{max}}$, $k = 0.62$ for $w < 1$ and $k = 0.25$ for $w > 1$; δ_{max} is the maximum value of δ at $E = E_{\text{max}}$, which are functions of the impact angle ξ , given by

$$\begin{aligned} \delta_{\text{max}} &= \delta_{\text{max}0}(1 + k_s \xi^2 / 2\pi), \\ E_{\text{max}} &= E_{\text{max}0}(1 + k_s \xi^2 / \pi), \end{aligned} \quad (5.7)$$

and k_s is a surface smoothness factor ranging from 0 (for a rough surface) to 2 (for a polished surface). For simplicity, we set $k_s = 1$ to represent a typical dull surface. Note $\delta_{\text{max}0}$ and $E_{\text{max}0}$ are the material-dependent secondary electron emission (SEE) parameters at normal incidence ($\xi = 0$), and the typical values for alumina (Al_2O_3) are $\delta_{\text{max}0} = 1.5$ to 9 and $E_{\text{max}0} = 350$ to 1300 eV [159].

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Figure 5.2: (a) Dependence of secondary electron yield δ on normalized impact energy $E_i/E_{\max 0}$ for different $\delta_{\max 0}$; (b) The normalized first, second crossover energy $E_{1,2}/E_{\max 0}$ as a function of $\delta_{\max 0}$ (dashed lines), and their normalized differences $\Delta E/E_{\max 0}$ (solid line).

5.3 Susceptibility Diagram

The secondary electron yield δ at $\xi = 0$ as a function of normalized impact energy $E_i/E_{\max 0}$ is shown in Fig. 5.2(a) for different $\delta_{\max 0}$. The first and second crossover points E_1 and E_2 with $\delta = 1$ and their difference $\Delta E = E_2 - E_1$ (in term of $E_{\max 0}$) are also plotted in Fig. 5.2(b) as a function of $\delta_{\max 0}$. It is clear that multipactor discharge only occurs if the impact energy E_i is between E_1 and E_2 .

5.3 Susceptibility Diagram

In this section, a kinematic calculation is performed to determine the susceptibility diagram of a multipactor discharge for a given set of F_{rf} , F_{dc} , $E_{\max 0}$ and $\delta_{\max 0}$. The susceptibility diagram, which is based on a statistical method, is a useful tool to analyze whether a multipactor discharge will take place over a range of rf and dc electric fields at fixed values of $E_{\max 0}$ and $\delta_{\max 0}$. In our study, the default parameters of the DLA structure (for all the calculations unless mentioned otherwise) are $f = 11.424$ GHz, $E_{0m} = 2.1$ eV, $a = 5$ mm, $b = 7.185$ mm and length $L = 0.3$ m [25]. The method of our calculation is similar to previous approach [87, 159]. From the susceptibility diagrams, we report and explain a resonant condition due to phase focusing, for which the transit time of the multipactor electrons is equal to the inverse of the rf frequency, and the growth is maximized with a yield close to $\delta_{\max 0}$. The resonant condition is derived analytically, which agrees very well with numerical results. Various specified points in the susceptibility diagram (of different growth rates) are also discussed.

5.3.1 Kinematic Calculation

Consider an arbitrary initial rf phase θ_0 at the time of primary electron emission ($t = 0$), whose trajectory is traced continuously till it impacts on the surface after a transit time of $t = \tau_1$. After the first impact, the impact energy E_{i1} and its related secondary

5.3 Susceptibility Diagram

electron yield δ_1 are calculated according to the model described in Section 5.2. The secondary electrons generated during the first impact will see a new rf phase, which is updated through $\theta_1 = \theta_0 + \omega\tau_1$. Likewise we can repeat the same procedure to obtain a series of yields $(\delta_1, \delta_2, \dots, \delta_N)$ for a large number of impacts. For each value of θ_0 , the average values of impact energies and secondary yields over N impacts are calculated by

$$\begin{aligned} E_i(\theta_0) &= \frac{1}{N} [E_{i1} + E_{i2} + \dots + E_{iN}], \\ \delta(\theta_0) &= \sqrt[N]{\delta_1 \times \delta_2 \times \dots \times \delta_N}. \end{aligned} \quad (5.8)$$

Assuming that the initial rf phase θ_0 is uniformly distributed from 0 to 2π by 100 samples ($M = 100$), $N = 500$ impacts will be used in the calculation for each sample. Thus the mean values for the impact energy and the electron yield (sampling over the 100 initial rf phases θ_0) are

$$\begin{aligned} \bar{E}_i(F_{\text{rf}}, F_{\text{dc}}) &= \frac{1}{M} \left\{ [E_i(\theta_0)]_1 + [E_i(\theta_0)]_2 + \dots + [E_i(\theta_0)]_M \right\}, \\ \bar{\delta}(F_{\text{rf}}, F_{\text{dc}}) &= \sqrt[M]{[\delta(\theta_0)]_1 \times [\delta(\theta_0)]_2 \times \dots \times [\delta(\theta_0)]_M}. \end{aligned} \quad (5.9)$$

By plotting $\bar{\delta}(F_{\text{rf}}, F_{\text{dc}})$ as a function of F_{rf} and F_{dc} for fixed $\delta_{\text{max}0}$ and $E_{\text{max}0}$, we are able to determine the conditions for multipactor growth ($\bar{\delta} > 1$) or decay ($\bar{\delta} < 1$).

Fig. 5.3 shows the contour plots of $\bar{\delta}$ for different values of $E_{\text{max}0}$ ($= 350 - 1300$ eV) and $\delta_{\text{max}0}$ ($= 1.5 - 9$) as a function of $|F_{\text{dc}}|$ (x axis) and F_{rf} (y axis). From the figures, the growth (decay) of multipactor discharge refers to the region with $\bar{\delta} > 1$ ($\bar{\delta} < 1$), where the boundary at $\bar{\delta} = 1$ is highlighted in bold. For the cases with fixed $E_{\text{max}0} = 350$ eV and various $\delta_{\text{max}0} = 1.5$ to 9, the size of the growth region (bounded by $\bar{\delta} = 1$) decreases as $\delta_{\text{max}0}$ becomes smaller, due to the smaller energy difference ΔE between the two crossover points E_1 and E_2 [see Fig. 5.2(b)]. For the cases with fixed $\delta_{\text{max}0} = 9$, as $E_{\text{max}0}$ increases from 350 to 1300 eV, the growth region is shifted upwards due to the increase of the first crossover point E_1 .

5.3 Susceptibility Diagram

Figure 5.3: The contour plots of average yield $\bar{\delta}$ in the $x-y$ plane of $(x = |F_{dc}|, y = F_{rf})$ (MV/m), using different combinations of $(E_{\max 0}, \delta_{\max 0}) =$ (a) (350 eV, 1.5), (b) (350 eV, 3), (c) (350 eV, 6), (d) (350 eV, 9), (e) (700 eV, 9), (f) (1300 eV, 9). The bold lines denote the $\bar{\delta} = 1$ boundary and the white dashes lines denote the region of maximum growth with $\bar{\delta} \approx \delta_{\max 0}$.

5.3 Susceptibility Diagram

At the center of each susceptibility diagram, there is always a maximum growth region whose yield is nearly equal to the maximum yield ($\bar{\delta} \approx \delta_{\max 0}$), which is highlighted by the straight white dashed lines in the figure. For example, the maximum growth region of $\bar{\delta} \approx 1.44$ ($\approx \delta_{\max 0} = 1.5$) is bounded by point 5 and 8 as denoted in Fig. 5.3(a). Similarly, the maximum growth region of $\bar{\delta} \approx 5.76$ ($\approx \delta_{\max 0} = 6$) is bounded by same points 5 and 8 as denoted in Fig. 5.3(c). It is important to note that the maximum growth region reported here is characterized by a universal ratio (the white dashed lines), which measures the ratio of the magnitude of the dc field to the rf field. This ratio is independent of SEE parameters, and it is a function of the rf frequency and the radius of the DLA structure [see Eq. (5.10) below]. From the figure, the ratio is about $\gamma_{re} = |F_{dc}/F_{rf}| = 0.2$.

5.3.2 Resonant Condition

The maximum growth region shown in Fig. 5.3 is due to a resonant condition, which is based on a phase focusing mechanism. To understand this behavior, we define two types of electrons according to the rf phase at the instant of their emission, namely θ_α with $\sin(-k_z z + \theta_\alpha) < 0$ and θ_β with $\sin(-k_z z + \theta_\beta) > 0$, which will determine the direction of the radial rf electric field during the multipactor discharge [see Eq. (5.2)]. Note that the radial direction of the dc electric field F_{dc} (due to accumulated positive charges) is always negative, $F_{dc} < 0$. For electrons in the θ_α group, $F_r < 0$ is in the same direction with $F_{dc} < 0$, which will attract the emitted electrons back to the same emitting surface during a relatively short transit time τ_α . For electrons in the θ_β group, we have the opposite direction between the rf and dc fields, and the transit time τ_β of the emitted electrons is much longer.

Figure 5.4 shows the calculated impact energy E_i and transit time τ at some of the points (F_{dc}, F_{rf}) specified in Fig. 5.3 (a) and (c). The points denoted as 2, 5, 8, 11 are near or in the maximum growth region with $\bar{\delta} \approx \delta_{\max 0}$. The other points (1, 4,

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7, 10 and 3, 6, 9, 12) are, respectively, located on the left and right hand side of the maximum growth region. At each point, we have used $N = 50$ impacts with an initial rf phase $\theta_0 = 0$ in our calculation. After each impact, we record the transit time τ (triangles) and the impact energy E_i (squares), where the two different phase groups (θ_α and θ_β) are labeled in solid and open symbols, respectively, as shown in Fig. 5.4. Note single-surface multipactor discharge always occurs for large F_{dc} of a few MV/m or higher, but single-surface or two-surface multipactor discharge can occur at small F_{dc} (see Section 5.4).

As an example, consider a case [see Fig. 5.3(a)] with $E_{max0} = 350$ eV and $\delta_{max0} = 1.5$, where the two crossover energies (at normal incidence) are $E'_1 = 87.5$ eV and $E'_2 = 1.4$ keV, marked as the two dotted horizontal lines in Fig. 5.4. In Fig. 5.4(a), the transit time τ and impact energy E_i at the four points (2, 5, 8 and 11) are plotted for the 50 impacts. Note that these four points are all located in the region of multipactor growth ($\bar{\delta} > 1$), where almost all the impact energies are within E'_1 and E'_2 . It is clear that the emitted electrons (at these four points) mainly belong to θ_β group (open symbols) and have a fixed transit time of $\tau = \tau_\beta \approx T_{rf} = 8.75 \times 10^{-2}$ ns, which is equal to the inverse of the rf frequency ($f = 11.424$ GHz). At this resonant condition, there is no net work done by the axial rf electric field F_z within the transit time, and all the 50 impacts are near normal incidence ($\xi \approx 0$). In this case, the electrons will gain energy from the radial rf electric field. Under the condition of same transit time $\tau = 1/f$ for points 2, 5, 8 and 11, the energy gain at point 2 is highest because of the largest magnitude of rf field. From the figure, we also observe that the impact energy is bounded by the second crossover energy at point 2 and the first crossover energy at point 11. Thus the region bounded from point 2 to point 11 [in Fig. 5.3(a)] can be considered as a resonant region, which has a maximum growth of $\bar{\delta} \approx \delta_{max0}$ located between point 5 and point 8. It is worth noting that the location of this resonant region is not sensitive to the SEE parameters, for which the ratio of the magnitude

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Figure 5.4: Calculated transit time τ (triangle) and impact energy E_i (square), at two situations: $F_r < 0$ (solid symbols, θ_α group) and $F_r > 0$ (open symbols, θ_β group) at the instant of emission for the points highlighted in the susceptibility diagrams shown in Fig. 5.3 (a) and (c). (a) Resonant condition at $F_{rf} = 8, 6, 4$ and 2 MV/m (for points 2, 5, 8 and 11), (b) Three different F_{dc} at fixed $F_{rf} = 6$ MV/m (for points 4, 5 and 6). The horizontal lines represent the two crossover impact energies for $(E_{max0}, \delta_{max0}) = (350 \text{ eV}, 6)$ (dashed) and $(350 \text{ eV}, 1.5)$ (dotted) at normal incidence.

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of the dc electric field to the rf electric field defined as $\gamma_{re} = |F_{dc}/F_{rf}|$ depends only on rf frequency and the radius of the DLA structure.

To derive a simple analytical formula for the resonant condition observed in our numerical calculations, we made the following approximations (only in the derivation here): (i) zero initial velocity, (ii) no z -dependence in the sine function of F_r field, and (iii) $r \approx a$ is valid near the surface for the single-surface multipactor. At the resonant condition, the electrons are emitted from dielectric surface at $r = a$ and back to the same surface after a transit time $\tau = 1/f = T_{rf}$. The equation of motion (including the assumptions above) $m\ddot{r} = -eF_{dc} - eF_{rf}(\frac{k_z a}{2}) \sin(\omega t + \theta)$ gives the analytical solutions of time-dependent electron's velocity $\dot{r}(t) = -\frac{eF_{dc}}{m}t + \frac{eF_{rf}}{m\omega} \frac{k_z a}{2} [\cos(\omega t + \theta) - \cos(\theta)]$, and electron's position $r(t) = a - \frac{eF_{dc}}{2m}t^2 + \frac{eF_{rf}}{m\omega^2} \frac{k_z a}{2} [\sin(\omega t + \theta) - \sin(\theta)] - \frac{eF_{rf}}{m\omega} \frac{k_z a}{2} \cos(\theta)t$. During one transit from 0 to $\tau = 1/f$, the electron's traveling distance is zero $r(\tau) - r(0) = 0$, and $-\frac{eF_{dc}}{2m}\tau^2 - \frac{eF_{rf}}{m\omega} \frac{k_z a}{2} \cos(\theta)\tau = 0$. If $|\cos(\theta)| = 1$ (which is required for transit time $\tau = 1/f$), the ratio of the magnitude of dc and rf electric fields at the resonant condition is

$$\gamma_{re} = |F_{dc}/F_{rf}| = \frac{af}{c}. \quad (5.10)$$

At $f = 11.424$ GHz and $a = 5$ mm, the formula gives $\gamma_{re} = 0.19$, which agrees rather well with the numerical results of $\gamma_{re} = 0.175 - 0.2$ over a wide range of E_{max0} and δ_{max0} (see the straight white dashed lines plotted in Fig. 5.3). The requirement of $|\cos(\theta)| = 1$ can be met because the phase increment after each transit is $\omega\tau = 2\pi$ at the resonant condition. Once the phase somehow comes to $|\cos(\theta)| = 1$, it can be focused there subsequently. But it is important to note that in real simulation, the radial rf electric field varies with r , the term $-k_z z$ inside the sine function of Eq. (5.2) is not exactly zero, and the transit time τ is not exactly equal to T_{rf} , which cause the minor difference between the numerical results of γ_{re} and the analytical solution in Eq. (5.10). Although the assumptions to derive the simple analytic relation are relatively crude, it is able to tell the experimentalist what the dangerous value of

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Figure 5.5: The contour plots of the susceptibility diagram similar to Fig. 5.3 but with zero radial rf field in the plane of x - y plane ($x = |F_{dc}|$, $y = F_{rf}$) (MV/m), using the same combinations of $(E_{max0}, \delta_{max0}) =$ (a) (350 eV, 1.5), (b) (350 eV, 3), (c) (350 eV, 6), (d) (350 eV, 9), (e) (700 eV, 9), (f) (1300 eV, 9). The bold lines denote the $\bar{\delta} = 1$ boundary.

dc charging filed is for their operating condition (inner radius a , frequency f and magnitude of rf field F_{rf}).

It is important to note that the resonant condition described above can only occur in a DLA structure as it is due to the radial rf electric field, which is absent from the simple dielectric window cases studied before [87, 159]. In comparison to the susceptibility diagrams for the DLA structure shown in Fig. 5.3, we have artificially turned off the radial rf electric field in our simulation, and constructed the equivalent susceptibility diagrams, which are plotted in Fig. 5.5 using the same SEE parameters. In this case without the radial rf field, the transit time is inversely proportional to the

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magnitude of the dc field only. The electrons gain energy only from the longitudinal rf electric field (in a direction parallel to the surface). The impact energy is higher for smaller dc field (longer time to gain energy) at a fixed rf field, and also higher for larger rf field at a fixed dc field. The lower and upper boundaries of the growth region correspond to E_1 and E_2 , respectively. There is also a maximum growth region but at a smaller dc electric field. The resonant condition (the universal ratio and fixed transit time) for maximum growth is not found here. The reason is that the transit time τ for the DLA structure is determined by both dc and rf fields, which is different from the rf dielectric window.

5.3.3 More Discussion on Susceptibility Diagrams

Compared to the points (2, 5, 8 and 11) located in the resonant region as shown in Fig. 5.3(a), all the other points outside the growth region (e.g. points 1, 4, 7, 10 and 3, 6, 9, 12) have impact energies outside the first and second crossover energies. In this case, the electrons gain energy from both the longitudinal and the radial rf electric fields, and the role of dc charging field is to determine the transit time of the electrons. A comparison between three points (4, 5 and 6) of different F_{dc} but the same $F_{rf} = 6$ MV/m is shown in Fig. 5.4(b). It is expected that with same magnitude of rf field, larger dc field will result in shorter transit time and then less energy gain. At point 5, we have the resonant condition discussed above, which shows that the transit time τ is equal to the T_{rf} and the impact energy satisfies $E'_1 < E_i < E'_2$.

At point 6, we have a relatively large F_{dc} and thus a short transit time in the range of $\tau_\alpha < \tau_\beta < T_{rf}$, for which majority of the electrons are characterized by the θ_α group (solid symbols). In this case, if the phase is within the θ_α group where the transit time is $\tau = \tau_\alpha$, the subsequent impacts will be most likely in the same phase group, as the increment of phase ($\Delta\theta = \omega\tau$) is very little due to short τ_α . If the phase goes to θ_β group, the transit time is longer with $\tau = \tau_\beta$, the increment of rf

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phase becomes larger, which may bring the emitted electrons out of the θ_β group. The overall count of phases will be in favor of θ_α with shorter transit time, which is indicated by the relatively more solid symbols compared to the open symbols. Thus most of the electrons at point 6 will acquire less energy from rf field due to short transit time, and the impact energy (squares) is less than the first crossover point ($E_i < E'_1$) as shown in the figure. At point 4 with relatively small F_{dc} , the transit time for both θ_α and θ_β groups is larger in the range of $\tau_\alpha < T_{rf} < \tau_\beta$. This implies that the electrons have longer time to acquire energy from rf field in order to have higher impact energy. But if the transit time becomes too long, the impact energy may be larger than the second crossover point $E_i > E'_2$ and thus $\delta < 1$.

By considering another case with $E_{\max 0} = 350$ eV and $\delta_{\max 0} = 6$, whose susceptibility diagram is shown in Fig. 5.3(c), the crossover energies are expanded to $E_1 = 7$ eV and $E_2 = 3.5$ keV [see dashed horizontal lines in Fig. 5.4(b)]. In this case, it is more likely to have impact energy within the range of E_1 and E_2 , hence higher probability to have $\delta > 1$. For the previous case of $(E_{\max 0}, \delta_{\max 0}) = (350 \text{ eV}, 1.5)$, there are 19 and 3 counts (out of 50) with $\delta > 1$ for points 4 and 6. The number is increased, respectively, to 28 and 14, when $\delta_{\max 0}$ is increased from 1.5 to 6 at fixed $E_{\max 0} = 350$ eV. This comparison explains why points 3, 6, 9 and 12 are still outside the multipactor growth region but points 1, 4, 7 and 10 can have modest multipactor growth with $1 < \bar{\delta} < 2$ as shown in Fig. 5.3(c), when $\delta_{\max 0}$ is increased to 6. For the ease of explanation, we have simply used values of E_1 and E_2 at impact angle $\xi = 0$ in comparing the two cases. But in a real simulation, the impact angles are calculated from solving the equation of motion, which is not necessarily at normal incidence.

From the detailed analysis of the susceptibility diagrams shown above, we conclude that the lower boundary (point 11) of the resonant growth region is determined by the first crossed-cover energy E'_1 , and the upper boundary (point 2) is by the second crossed-cover energy E'_2 . The right boundary with $\bar{\delta} = 1$ (which

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divides the growth region from the points 3, 6, 9 and 12) is mainly affected by E'_1 . The left boundary (which divides the growth region from the points 1, 4, 7 and 10) is sensitive to both E'_1 and E'_2 .

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Kinematic calculation shown in Section 5.3 has ignored the beam loading effect on the rf field. In this section, we will use a similar dynamic calculation [87] to determine the effects of beam loading for multipactor discharge in a DLA structure, and to calculate the power absorption by the multipactor discharge at a saturation condition. It is found that the saturation condition always occurs at the right boundary (or the first crossover energy) of the susceptibility diagram. The power absorption is estimated by a single-step method based on the saturated dc and rf fields obtained from the susceptibility diagram. The reason for the much higher power absorption by multipactor discharge in a DLA structure as compared to a simple dielectric window will be given. The calculated results of the power absorption are compared with experimental findings over a wide range of SEE parameters.

To study the evolution and power absorption of multipactor discharge, it is useful to construct the susceptibility diagrams for various SEE parameters i.e. $E_{\max 0}$ and $\delta_{\max 0}$, which are shown in Fig. 5.6 and Fig. 5.7. In Fig. 5.6, the SEE parameters are $(E_{\max 0}, \delta_{\max 0}) =$ (a) (700 eV, 5), (b) (500 eV, 4), (c) (320 eV, 3) and (d) (140 eV, 2), where the shaded region represents the growth region with $\bar{\delta} > 1$. These specific SEE parameters are chosen in order to have exactly the same first crossover energy of $E_1 = 21$ eV, but different second crossover energy of E_2 . Moreover the other three cases in Fig. 5.7 are $(E_{\max 0}, \delta_{\max 0}) =$ (a) (350 eV, 5) to have $E_1 = 10$ eV and $E_2 = 3.4$ keV; (b) (180 eV, 2) to have slightly larger $E_1 = 27$ eV but smaller $E_2 = 985$ eV;

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and (c) (32.5 keV, 9) to have much greater $E_1 = 384$ eV and $E_2 = 400$ keV. Note all the E_1 and E_2 are referred to the impact energy at normal angle ($\xi = 0$).

5.4.1 Dynamic Calculation

In the dynamic calculation, the dc charging field on the surface of the dielectric is assumed to have two components, $F_{dc} = F_{dcc} + F_{dct}$. The first component F_{dcc} is a constant dc field, which exists prior to the multipactor discharge in order to initiate the discharge. It could come from several practical issues, for example, nonuniform surface charging, the material's intrinsic defects, the adsorbates, and the geometric unevenness. The second component F_{dct} is a time-varying dc field, which changes according to the positive charges accumulated on the surface (at each impact). The space charge effect during the time of flight for each impact is ignored [160] and the dc field is only updated after each impact.

For a given initial rf electric field F_{rf0} , proper initial dc field $|F_{dcc}| \geq 0$ is used to initiate the multipactor growth. If the initial dc field F_{dcc} is zero, the buildup of dc field F_{dc} remains very small at first, so it is possible for electrons to undergo a single-surface or a two-surface multipactor. Specifically, the multipactor will be initiated at some point on the dielectric surface, and the emitted secondary electrons will subsequently impact at other points on the dielectric surface with different secondary yields. Hence initially the buildup of dc electric field on the dielectric surface will be nonuniform. To model this nonuniformity, we distinguish the two surfaces as shown in Fig. 5.1(d) as lower surface ($r = a, \varphi = 0, z$) and upper surface ($r = a, \varphi = \pi, z$) respectively. After a few impacts (when the dc field grows to a value larger than 0.02 MV/m), one of the two surfaces will accumulate more positive charges, which attract almost all the subsequent secondary electrons to impact on it. The single-surface multipactor becomes dominant.

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Figure 5.6: Susceptibility diagrams ($x = F_{dc}$, $y = F_{rf}$) (MV/m) for four different combinations of $(E_{\max 0}, \delta_{\max 0}) =$ (a) (700 eV, 5), (b) (500 eV, 4), (c) (320 eV, 3) and (d) (140 eV, 2), which have the same first crossover impact energy $E_1 = 21$ eV. The bold lines denote the $\bar{\delta} = 1$ boundary, $\tilde{R}$ and $\tilde{L}$ indicates, respectively, the right boundary (impact energy roughly equals to first crossover energy E_1) and left boundary.

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In the calculation, the number of multipactor electrons is updated by $N_{e(i)} = \delta_{(i)}N_{e(i-1)}$ upon the i th impact. By defining N_{upper} (and N_{lower}) as the total number of charges on the upper (and lower) dielectric surface, the $N_{\text{upper}(i)}$ or $N_{\text{lower}(i)}$ is updated by adding $\Delta N = N_{e(i)} - N_{e(i-1)}$, which equals the outgoing electrons minus the incoming electrons at each impact. Hence the buildup of the varying dc field at each impact is expressed as

$$F_{\text{dct}(i)} = \pm \frac{e}{2A_s\epsilon_0} [N_{\text{lower}(i)} - N_{\text{upper}(i)}], \quad (5.11)$$

where ϵ_0 is the free space permittivity, $A_s = \pi a L_{\text{eff}}$ is the area for multipactor to occur, a is the radius of the DLA structure, and L_{eff} is the propagation distance along the z direction for multipactor discharge. For simplicity, we set L_{eff} equal to the total length of the DLA structure ($L = 0.3$ m), which is comparable to the real values of L_{eff} observed in the simulation. The $+$ and $-$ signs denote, respectively, the radial direction of the dc electric field on the upper and lower surfaces. Once the magnitude of the dc field evolves to a large value (> 0.02 MV/m), where the system becomes a single-surface multipactor discharge either at the lower or upper surface, the dc field becomes $-eN_{e(i)}/2A_s\epsilon_0$.

During the transit time $\tau_{(i)}$, there is an amount of power $P_{m(i)}$ absorbed by the $N_{e(i-1)}$ number of electrons in both axial and radial directions, and it is calculated by

$$P_{m(i)} = -\frac{eN_{e(i-1)}}{\tau_{(i)}} \int_0^{\tau_{(i)}} [F_{z(i-1)}v_z + F_{r(i-1)}v_r] dt, \quad (5.12)$$

where $F_{z(i-1)}$ and $F_{r(i-1)}$ are determined by the Eq. (5.2) numerically. The beam loading of the rf field is then calculated by (the detailed transmission line model [87] is described in Appendix C)

$$\frac{F_{\text{rf}(i)}}{F_{\text{rf0}}} = \frac{1}{1 + Z_0 K_{(i)}/2}, \quad \text{where } K_{(i)} = \frac{P_{m(i)}}{A_c \times F_{\text{rf}(i-1)}^2}. \quad (5.13)$$

Here the characteristic impedance of TM_{01} mode in a dielectric-loaded accelerating structure is $Z_0 = k_z/\omega\epsilon_0$ [164], which is 377Ω at synchronous frequency $f = 11.424$

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GHz (where phase velocity $v_p = c$) in alumina DLA structure with $a = 5$ mm and $b = 7.185$ mm. The $A_c = \pi a^2$ is the cross sectional area of the DLA structure. Note the value of A_c can also be determined using the known experimental parameters through the relation of $P_{\text{in}} = F_{\text{rf0}}^2 A_c / 2Z_0$ if the value of the input power P_{in} and rf field F_{rf0} are given. For example, we have $A_c = 6.032 \times 10^{-5} \text{ m}^2$ at $P_{\text{in}} = 80 \text{ kW}$ and $F_{\text{rf0}} = 1 \text{ MV/m}$, which is roughly equal to $\pi a^2 = 7.854 \times 10^{-5} \text{ m}^2$ at $a = 5 \text{ mm}$ [25]. Thus for an input rf electric field with magnitude F_{rf0} , the instantaneous fraction of power absorbed after i th impact is $P_{m(i)}/P_{\text{in}}$.

For each impact, $F_{\text{dc}(i)} = F_{\text{dcc}} + F_{\text{dct}(i)}$ and $F_{\text{rf}(i)}$ are updated using Eq. (5.11) and Eq. (5.13) based on the calculated $N_{e(i)}$ and $P_{m(i)}$. The number is thereafter updated by using $N_{e(i+1)} = \delta_{(i+1)} N_{e(i)}$, which will give a new $F_{\text{dc}(i+1)}$ to repeat the process. The amount of power absorption $P_{m(i+1)}$ by the $N_{e(i)}$ number of electrons is calculated using Eq. (5.12), and the fraction of power absorbed is $P_{m(i+1)}/P_{\text{in}}$. This new $P_{m(i+1)}$ provides us a new $F_{\text{rf}(i+1)}$ to continue the evolution in a like manner.

5.4.2 Saturation Condition

Using this multi-step method, we show the evolutions of N_e (dotted lines), the magnitude of F_{dc} and F_{rf} (solid lines) from its known initial condition at point A shown in Fig. 5.7, where point A is at $(F_{\text{rf0}}, F_{\text{dcc}}) [\text{MV/m}] =$ (a) (3, 0), (b) (3, 0.5) and (c) (6, 1), with initial $N_{e0} = 1$ and $\theta_0 =$ (a) 0, (b) $\pi/2$, (c) π . From the figure, we see that the number of multipactor electrons N_e increases until it reaches a saturation condition at point B with a yield of $\bar{\delta} = 1$. The magnitude of the dc electric field F_{dc} also increases due to multipactor discharge, and the rf electric field F_{rf} decreases due to beam loading. This finding suggests the route to saturation is always from point A to point B, similar to the dielectric window case [87], but with a much higher power absorption (see below). Note several tests have been performed by using different initial rf phases θ_0 for various F_{rf0} , F_{dcc} , E_{max0} and δ_{max0} . It is confirmed

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Figure 5.7: Susceptibility diagrams (left) and evolution of multipactor discharge from point A to point B (right): number of multipactor electrons N_e (dotted) and electric fields (solid), for three different cases of $(E_{\max 0}, \delta_{\max 0}) =$ (a) (350 eV, 5), (b) (180 eV, 2), (c) (32.5 keV, 9). The dashed lines (right figures) represent the saturation conditions at point B (estimated using the one-step method).

that saturation condition of the dc and rf fields ($F_{\text{dc}}^{\text{sat}}, F_{\text{rf}}^{\text{sat}}$) is always located at the right boundary of susceptible region with a yield of $\bar{\delta} = 1$ at the first crossover energy E_1 , which is denoted as $\tilde{R}$ in Fig. 5.6 and Fig. 5.7.

The reason of this saturation can be understood as follows. If $F_{\text{dc}} < F_{\text{dc}}^{\tilde{R}}$, we have $\bar{\delta} > 1$ to provide more secondary electrons, which will increase the value of F_{dc} toward the $F_{\text{dc}}^{\tilde{R}}$ value. If $F_{\text{dc}} > F_{\text{dc}}^{\tilde{R}}$, we have $\bar{\delta} < 1$, which will decrease the value of F_{dc} toward $F_{\text{dc}}^{\tilde{R}}$. Thus this saturation condition is at a stable equilibrium. On the other hand the left boundary in the susceptibility diagram also has a yield of $\bar{\delta} = 1$,

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but it is unstable, which is denoted as $\tilde{L}$ in Fig. 5.6 and Fig. 5.7. When $F_{dc} < F_{dc}^{\tilde{L}}$, we have $\bar{\delta} < 1$, which will further decrease the F_{dc} . Similarly, the $\bar{\delta} > 1$ condition will increase further the F_{dc} value if $F_{dc} > F_{dc}^{\tilde{L}}$.

5.4.3 Steady-State Power Absorption

By knowing the stable saturation point B shown in the susceptibility diagrams, we propose a simple backward one-step method to estimate the amount of power absorption by the multipactor discharge (at saturation condition) for a given input rf field of F_{rf0} . The approach is as follows. Assuming that the initial F_{rf0} is unknown for a given saturation point, namely F_{rf}^{sat} and F_{dc}^{sat} , which is located at the saturation boundary of $\tilde{R}$ based on the constructed susceptibility diagram. At saturation, the process is a single-surface multipactor discharge due to the large F_{dc}^{sat} field. The number of multipactor electrons N_e^{sat} is inferred by the buildup of dc field, which is $|F_{dct}^{\text{sat}}| \approx eN_e^{\text{sat}}/2A_s\epsilon_0$. Thus only one impact number is required to compute for the N_e^{sat} electrons at the given values of F_{dc}^{sat} and F_{rf}^{sat} . We can numerically calculate (for one transit) the P_m^{sat} and K_{sat} using Eq. (5.12). The unknown value of F_{rf0} is determined by Eq. (5.13), which also provides the unknown input power $P_{\text{in}} = F_{rf0}^2 A_c / 2Z_0$. Using this approach, the normalized power absorption $P_m^{\text{sat}}/P_{\text{in}}$ can be determined consistently as a function of initial rf field (or input power).

This method is only a single trajectory calculation for one impact that requires only one input parameter $\gamma_{\text{sat}} = F_{dc}^{\text{sat}}/F_{rf}^{\text{sat}}$, which measures the ratio of the magnitude of the dc field to the rf field at the saturation point. The value of γ_{sat} is simply the inverse local slope of any points along the saturation boundary ($\tilde{R}$) shown in the susceptibility diagrams (see Fig. 5.6 and Fig. 5.7). Exact value of $E_{\text{max}0}$ and $\delta_{\text{max}0}$ are not required if arbitrary γ_{sat} is assumed in the calculation. Using this simplified one-step method, the power absorption (in terms of input power) and its corresponding initial rf field F_{rf0} are plotted as a function of F_{rf}^{sat} in Fig. 5.8(a) for various arbitrary

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$\gamma_{\text{sat}} = 0.1$ to 0.3 . From the figure, we see that P_m/P_{in} (solid line) is an increasing function of both $F_{\text{rf}}^{\text{sat}}$ and $F_{\text{rf}0}$ (dashed line) at fixed γ_{sat} . At any given $F_{\text{rf}0}$, this figure also implies that the normalized power absorption increases with γ_{sat} .

The exact value of γ_{sat} is not a constant at the saturation boundary of $\tilde{R}$. From the susceptibility diagram, we see that it is an increasing (and decreasing) function at small (and large) $F_{\text{rf}}^{\text{sat}}$ as shown in Fig. 5.6 and Fig. 5.7. By using the accurate values of γ_{sat} given by the susceptibility diagram, we calculate the normalized power absorption as a function of the respective initial rf field $F_{\text{rf}0}$, which is plotted in Fig. 5.8(b) for the three susceptibility diagrams shown in Fig. 5.6 (a) - (c). Since the slope of the saturation boundary $\tilde{R}$ or γ_{sat} is nearly the same for all the three cases due to same first crossover energy of $E_1 = 21$ eV, the power absorption, which is about 30% to <50% in the range of $F_{\text{rf}0} = 2$ to 8 MV/m, does not change much. Here, we have assumed zero initial dc field ($F_{\text{dcc}} = 0$) to initiate the discharge, thus there is no power absorption for rf field less than 2 MV/m as it is outside the growth region (with zero initial dc field). In contrast to case 5.6(a) of (700 eV, 5), case 5.7(a) of (350 eV, 5) has a larger γ_{sat} and thus higher power absorption. In this case, the power absorption can also occur at a lower rf field like $F_{\text{rf}0} = 0.7$ to 2 MV/m as multipactor discharge can be initiated at lower rf field. At high rf electric field, the power absorption can be as high as 50% of incident power. Note that the saturation of high power absorption at high $F_{\text{rf}0}$ is due to the decrease of γ_{sat} indicated in the susceptibility diagram.

For the other susceptibility diagrams of Fig. 5.6(d), 5.7(b) and 5.7(c), we see that an initial nonzero dc field (F_{dcc}) is required to initiate multipactor discharge for some given values of $F_{\text{rf}0}$. First, we assume that the initiation of multipactor discharge (e.g. point A) is around the left boundary $\tilde{L}$ of the growth region. As an example, we need about $F_{\text{dcc}} = 0.5$ MV/m at $F_{\text{rf}0} = 3$ MV/m for case 5.7(b). In Fig. 5.8(c), the normalized power absorption with nonzero initial dc field F_{dcc} is plotted as a function of $F_{\text{rf}0}$ on two different situations. The first situation (solid lines) assumes that the

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Figure 5.8: (a) Normalized power absorption P_m/P_{in} (solid) and initial rf field F_{rf0} (dashed) as a function of F_{rf}^{sat} for various arbitrary γ_{sat} . (b) and (c) are P_m/P_{in} as a function of F_{rf0} by using the susceptibility diagrams given in Fig. 5.6 and Fig. 5.7 at various initial dc fields (b) zero field, (c) nonzero continuous field (solid) and nonzero impulse field (dotted).

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initial dc field is continuously applied during the evolution of multipactor discharge from the initiation point A to the saturation point B. The second condition (dotted lines) assumes that the initial dc field is turned off immediately once the initiation of multipactor discharge has started. With a continuous external F_{dcc} , it is obvious that fewer secondary electrons are required in order to reach the saturated dc field at point B, and thus lower power absorption is expected (see the solid lines). For an impulse F_{dcc} (just to initiate the discharge), more secondary electrons are required to reach the same level of saturated dc field, leading to higher power absorption (see the dotted lines). The power absorption can only occur within a certain range of rf field, for which the multipactor growth is possible. The range is about $1.5 \text{ MV/m} < F_{\text{rf0}} < 6 \text{ MV/m}$ for 5.6(d) and 5.7(b), while $F_{\text{rf0}} > 4 \text{ MV/m}$ for case 5.7(c).

In comparison to the previous studies of a 1D dielectric window [159, 87, 88, 160], power absorption (due to multipactor discharge) in a DLA structure [25, 155] is much larger, which can be explained as follows. In a DLA structure, the incident power flux is *parallel* to the cylindrical dielectric surface with a cross sectional area of about $A_c = \pi a^2$, where a is the radius of the DLA structure. The charge accumulation on DLA structure, however, has an effective area of $A_s = \pi aL$, where $L \gg a$ is the length of the DLA structure. Since the power absorption by the multipactor discharge is proportional to the number of secondary electrons ($P_m \propto N_e^{\text{sat}} \propto A_s$), and the power input is $P_{\text{in}} \propto A_c$, the normalized power absorption for the DLA structure is $P_m/P_{\text{in}} \propto A_s/A_c = L/a$, which can be large if $L \gg a$. For a dielectric window, the rf field is parallel to the dielectric surface, and the direction of the incident power flux is *perpendicular* to the surface. Both charge accumulation and input power flow have the same characteristic area, therefore the normalized power absorption is independent of the surface area for dielectric window. In particular, Ang *et al.* [87] predicts the fraction of saturated power absorption is less than 1% for the dielectric

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window case (over a wide range of parameters), but the value can be up to 50% in the DLA structure due to $L \gg a$ condition, as reported in this research.

5.4.4 Comparison with Experiments

It is difficult to have a quantitative comparison between our calculated power absorption with the experimental measurements, as the SEE properties are not specified in the papers [25, 155]. However, some qualitative discussions are made here by using the calculated results, which cover a wide range of SEE parameters. The materials used in the first experiment [25] is alumina, whose SEE parameters are $E_{\max 0} = 350 - 1300$ eV and $\delta_{\max 0} = 1.5 - 9$ [159]. In our calculations, we have used various values of $(E_{\max 0}, \delta_{\max 0})$ to calculate the normalized power absorption P_m/P_{in} as a function of $F_{\text{rf}0}$. All these cases have similar first crossover energy E_1 (around 10 - 20 eV) and very large second crossover energy E_2 (1 keV or more). From the results shown above, we notice that E_1 is an important parameter in determining the threshold value of the rf field to have multipactor discharge, and also the saturation condition at $\tilde{R}$. On the other hand, the left boundary of a susceptibility diagram is influenced by both E_1 and E_2 . For a typical case of alumina [Fig. 5.6 (a) - (c) and Fig. 5.7(a)], small E_1 (10 - 20 eV) and large E_2 (3.4 - 16 keV) will enable the initiation of multipactor at $F_{\text{rf}} \approx 1$ MV/m with zero initial dc electric field. And the calculations shown in Fig. 5.8(b) indicate that significant power absorption as high as 50% of the incident power is possible, which confirm the threat of multipactor discharge and its large power absorption, if uncoated alumina is used at high rf field in a DLA structure [25].

To avoid multipactor discharge, some coatings or new materials with suitable SEE properties have been proposed, such as TiN coating on alumina [155]. It is qualitatively known that TiN coating on alumina will have smaller SEE parameters as compared to alumina [165, 166]. Experimental testings have also suggested that

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the coating dose not change the threshold rf field (for initiating multipactor), but is able to decrease the power absorption. Here, we speculate that case 5.6(d) of (140 eV, 2) or case 5.7(b) of (180 eV, 2) may describe such behavior of lower power absorption in Fig. 5.8(c) due to invariant E_1 and reduced E_2 as compared to pure alumina. The other possible reason of using TiN to fight multipactor is to drain the charges accumulated on the dielectric surface.

In addition to TiN coating, a new material called MCT-20 has also been used to avoid multipactor discharge at relatively small rf field, and to decrease power absorption at large rf field [155]. According to our model, such materials will require higher value of E_1 , which can shift the growth region upwards (to increase threshold value of F_{rf}), and decrease the size of the growth region (to decrease power absorption). Thus SEE parameters like $(E_{\text{max0}}, \delta_{\text{max0}}) = (1300 \text{ eV}, 1.5)$ or $(32.5 \text{ keV}, 9)$ studied above may be suited for such MCT-20 materials. In particular, the multipactor discharge for case 5.7(c) has a threshold of $F_{\text{rf}} = 4 \text{ MV/m}$ and the power absorption is less than 20% as shown in Fig. 5.8(c).

5.5 Summary

In summary, a statistical model has been developed to explain the observation of multipactor discharge during a high-power testing of a dielectric-loaded accelerating structure [26]. The susceptibility diagram, dynamic evolution and steady-state power absorption of the multipactor discharge are calculated. Our results confirm the experimental findings [25, 155] by using various values of $(E_{\text{max0}}, \delta_{\text{max0}})$. In such a DLA structure, two-surface multipactor discharge may occur at early stage when the dc field on the dielectric is smaller than 0.02 MV/m, and it becomes a single-surface multipactor discharge when the dc field gets larger. A resonant condition with the transit time equal to the inverse of the rf frequency is derived, which is able

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to provide the maximum growth of multipactor discharge close to $\delta_{\max 0}$. It is found that the saturation condition is always a single-surface multipactor discharge, which occurs at the first crossover impact energy. An efficient one-step method is introduced to calculate the steady-state power absorption of the multipactor discharge based on the susceptibility diagram.

In order to avoid the large power absorption in DLA structure, materials with large first crossover impact energy and small growth region are suggested. Another method is probably to decrease the surface area by reducing the length of DLA structure. With reduced area, we will have less accumulated positive charges at the same saturated dc field, which may reduce the power absorption due to the small amount of secondary electrons. Finally, our model is readily to be extended to other DLA structures with different operating conditions, such as size, shape and frequency.

CHAPTER 6

CONCLUSIONS AND FUTURE WORK

Section 6.1 summarizes the major results of this dissertation. Section 6.2 addresses some interesting issues for future work.

6.1 Conclusions

This dissertation deals with various manifestations of electron emission from a free-electron based metal, which are thermionic emission, field emission, photoemission and secondary electron emission. This research differs from previous studies in that we focus on the modeling and understanding of the latest observed phenomena, new physical mechanisms and novel applications of electron emission.

In the first part of this dissertation, we propose a nonequilibrium model to describe the low-power ultrafast laser excited electron emission from a metallic surface with a dc bias. Using a microscopic kinetic approach, we determine the nonequilibrium electron distribution after the laser excitation, and calculate the time-dependence of the emitted electron charges and current density. It is found that the classical two temperature model, which is accurate for picosecond laser excited

6.1 Conclusions

electron emission process, is no longer valid when the laser pulse duration is less than 100 femtosecond. Our calculation validates the known experimental observations [13, 14] of a nonlinear dependence of electron counts on laser power.

In the second part of this dissertation, we study the electron shot noise of high current space-charge-limited (SCL) field emission, including the effects of both quantum partitioning and Coulomb correlation of the emitted tunneling electrons inside a gap. The Fano factor (γ) is calculated over a wide range of applied voltages, gap spacings and electron pulse lengths in classical, quantum and relativistic regimes. It is found that the effect of space charge smoothing (observed in thermionic emission) is no longer valid for high current field emission, as the space charge field will increase the potential barrier and thus decrease the degree of quantum partitioning (larger γ). However, the shot noise of SCL field emission in a nanogap may be suppressed due to the combination of Coulomb repulsion and exchange-correlation potential among the tunneling electrons, where the dynamics of the electrons inside the gap are treated by using a quantum mean field model. Coulomb correlation can be ignored when the pulse length of the electron beam is much smaller than the gap transit time. Possible experimental settings are discussed in order to observe the shot noise suppression of field emission with and without the space charge effects.

In the third part of this dissertation, we explore new possibilities of refrigeration by using thermal-field emission of electrons from nanoscale emitters in a planar diode or from the cathode (inner electrode) in a coaxial cylindrical diode. Our calculation shows that it is possible to provide cooling at temperature down to 200 K if the work function of the cathode is about 1 eV. The limitation on using low work function cathode can be improved by applying an external crossed magnetic field to create an additional potential barrier near anode, in order to restrict the emission of low energy electrons (below the Fermi energy level) more efficiently. Because of this extra filtering process, emitters of arbitrary work functions can be used to provide

6.2 Recommendations for Further Research

an improved cooling capability from 300 K down to 10 K. The optimal conditions to achieve maximum cooling power density are determined both numerically and analytically. The space charge effects of the emitted electrons in the gap are included self-consistently for the coaxial cylindrical diode geometry, which will degrade the predicted cooling power density to a certain extent.

In the last part of this dissertation, we present a Monte-Carlo model to explain the multipactor discharge and its high-power absorption in a dielectric-loaded accelerating (DLA) structure reported recently [25]. Susceptibility diagrams are constructed to determine the conditions of multipacting. Dynamic calculations for beam loading and its steady-state power absorption by the multipactor discharge are performed. It is found that the fraction of power absorbed by multipactor discharge at saturation is much larger than the case of a simple rf window, and it is sensitive to the incident power, which confirms the prior experimental results. This enhanced power absorption is due to the fact that the length of a DLA structure is much larger than the radius of the structure. A resonant condition of a maximum growth region has also been determined numerically and analytically. The difference between the resonant condition (due to phase focusing) and the saturation condition (due to beam loading) is clarified. To avoid the high power absorption in DLA structure, we suggest to adopt materials with large first crossed-over impact energy and small growth region, or to decrease the surface area by reducing the length of the DLA structure.

6.2 Recommendations for Further Research

We now address some possible extensions of this research work. First of all, the main difficulty of the nonequilibrium model for the ultrafast laser excited electron field emission consists in the accurate estimation of geometrical field enhancement for a

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sharp field emitter. The current model is one-dimensional for which we assume the assigned arbitrary values of F_L and F_{dc} have included the geometrical enhancement factor of both laser field and dc field on the sharp tip. An improvement of calculating the enhancement factor will be useful to have a direct connection to the experimental parameters such as applied dc voltage and laser power. The model also assumes that the power of the laser is low enough that effects such as optical field emission and the electron space charge field can be ignored. This assumption should be corrected when the laser power is increased. Finally, we ignore the effects of finite tunneling time, which should be valid when the time-varying laser field does not modulate the potential barrier significantly. This limitation will require revision when the effect of optical tunneling is included in future works.

The model of shot noise proposed in the second part of this dissertation is an equilibrium model, where the electronic properties of the metal surfaces are assumed to be at equilibrium. The main restrictions of the model are as follows. The image charge is a consequence of exchange-correlation related to variation in electron density. Under high electric fields, the form of the image charge requires revision when the density near the surface is quite altered. Another practical complication is that fields larger than 10 V/nm cause the emitter surface to become dynamic rather than static, for example, a low work function coating like Barium will be desorbed. Future work should be focused on extending the current exploration of the basic physics to those more realizable situations. Moreover, in order to experimentally observe the interesting phenomena of shot noise, delicate measurements of electron emission current with high temporal resolution deserve significant attention.

For a nano-scale field emitter used in refrigeration applications based on electron thermal-field emission, space charge effects have been ignored. It could become important if a large number of emitters are used, so that the electron transport will be limited by space charge. The one-dimensional model also considered that most

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electrons are emitted from the centerline of the emitter, which have the largest field enhancement. This approximation is valid for the macroscopic electron transport (far away from the emitter) in a gap of typical size that is much larger than the radius of emitter. To include the electrons emitted off the centerline and space charge effects, a complete model is required to solve the two-dimensional Schrödinger equation and Poisson equation. On the other hand, to realize the proposed novel refrigeration idea, experimental work to demonstrate our theoretical concept is important and necessary.

Finally it would be of great interest to work on PIC (particle-in-cell) simulations for the multipactor discharge phenomenon in the dielectric-loaded accelerating structures. The simulation is able to take into account the space charge effects during the electron transit time, which are neglected in our numerical calculations. Furthermore our model is readily to be extended to other accelerating structures with different operating conditions, such as size, shape and frequency.

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Journal Papers

1. L. Wu and L. K. Ang. "Low temperature refrigeration by electron emission in a crosses-field gap", *Appl. Phys. Lett.*, **89**:133503 (2006).
2. L. Wu and L. K. Ang. "Multipactor discharge in a dielectric-loaded accelerating structure", *Phys. Plasmas*, **14**:013105 (2007).
3. L. Wu, L. K. Ang and W. S. Koh. "Theory of shot noise in high-current space-charge-limited field emission", *Phys. Rev. B*, **77**:115351 (2008).
4. L. Wu and L. K. Ang. "Low temperature refrigeration by using thermal-field emission in a coaxial cylindrical diode", *J. Appl. Phys.*, **104**:084506 (2008).
5. L. Wu and L. K. Ang. "Nonequilibrium model of ultrafast laser-induced electron photofield emission from a dc-biased metallic surface", *Phys. Rev. B*, **78**:224112 (2008).

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2. L. Wu and L. K. Ang. “Multipactor discharge in a dielectric - loaded accelerating structure”, *The 19th International Vacuum Nanoelectronics Conference and 50th International Field Emission Symposium, Guilin, China*, PE137 (2006)
3. L. Wu and L. K. Ang. “Low temperature cooling by thermal-field electron emission in a crossed-field gap”, *2007 IEEE Pulsed Power and Plasma Science Conference, Albuquerque, New Mexico, United States*, 5E4 (2007) [supported by IEEE student travel grant and selected as a finalist for a Student Paper Award]
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6. L. Wu and L. K. Ang. “Nonequilibrium model of ultrafast laser induced electron emission from a dc-biased metallic surface”, *The 50th Annual Meeting of the Division of Plasma Physics, American Physical Society, Dallas, Texas, United States*, TO3.00006 (2008) [supported by IHPC-EEE joint lab]
7. L. Wu and L. K. Ang. “Low temperature refrigeration by using thermal-field emission in a coaxial cylindrical diode”, *The 50th Annual Meeting of the*

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APPENDIX A

FORMULATION OF SPACE CHARGE LIMITED FLOW

Assume that we have a supply of free electrons at rest (at the grounded cathode) and apply a voltage V_g to an anode at a distance D from the cathode, current density J will be drawn across this gap in the steady state. The emitted electrons of density profile $n(x)$ inside the gap will result in a space charge potential $V_{sc}(x)$, which must obey the one-dimensional (1D) Poisson equation (the diode is assumed to be of infinite extent in the y and z directions)

$$\frac{d^2 V_{sc}}{dx^2} = \frac{en(x)}{\epsilon_0} \quad (\text{A.1})$$

where e is the electron charge, ϵ_0 is the permittivity of free space.

Besides a classical formulation for a moderate gap spacing and gap voltage (Section A.1), the quantum dynamics needs be considered for the case of a nano-scale gap spacing D [nm] (Section A.2) and a relativistic formulation is required for the case of a large gap voltage V_g [MV] (Section A.3). For convenience, the physical quantities are mathematically normalized, which are summarized in Table A.1. The most important two are: (i) the normalized gap spacing with respect to the electron

A.1 Classical Regime

de Broglie wavelength $\lambda = D/\lambda_0$ to clearly show the transition from quantum regime ($\lambda < 1$) to classical regime ($\lambda \gg 1$), and (ii) the normalized gap voltage with respect to the electron rest energy $U_0 = eV_g/(mc^2)$ to expressly demonstrate the transition from relativistic regime ($U_0 > 1$) to classical regime ($U_0 \ll 1$).

Table A.1: Normalized Physical Quantities

Normalization	Physical Quantity	Normalizing Scale
$\bar{x} = x/D$	position	D = gap spacing
$\phi_v = V_v/V_g$	applied electric potential	V_g = gap voltage
$\phi_{sc} = V_{sc}/V_g$	space charge potential	V_g = gap voltage
$\mu = J/J_{CL}$	current density	J_{CL} = classical CL law
$q^2 = n/n_0 = \psi ^2/n_0$	electron density	$n_0 = 2\epsilon_0 V_g/3eD^2$
$\epsilon = E_0/eV_g$	electron emission energy	eV_g = anode potential energy
$\lambda = D/\lambda_0$	normalized gap spacing	$2\pi\lambda_0$ = de Broglie wavelength
$\phi_g = eV_g/E_H$	normalized gap voltage	E_H = Hartree energy
$\phi_{xc} = U_{xc}/eV_g$	exchange-correlation potential	eV_g = anode potential energy
$U_0 = eV_g/(mc^2)$	normalized gap voltage	mc^2 = electron rest energy

A.1 Classical Regime

In a classical gap [123, 124], the current density $J = en(x)v(x)$ will be drawn across the gap in the steady state, where n and v are the density and velocity of the electrons, respectively, in the gap as a function of the position x between two plates. Now $v(x)$ can be found from the energy conservation [136],

$$\frac{1}{2}mv^2(x) - e[V_{sc}(x) + V_v(x)] = \text{constant} = 0 \quad (\text{A.2})$$

A.2 Quantum Regime

where m and e are the electron mass and charge, respectively, $V_{sc}(x) + V_v(x)$ is the potential field in the gap, and for simplicity the total energy has been set to zero (for electrons initially at rest at the grounded cathode). The Poisson equation in Eq. (A.1) is therefore [123, 124]

$$\frac{d^2 V_{sc}}{dx^2} = \frac{J}{\epsilon_0 v(x)} = \frac{J}{\epsilon_0 \sqrt{2e[V_{sc}(x) + V_v(x)]/m}}. \quad (\text{A.3})$$

In terms of the normalized parameters $\bar{x}$, μ , ϕ_{sc} and $\phi_v = \bar{x}$, we have

$$\phi_{sc}'' = \frac{4}{9} \frac{\mu}{\sqrt{\phi_{sc} + \bar{x}}}, \quad (\text{A.4})$$

which is subjected to boundary conditions $\phi_{sc}(0) = 0$ and $\phi_{sc}(1) = 0$. Hence for any value of current density $\mu \leq \mu_C$, we can obtain a spatial profile of space charge potential $\phi_{sc}(\bar{x})$ or $V_{sc}(x)$. For classical case, $\mu_C = 1$ is the maximum steady-state current density that can be transported across the gap, and there are no solutions to Eq. (A.4) for $\mu > \mu_C$.

A.2 Quantum Regime

In a planar nanogap, using mean field theory for electrons in a one-dimensional potential energy barrier $U(x) = -eV_{sc}(x) - eV_v(x) + U_{xc}(x)$, the 1D time-independent Schrödinger equation and the Poisson equation (with $n = \psi\psi^*$) are [132, 55]

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = (E_0 + eV_{sc} + eV_v - U_{xc})\psi \quad (\text{A.5})$$

$$\frac{d^2 V_{sc}}{dx^2} = \frac{e\psi\psi^*}{\epsilon_0} \quad (\text{A.6})$$

where $\psi(x)$ is the complex electron wave function, E_0 is the electron emission energy, V_{sc} is the space charge potential, V_v is the applied electric potential, $U_{xc} = \bar{U}_{xc} \times E_H$ is the electron exchange-correlation potential energy with E_H the Hartree energy. The dimensionless $\bar{U}_{xc}$ is calculated by Kohn-Shan density functional theory (DFT) [167]

$$\bar{U}_{xc} = \epsilon_{xc} - \frac{r_s}{3} \frac{d\epsilon_{xc}}{dr_s}, \quad (\text{A.7})$$

A.2 Quantum Regime

where r_s is the local Seitz radius $[4\pi n(r_s a_0)^3 = 1]$ in terms of the Bohr radius a_0 . The exchange-correlation energy $\epsilon_{xc} = \epsilon_x + \epsilon_c$ consist of the exchange energy ϵ_x [168] and correlation energy ϵ_c [122] of each electron for a uniform electron gas of density n under the Kohn-Sham local density approximation (LDA). They are

$$\epsilon_x = -\frac{3}{4} \left(\frac{3}{2\pi} \right)^{2/3} \frac{1}{r_s}, \quad (\text{A.8a})$$

$$\epsilon_c = -2A(1 + a_1 r_s) \ln \left[1 + \frac{1/2A}{\kappa} \right], \quad (\text{A.8b})$$

where $\kappa = b_1 \sqrt{r_s} + b_2 r_s + b_3 r_s^{3/2} + b_4 r_s^{c+1}$ and $(c, A, a_1, b_1, b_2, b_3, b_4)$ are parameterized constants obtained using the random phase approximation [122].

We represent the complex wave function $\psi(x)$ in terms of the non-dimensional wave amplitude $q(\bar{x})$ and phase $\theta(\bar{x})$, both assumed real [55]

$$\psi(x) = \sqrt{n_0} q(\bar{x}) e^{i\theta(\bar{x})}. \quad (\text{A.9})$$

The charge conservation requires that the current density $J = e(i\hbar/2m)(\psi\psi^{*'} - \psi^*\psi')$ be constant for all x , where the prime denotes a derivative with respect to x . Deriving from the definition of J , we will have $\theta'(\bar{x}) = \frac{2}{3}\mu\lambda q^{-2}$ where μ and λ is, respectively, the normalized current density and gap spacing as shown in Table A.1. By taking this precise expression of ψ into Eqs. (A.5) and (A.6), we are able to obtain the normalized 1D time-independent Schrödinger equation and the Poisson equation [55]

$$q'' + \lambda^2 \left[\epsilon + \phi_{sc} + \bar{x} - \phi_{xc} - \frac{4}{9} \frac{\mu^2}{q^4} \right] q = 0, \quad (\text{A.10})$$

$$\phi_{sc}'' = \frac{2}{3} q^2, \quad (\text{A.11})$$

where the prime denotes the derivative with respect to $\bar{x}$. The boundary conditions for Eqs. (A.10) and (A.11) are $\phi_{sc}(0) = 0$, $\phi_{sc}(1) = 0$, $q(1) = (2\mu/3)^{1/2}(1 + \epsilon)^{-1/4}$, $q'(1) = 0$. With these boundary conditions, we can determine the profile of wave amplitude $q(\bar{x})$ and space charge potential $\phi_{sc}(\bar{x})$ for any value of injected current density $\mu \leq \mu_Q$, at given gap spacing λ and gap voltage ϕ_g . Here $\mu_Q > 1$ is the

A.3 Relativistic Regime

maximum space charge limited electron current density in quantum regime, as no solutions can be found to Eqs. (A.10) and (A.11) for $\mu > \mu_Q$.

It can be easily shown that the classical limit is obtained by simply ignoring the first term in Eq. (A.10) because the quantum behavior disappears when $\lambda \gg 1$, i.e., large gap spacing. For electrons initially at rest ($\epsilon = 0$) at the grounded cathode in a large gap spacing ($\phi_{xc} \approx 0$), we have from Eq. (A.10) that $\phi_{sc} + \bar{x} - \frac{4}{9} \frac{\mu^2}{q^4} = 0$, which when cast back into Eq. (A.11), will lead to the normalized classical Poisson equation as shown in Eq. (A.4).

A.3 Relativistic Regime

It has been shown from Eq. (A.2) that electron velocity v increases as the square root of potential $V_{sc} + V_v$. This is true up to velocities of about one-tenth the speed of light c , which is attained at about 2,600 volts. Beyond this value of potential the velocity increases less rapidly. This comes about because one of the fundamental postulates of the theory of relativity is that no object can acquire speeds greater than the velocity of light. If this is true, then the mass of a particle must increase as it is accelerated, for otherwise a constant accelerating force would in time bring it to velocities greater than that of light. This is consistent with another postulate of relativity, namely, that mass is a manifestation of energy. When a particle is accelerated, it acquires kinetic energy, which manifests itself as an increase in mass. In developing special relativity, Einstein found that the kinetic energy of a moving body [169] is

$$K.E. = \frac{mc^2}{\sqrt{1 - v^2/c^2}} - mc^2 = m_r c^2 - mc^2, \quad (\text{A.12})$$

where v is velocity, m is rest mass, and m_r is relativistic mass which represents the total quantity of energy in a body.

The Lorentz factor or Lorentz term appears in several equations in special relativity, including time dilation, length contraction and the relativistic mass

A.3 Relativistic Regime

formula. Because of its ubiquity, physicists generally represent it with the shorthand symbol Γ (note that the more commonly used symbol γ for Lorentz factor has been taken to denote the Fano factor of shot noise in Chapter 3, so the symbol Γ is chosen here to avoid confusion), which is defined as

$$\Gamma \equiv \frac{1}{\sqrt{1 - v^2/c^2}}. \quad (\text{A.13})$$

The relation of $m_r = \Gamma m$ can be found from Eq. (A.12), which tells how the relativistic mass m_r increases as a function of velocity v . It is independent of how the velocity is acquired. If the kinetic energy is acquired by acceleration through a potential $V_{sc} + V_v$, then [42]

$$\Gamma = 1 + \frac{e(V_{sc} + V_v)}{mc^2}. \quad (\text{A.14})$$

Therefore the Poisson equation in Eq. (A.1) becomes now

$$\frac{mc^2}{e} \frac{d^2\Gamma}{dx^2} = \frac{J}{\epsilon_0 v(x)} = \frac{J}{\epsilon_0 c \sqrt{1 - \Gamma^{-2}}}. \quad (\text{A.15})$$

By introducing the normalized gap voltage $U_0 = eV_g/(mc^2)$, we have the normalized Poisson equation in relativistic regime [102, 125]

$$\Gamma'' = \mu \frac{4\sqrt{2}}{9} U_0^{3/2} \frac{\Gamma}{\sqrt{\Gamma^2 - 1}}, \quad (\text{A.16})$$

where the prime denotes the derivative with respect to $\bar{x}$, and the boundary conditions are $\Gamma(0) = 1$ and $\Gamma(1) = 1 + eV_g/(mc^2)$. For any value of current density $\mu \leq \mu_R$ (where $\mu_R < 1$ is the maximum space charge limited electron current density in relativistic regime), the solution of $\Gamma(\bar{x})$ as well as the space charge potential profile $V_{sc}(x)$ can be found. At small gap voltage $U_0 \ll 1$, i.e. $\alpha = \frac{e(V_{sc} + V_v)}{mc^2} \ll 1$, we can recover the classical limit as follows:

$$\begin{aligned} \frac{eV_g}{mc^2} \phi_{sc}'' &= \mu \frac{4\sqrt{2}}{9} \left(\frac{eV_g}{mc^2} \right)^{3/2} \frac{1 + \alpha}{\sqrt{1 + \alpha^2 + 2\alpha - 1}} \\ \phi_{sc}'' &\approx \mu \frac{4\sqrt{2}}{9} \left(\frac{eV_g}{mc^2} \right)^{1/2} \frac{1}{\sqrt{2\alpha}} \\ \phi_{sc}'' &\approx \frac{4}{9} \frac{\mu}{\sqrt{\phi_{sc} + \bar{x}}}. \end{aligned} \quad (\text{A.17})$$

APPENDIX B

DERIVATION OF TRANSMISSION COEFFICIENT

For any transmission problem over a potential energy profile $U(x)$, the transmission coefficient $\mathcal{T}(E_x)$, defined as the probability that an electron with normal energy E_x can penetrate the profile $U(x)$, can be derived universally in this Appendix, for a single barrier or a dual barrier (see Fig. B.1) [38].

B.1 Single Barrier

The analysis starts from the time-independent Schrödinger equation, where $\psi(x)$ is the electron wave function, both potential energy $U(x)$ and electron normal energy E_x are referring to the Fermi energy level,

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E_x\psi(x). \quad (\text{B.1})$$

As shown in Fig. B.1, the whole region from cathode $x = a$ to anode $x = b$ are divided into five parts: (I) $a < x < x_1$, (II) $x_1 < x < x_2$, (III) $x_2 < x < x_3$, (IV) $x_3 < x < x_4$, (V) $x_4 < x < b$, where x_1, x_2, x_3, x_4 are the roots of $E_x - U(x) = 0$. For simplicity, only the first barrier over region I, II, III is analyzed and the results can be extended to the second barrier.

B.1 Single Barrier

Figure B.1: Schematic diagram of a single barrier between x_1 and x_2 , and a dual barrier between x_1 and x_4 in a vacuum gap between cathode and anode, for an incident electron of x -direction energy E_x .

Let define $\phi(x) = E_x - U(x)$ and $\lambda^2 = 2m/\hbar^2$, the time-independent Schrödinger equation Eq. (B.1) can be simplified as

$$\frac{d^2\psi(x)}{dx^2} + \lambda^2\phi(x)\psi(x) = 0, \quad (\text{B.2})$$

where the possible solution of $\psi(x)$ can be written for the known values of $\phi(x)$ in region I, II and III, respectively [38]:

$$\psi_1(x) = \frac{1}{\phi^{1/4}} \left[A \exp \left(i\lambda \int_{x_1}^x \sqrt{\phi(x)} dx \right) + B \exp \left(-i\lambda \int_{x_1}^x \sqrt{\phi(x)} dx \right) \right], \quad (\text{B.3a})$$

$$\psi_2(x) = \frac{1}{|\phi|^{1/4}} \left[C \exp \left(-\lambda \int_{x_1}^x \sqrt{|\phi(x)|} dx \right) + D \exp \left(\lambda \int_{x_1}^x \sqrt{|\phi(x)|} dx \right) \right], \quad (\text{B.3b})$$

$$\psi_3(x) = \frac{1}{\phi^{1/4}} \left[E \exp \left(i\lambda \int_{x_2}^x \sqrt{\phi(x)} dx \right) + F \exp \left(-i\lambda \int_{x_2}^x \sqrt{\phi(x)} dx \right) \right]. \quad (\text{B.3c})$$

Firstly, we will perform the analysis around $x = x_1$ (region I and II) by approximating $\phi(x) \approx \phi(x_1) + \phi'(x_1)(x - x_1)$, and defining $\nu_1^2 = -\phi'(x_1)$, $\zeta_1 =$

B.1 Single Barrier

$(\lambda\nu_1)^{2/3}(x_1 - x)$, we will obtain

$$\frac{d^2\psi}{d\zeta_1^2} + \zeta_1\psi = 0, \quad (\text{B.4})$$

with solution $\psi = a\psi_a(\zeta_1) + b\psi_b(\zeta_1)$ for any arbitrary constants a and b , if $\psi_a(\zeta_1)$ and $\psi_b(\zeta_1)$ are two solutions of Eq. (B.4). Secondly, we will perform the similar analysis around $x = x_2$ (region II and III) by approximating $\phi(x) \approx \phi(x_2) + \phi'(x_2)(x - x_2)$, and defining $\nu_2^2 = \phi'(x_2)$, $\zeta_2 = (\lambda\nu_2)^{2/3}(x - x_2)$, we will have:

$$\frac{d^2\psi}{d\zeta_2^2} + \zeta_2\psi = 0, \quad (\text{B.5})$$

with solution $\psi = c\psi_c(\zeta_2) + d\psi_d(\zeta_2)$ for any arbitrary constants c and d , if $\psi_c(\zeta_2)$ and $\psi_d(\zeta_2)$ are two solutions of Eq. (B.5).

The Eqs. (B.4) and (B.5) are both mathematically in form of the second order differential equation

$$\frac{d^2y}{dx^2} + xy = 0, \quad (\text{B.6})$$

where its solutions can be expressed as follows,

$$\begin{aligned} y(x > 0) &= \frac{c_1}{\sqrt{\pi}x^{1/4}} \sin \left[\frac{2}{3}x^{3/2} + \frac{\pi}{4} \right] + \frac{c_2}{\sqrt{\pi}x^{1/4}} \cos \left[\frac{2}{3}x^{3/2} + \frac{\pi}{4} \right], \\ y(x < 0) &= \frac{c_1}{2\sqrt{\pi}|x|^{1/4}} \exp \left[-\frac{2}{3}|x|^{3/2} \right] + \frac{c_2}{\sqrt{\pi}|x|^{1/4}} \exp \left[\frac{2}{3}|x|^{3/2} \right]. \end{aligned} \quad (\text{B.7})$$

Based on this mathematics, we can solve Eq. (B.4) in region I ($x < x_1, \zeta_1 > 0$) and region II ($x > x_1, \zeta_1 < 0$) respectively, and match the solution of $\psi(x)$ in the respective region to $\psi_1(x)$ and $\psi_2(x)$ in Eq. (B.3), i.e. to correlate the coefficients (A, B) with (a, b) and (C, D) with (a, b) . This will subsequently lead to a matrix which links the coefficients (A, B) and (C, D) ,

$$\begin{bmatrix} A \\ B \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1+i & \frac{1-i}{2} \\ 1-i & \frac{1+i}{2} \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix}.$$

Similarly, Eq. (B.5) in regions II ($x < x_2, \zeta_2 < 0$) and III ($x > x_2, \zeta_2 > 0$) can also be solved, and solutions in each region can be matched to $\psi_2(x)$ and $\psi_3(x)$ in Eq. (B.3),

B.2 Dual Barrier

through which the relation of (C, D) with (c, d) and (E, F) with (c, d) can be found. By doing so, the coefficients (C, D) and (E, F) can be linked through the following matrix where $\alpha = \exp\left(\lambda \int_{x_1}^{x_2} \sqrt{|\phi(x)|} \, dx\right)$,

$$\begin{bmatrix} C \\ D \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} (1-i)\alpha & (1+i)\alpha \\ \frac{1+i}{2\alpha} & \frac{1-i}{2\alpha} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix}.$$

Finally we can correlate the coefficients (A, B) and (E, F) through the medium (C, D)

$$\begin{bmatrix} A \\ B \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 2\alpha + \frac{1}{2\alpha} & i(2\alpha - \frac{1}{2\alpha}) \\ -i(2\alpha - \frac{1}{2\alpha}) & 2\alpha + \frac{1}{2\alpha} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix}.$$

If only waves transmitting in positive x -direction are considered, the transmission coefficient $\mathcal{T}(E_x)$ will be approximately (assuming large α),

$$\mathcal{T}(E_x) = \left| \frac{E}{A} \right|^2 = \frac{4}{\left(2\alpha + \frac{1}{2\alpha}\right)^2} \approx \exp \left[-\frac{2}{\hbar} \int_{x_1}^{x_2} \sqrt{2m[U(x) - E_x]} \, dx \right], \quad (\text{B.8})$$

which is identical with the ordinary WKB expression in Eq. (1.9) in Chapter 1.

B.2 Dual Barrier

Similar to the derivation of the transmission probability over the single barrier between x_1 and x_2 , the wave functions in region III, IV and V can be written as,

$$\psi_3(x) = \frac{1}{\phi^{1/4}} \left[E' \exp \left(i\lambda \int_{x_3}^x \sqrt{\phi(x)} \, dx \right) + F' \exp \left(-i\lambda \int_{x_3}^x \sqrt{\phi(x)} \, dx \right) \right], \quad (\text{B.9a})$$

$$\psi_4(x) = \frac{1}{|\phi|^{1/4}} \left[G \exp \left(-\lambda \int_{x_3}^x \sqrt{|\phi(x)|} \, dx \right) + H \exp \left(\lambda \int_{x_3}^x \sqrt{|\phi(x)|} \, dx \right) \right], \quad (\text{B.9b})$$

$$\psi_5(x) = \frac{1}{\phi^{1/4}} \left[I \exp \left(i\lambda \int_{x_4}^x \sqrt{\phi(x)} \, dx \right) + J \exp \left(-i\lambda \int_{x_4}^x \sqrt{\phi(x)} \, dx \right) \right]. \quad (\text{B.9c})$$

The relation between (E', F') and (I, J) can be represented using a similar matrix as the one between (A, B) and (E, F) , by defining $\beta = \exp\left(\lambda \int_{x_3}^{x_4} \sqrt{|\phi(x)|} \, dx\right)$.

$$\begin{bmatrix} E' \\ F' \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 2\beta + \frac{1}{2\beta} & i(2\beta - \frac{1}{2\beta}) \\ -i(2\beta - \frac{1}{2\beta}) & 2\beta + \frac{1}{2\beta} \end{bmatrix} \begin{bmatrix} I \\ J \end{bmatrix}$$

B.2 Dual Barrier

Note the wave function $\psi_3(x)$ in region III has been represented in two different forms, as a transmitted wave from the first barrier at x_2 in Eq. (B.3) and an incident wave into the second barrier at x_3 in Eq. (B.9), which is characterized by coefficients (E, F) and (E', F') , respectively. It is easy to show that both coefficients can be related to each other by the parameter $\gamma = \lambda \int_{x_2}^{x_3} \sqrt{\phi(x)} dx$,

$$\begin{bmatrix} E \\ F \end{bmatrix} = \begin{bmatrix} \cos \gamma - i \sin \gamma & 0 \\ 0 & \cos \gamma + i \sin \gamma \end{bmatrix} \begin{bmatrix} E' \\ F' \end{bmatrix}.$$

By summarizing the transmission problem over the whole gap ($a < x < b$), we can link (A, B) and (I, J) through matrix manipulation to get

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix} \begin{bmatrix} I \\ J \end{bmatrix}.$$

By only considering the wave propagating in positive x -direction, the important parameter will be m_{11} that relates the magnitude of A and I ,

$$m_{11} = \frac{1}{2} \left[\cos \gamma \left(4\alpha\beta + \frac{1}{4\alpha\beta} \right) - i \sin \gamma \left(\frac{\alpha}{\beta} + \frac{\beta}{\alpha} \right) \right]. \quad (\text{B.10})$$

Therefore the transmission coefficient over a dual barrier $\mathcal{T}(E_x)$ is determined:

$$\mathcal{T}(E_x) = \left| \frac{I}{A} \right|^2 = \frac{1}{|m_{11}|^2} = \frac{4}{\cos^2 \gamma \left(4\alpha\beta + \frac{1}{4\alpha\beta} \right)^2 + \sin^2 \gamma \left(\frac{\alpha}{\beta} + \frac{\beta}{\alpha} \right)^2}. \quad (\text{B.11})$$

APPENDIX C

REVIEW OF THE TRANSMISSION LINE MODEL

C.1 Review on Transmission Line Model

To analyze the amount of power delivered by multipactor discharge onto the dielectric, we use a transmission line model [87], which considers a plane electromagnetic wave incident through a dielectric-loaded accelerating (DLA) structure. In the absence of multipactor, this plane wave is assumed to be perfectly transmitted through the DLA structure with zero reflection. Such an incident plane wave may then be represented as a rightward traveling voltage pulse V^+ on a transmission line of characteristic impedance Z_0 , and terminated by a matched load of impedance $Z_L = Z_0$ [see Fig. C.1(a)]. The presence of multipactor will induce partial reflection and partial absorption of the incident wave, with the reminder being transmitted. All of these can be simply modeled by a variable impedance Z_m [see Fig. C.1(b)]. The multipactor impedance Z_m and load impedance Z_0 are grouped together to give a total equivalent impedance [see Fig. C.1(c)],

$$Z_{\text{eq}} = \frac{Z_m Z_0}{Z_m + Z_0}. \quad (\text{C.1})$$

C.1 Review on Transmission Line Model

Let V^+ be the incoming wave and V^- be the reflected wave at the load, the voltage across Z_{eq} is V_L as shown in Fig. C.1(c). The continuity of voltage and current at the load gives

$$V^+ + V^- = V_L, \quad (\text{C.2a})$$

$$\frac{V^+}{Z_0} - \frac{V^-}{Z_0} = \frac{V_L}{Z_{\text{eq}}}. \quad (\text{C.2b})$$

Combining Eq. (C.1) and Eq. (C.2), the ratio of $V_{L(i)}$ and V^+ could be related to the multipactor impedance $Z_{m(i)}$

$$\frac{V_{L(i)}}{V^+} = \frac{2Z_{m(i)}}{2Z_{m(i)} + Z_0}, \quad (\text{C.3})$$

where $V_{L(i)}$ is the load voltage after the i th impact which appears during the $(i+1)$ th transit, and $Z_{m(i)}$ is the multipactor impedance during the i th transit.

Furthermore the instantaneous power consumed by the multipactor electrons $P_{m(i)}$ during the i th transit from the circuit model is

$$P_{m(i)} = \frac{V_{L(i-1)}^2}{Z_{m(i)}} \equiv K_{(i)} V_{L(i-1)}^2, \quad (\text{C.4})$$

which is equivalent to the work done on the multipactor electrons by the rf field, and can be calculated numerically from Eq. (5.12) in Chapter 5. Consequently the beam loading effect in Eq. (C.3) can be therefore represented by

$$\frac{V_{L(i)}}{V^+} = \frac{2V_{L(i-1)}^2}{2V_{L(i-1)}^2 + Z_0 P_{m(i)}} = \frac{1}{1 + Z_0 K_{(i)}/2}. \quad (\text{C.5})$$

Note, the conversion between the rf electric field F_{rf} and the transmission line voltage V is through $V = F_{\text{rf}} A_c^{1/2}$. Here A_c is the area of surface that perpendicular to incident wave, which is πa^2 for the cylindrical DLA structure of radius a .

C.1 Review on Transmission Line Model

Figure C.1: Transmission line model (a) without or (b) and (c) with multipactor discharge.