Modeling of microstructure evolution during cold wire drawing process and properties determination

Rengarajan Karthic Narayanan

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Modeling of Microstructure Evolution During Cold Wire Drawing Process and Properties Determination

Rengarajan Karthic Narayanan

School of Mechanical and Aerospace Engineering

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Abstract

Wire drawing is the most widely employed process for manufacturing the micrometer sized gold wire ($\phi 10 - \phi 50 \mu m$) used for electronic interconnects. Currently, gold wire is applied in the bonding pad and miniaturization has resulted in need of higher quality of wire; wire quality is dependent on mechanical properties. The mechanical properties are based on microstructural behavior.

This thesis deals with constitutive modeling and development of a computational framework for the simulation of micromechanical and microstructural behavior of polycrystalline face centered cubic metal such as copper and gold. This is applied to simulate the cold wire drawing and wire bonding processes. Of particular interest are two important phenomena: texture evolution and bond pad cratering. To model the constitutive behavior, a rate independent crystal plasticity with finite strain is implemented as a user routine in commercial finite element (FE) package ABAQUS. An enhanced algorithm has been implemented that takes into account active crystallographic slip and orientation effects to improve the quality of predicted textures. This framework is used to study the micromechanical behavior of copper wire when subjected to drawing and bond pad cratering.

Initially, cold drawing process is simulated according to industrial process conditions based on a J_2 plasticity theory. The material under consideration is gold wire. The residual stresses on the transverse cross section of the cold drawn gold wire is studied to analyse the strain inhomogeneity which gives an approximate measure of the anisotropic properties in the wire. Micro indentation simulations are then conducted on the drawn wire at different positions across the transverse

cross section to understand the mechanical response due to cold work. The deformation characteristics of the wire are thus studied in detail using this finite model. The simulation results are compared with those from experiments to ascertain the trend of strain localization. This paved the way for modeling the microstructural and micromechanical behavior using a crystal plasticity finite element frame work. Due to the rising cost of gold wire and considering the volume used in wire bonding industry, attention has turned towards low cost copper as an alternative. The mechanical and electrical properties of copper are found to be superior compared to gold, which is also a major factor in this change.

The wire drawing of copper using the rate independent crystal plasticity finite element (CPFE) is thus also of interest in this thesis. The anisotropy of the copper single crystals with respect to crystallographic orientations are understood using nanoindentation finite element simulations. Then, the texture evolution of the drawn polycrystalline copper wire is studied in detail. The experimental texture evolution of the wire after drawing is compared with the simulated results. The enhanced model in this work is shown to improve texture predictions.

An additional point of interest is the application of crystal plasticity finite element model on the bond pad cratering. During the wire bonding process, the free air ball impacts on the soft aluminum metallization pad leading to squeeze out from the pad. The effect of copper free air ball texture during this impact stage on the bond pad is also analysed and explained. The failure of the aluminum pad affects the reliability of the process.

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Contents

Abstract	i
Acknowledgements	iii
List of Tables	ix
List of Figures	x
1 Introduction	1
1.1 Research Background	1
1.2 Crystallographic Texture and its Effects	3
1.3 Modeling Texture and its Evolution	5
1.4 Objectives	6
1.5 Scope	7
1.6 Thesis Outline	8
2 Literature Review	10
2.1 Effect of Process Parameters on Wire Drawing Process	10
2.2 Modeling of wire drawing process using continuum plasticity	19
2.3 Microstructure Modeling	20
2.3.1 Crystal Plasticity Models	22
2.3.1.1 Euler - Bunge angles	27
2.3.1.2 Representation of Texture	28
2.3.1.3 Updating the texture	30

2.4	Summary	30
3	Effect of Cold Work on the Mechanical Response of Drawn Ultra-Fine Gold Wire	32
3.1	Introduction	32
3.2	Numerical Modeling	33
3.2.1	Finite Element Implementation	33
3.2.2	Dimensional analysis for mechanical response	36
3.3	Results and Discussion	39
3.3.1	Validation of the model using slab analysis	39
3.3.2	Effect of area reduction (RA) and die angle (α) on the axial stresses	42
3.3.3	Influence of residual stress on $h_c/h_{\max}$, $(W_t - W_u)/W_t$ and p_m	44
3.4	Summary	49
4	Computational Framework of 3D rate independent crystal plasticity	50
4.1	Kinematics of deformation	50
4.2	Algorithm	53
4.2.1	Constitutive model for copper single crystal	53
5	Indentation Response of Single Crystal Copper Using Rate Independent Crystal Plasticity	62
5.1	Introduction	62
5.2	Finite element simulations	63
5.3	Results and discussion	67
5.3.1	Elastic-plastic contact response	67
5.3.2	Plastic zone size variation beneath the indenter	73
5.4	Summary	77

6	Experimental and Numerical Investigations of the Texture Evolution in Copper Wire Drawing	78
6.1	Introduction	78
6.2	Experimental procedures	79
6.2.1	Materials and methods	79
6.2.2	Mechanical testing	80
6.2.3	Scanning Electron microscopy	80
6.2.4	X-ray diffraction measurement	80
6.2.5	Finite element analysis	81
6.3	Results and discussion	84
6.3.1	Mechanical properties	85
6.3.2	Crystallographic texture	87
6.3.3	Surface texture	94
6.4	Summary	98
7	Effect of free air ball texture on copper bonding using a rate independent crystal plasticity	100
7.1	Introduction	100
7.2	Finite element model development	101
7.3	Results and discussion	103
7.3.1	Flow stress in the free air copper ball	103
7.3.2	Aluminum squeeze in the pad	108
7.4	Summary	110
8	Conclusions and Recommendations	112
8.1	Conclusions	112
8.2	Suggestions for future work	115
	References	117

A	Finite element simulation results of the drawn wire using a stepped die	134
B	Simulations of texture evolution in the drawn wire after coiling-uncoiling	137

List of Tables

2.1	Parameters influencing wire drawing process	16
2.3	As drawn fiber texture of ETP copper wire	17
4.1	Classification of FCC slip systems.	54

List of Figures

1.1	Wire bonding Process	2
1.2	Multiple cracks on the cold drawn wire	3
1.3	Shear stress-strain response for copper single crystals.	4
1.4	Fiber texture effect on mechanical properties of the drawn wire. . .	5
2.1	A typical wire drawing set-up	10
2.2	Drawing load Vs stroke of a low carbon iron wire	11
2.3	A schematic of wire drawing process	11
2.4	Normalised drawing stress with die angle and area reductions	12
2.5	Drawing stresses of copper wires tested slowly	13
2.6	Variation of drawing stress with die angles	14
2.7	Central burst zone in a drawn wire	15
2.8	Fracture observed in the wire	16
2.9	Tungsten wire uniaxial tests	18
2.10	Comparison between slab, FEM and upper bound method Vs ex- perimental drawing stress values	20
2.11	Modern finite element approaches for realistic metal-forming simu- lation	22
2.12	Single crystal subjected to tensile stress in x direction	23
2.13	Single crystal shear stress - strain response showing three stages of hardening	25
2.14	Stress - Strain curve from latent hardening experiment on virgin copper crystals	26

2.15	Euler Bunge angles	28
2.16	Pole figure representation	29
3.1	Power law fit to the stress-strain of gold wire at room temperature.	35
3.2	Finite element modeling procedure.	35
3.3	a. Spherical indentation Schematic and b. definition of irreversible work ($W_t - W_u$) and reversible work (W_u).	38
3.4	Variation of normalised drawing stress with area reduction	40
3.5	Equivalent plastic strain (PEEQ) obtained at the end of drawing step from FEM.	41
3.6	Axial residual stress (σ_{22}) distribution on drawn wire for area reductions (RA) a. 10%, b. 20% and c. 30%.	43
3.7	Equivalent plastic strain (PEEQ) during indentation loading and unloading to map the pile up.	45
3.8	Influence of residual stress on $h_c/h_{\max}$ (pile-up) Vs $h_{\max}/R$ (indentation depth)	48
4.1	Kinematics of deformation in crystalline material	51
4.2	Stereographic projection from [100] orientation showing the 24 standard triangles for FCC single crystal.	54
4.3	Shear stress - strain response of Cu (111)plane.	58
4.4	Flow chart of crystal plasticity model with finite element method implemented in ABAQUS.	61
5.1	Finite element discretization of the computational domain	66
5.2	Load displacement curves of single crystal copper in three crystallographic orientations.	70
5.3	Variation of mean effective pressure p_m as a function of geometric strain a/R	72
5.4	Shear stress and strain distribution in the copper single crystal in three different orientations	74

5.5	Pile up profile on single crystal copper	76
6.1	Finite element schematic of wire drawing process.	83
6.2	Initial texture of as recieved copper wire	83
6.3	Comparison of stress-strain curve in tension using 568 unweighted grain orientations with experimental measurements.	84
6.4	Mechanical properties of the wire.	86
6.5	Fracture micrographs of the wire specimen after the tensile test . .	87
6.6	Texture of drawn wire - single step	90
6.7	Texture of drawn wire - Intermediate step	90
6.8	Texture of drawn wire - Multiple step	90
6.9	ODFs ($\varphi_2 = 45^\circ$) for $\langle 111 \rangle + \langle 100 \rangle$ fiber texture components of the wires.	93
6.10	Inverse pole figures of drawn wire surface texture	97
6.11	Volume fraction for complex texture components	98
7.1	Cratering during copper wire bonding	101
7.2	Crystal plasticity finite element model of the impact stage	103
7.3	Flow stress in the free air ball with different crystallographic texture	106
7.4	Accumulated plastic slip of the FAB with different crystallographic texture	108
7.5	axial stress σ_{22} in the pad during the cratering with different free air ball texture	110
7.6	Aluminum pad squeeze	110
A.1	Skin pass die geometry.	134
A.2	Axial residual stress distribution on drawn wire for area reductions (RA) a. 10%, b. 20% and c. 30%	135
A.3	Influence of residual stress on a. $h_c/h_{\max}$ (pile-up) versus $h_{\max}/R$ (indentation depth) , b. $(W_t - W_u)/W_t$ versus $h_f/h_{\max}$ (elastic recovery parameter) and c. p_m/Y versus $E_e a/YR$	136

B.1	Texture evolution of the wire after coiling - uncoiling simulations.	138
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Nomenclature

α die angle

$\dot{\varepsilon}$ Strain rate tensor

λ Angle between the loading axis and slip direction

μ coefficient of friction

ϕ Angle between the loading axis and slip plane
normal direction

σ_d Drawing stress

τ Resolved shear stress

τ_c Critical resolved shear stress

$\Delta\sigma$ External stress increment

ε^p Plastic strain

ε^e Elastic strain component

ϑ_f Drawing velocity

E^e Fourth order elastic modulus tensor

F Total deformation gradient tensor

F^e Elastic deformation gradient tensor

F^p Plastic deformation gradient tensor

I Identity tensor

L Velocity gradient tensor

L^e Elastic velocity gradient tensor

L^p Plastic velocity gradient tensor

m Slip plane normal direction

m_x Schmid factor

P^α Symmetric space

R_f Final radius

R_i Initial radius

s Slip plane direction

W Spin tensor

K Strength coefficient

n Strain hardening exponent

a Contact radius

E_e Effective modulus

ETP Electrolytic tough pitch

F_l Indentation force

F_u Unloading force

FAB Free air ball

h_c Material pile-up

h_{max} Maximum indentation depth

IPF Inverse pole figure

ODF Orientation distribution function

p_m Mean contact pressure

RA Area reduction

SFE Stacking fault energy

T_m melting temperature

W_t Total work

W_u Reversible work

Chapter 1

Introduction

This chapter explains the motivation, objectives and thesis outline of this Ph.D research.

1.1 Research Background

Packaging of electronic circuits is the science and the art of establishing interconnections and a suitable operating environment for predominantly electrical circuits to process or store information. Since its first demonstration in 1957, wire bonding has been the major process used for making these interconnections [1]. This is due to the semiconductor industry's drive to lower the cost of the packaging without any loss in quality and reliability [2, 3]. The cost is much lower compared to wafer-level packaging, tape automated bonding and flip-chip, which are also widely used [4, 5]. The bonding wire forms the electrical interconnection between the die (semiconductor chip) and the lead-frame (chip package) as schematically shown in Figure 1.1. Problems associated with wire bond failures contribute to about 26% of overall failures in IC packages, making them the biggest source of IC package failure [6]. The wire bonding technology has many challenges to address such as rise in cost, decrease in bond pad pitch and reliability of the process [7–9].

Figure 1.1: Wire bonding Process [1]

Rapid development in the electronic packaging industry in the recent years has begun to witness the evolution of high power density and smaller size circuits. As the device dimensions are shrinking, the integrated chip has become smaller and its contact-pads are becoming closely spaced [10]. This fine-pitch necessitates the use of smaller diameter wires (few hundreds of micrometers or less) to provide the interconnects and this imposes a constraint on the mechanical properties of the micrometer diameter sized bonding wires [11]. There is particularly a need for improved mechanical properties and geometrical tolerances. For fine pitch packaging applications, low wire loops that do not sag and long span wires that do not sway are required [12]. Hence understanding the mechanical property of the wire becomes important for achieving a reliable bonding process.

Multi pass cold drawing is commonly used in the wire bonding industry to manufacture micrometer sized wires from cast bars. The manufacturing of these polycrystalline wires, requires an understanding of the role of deformation induced anisotropy on the plastic flow behavior of the material. Also, understanding the effect of the process parameters on the properties of the cold drawn wire will help in achieving improved process control. Cold drawing involves plastic cold working in which material undergoes large plastic deformation at temperatures

less than $0.3T_m$ (absolute melting temperature) in several stages with intermittent annealing steps to reduce the effect of material strain hardening. During this severe deformation process several defects such as cracks and inhomogeneous stress distributions can occur as shown in Figure 1.2 [13, 14]. The strain hardening also induces residual stresses in the multi drawn wire cross section that has a detrimental effect on the durability of the wire [15, 16]. Both stress inhomogeneity and residual stresses influence the mechanical properties and micro structures of the deformed materials [17, 18]. Stress inhomogeneity is strongly affected by the cold drawing process parameters such as die angle, coefficient of friction and area reduction (RA). This material inhomogeneity cannot be explained by investigating the mechanical properties at the macro scale. Understanding the material behavior at the microstructure level is essential to study the anisotropic properties of the wire.

Figure 1.2: Multiple cracks on the cold drawn wire [14].

1.2 Crystallographic Texture and its Effects

In face centered cubic materials (FCC) such as silver, gold, copper and brass, mechanical deformation as during rolling, drawing or extrusion leads to grains rotation towards a preferential orientation resulting in deformation induced crystallographic texture. Such texture studies [19–22] have revealed orientation dependent mechanical properties as shown in Figure 1.3.

Figure 1.3: Shear stress-strain response for copper single crystals of various orientations. The orientations are shown as an Inverse pole figure (IPF) map in the inset [23].

In polycrystalline materials, the crystallographic orientations of individual grains thus play an important role in the plasticity of the material [24, 25]. Anisotropic response associated with nanoindentation of various single crystals in different crystallographic orientations has been reported recently and are being studied widely [26, 27]. Kiely and Houston [28] report nanoindentation studies on single crystal gold (Au). Different crystallographic orientations were investigated to analyse the effect of anisotropy. Their results showed differences in indentation behavior on different crystallographic planes. Thus, anisotropy is seen to affect the mechanical properties. The quantitative characterization of the texture is hence critically important as textures induced by the forming operations involving mechanical deformation affect the quality of wire formed.

The microstructure and anisotropy of drawn polycrystalline electrolytic tough pitch (ETP) copper wire was investigated by Krishna Rajan and Ronald Petkie [29]. The texture of Cu wire had a mixture of $\langle 111 \rangle$ and $\langle 100 \rangle$ fiber components parallel to wire axis. The ratio of $\langle 111 \rangle$ to $\langle 100 \rangle$ with varying drawing strain

have been reported by Inakazu *et al* [30] where the fiber texture formation and the mechanical properties were analysed. The effect of stacking fault energy of FCC materials on the crystallographic texture was measured by English and Chin [31]. The results showed that, low stacking fault energy material such as silver had $\sim 90\%$ $\langle 100 \rangle$ fiber texture. In this context, Stout *et al* [32] observed that the initial texture strongly influences the final outcome. In copper and copper alloys, the intensity of $\langle 100 \rangle$ fiber texture decreases with increasing strain as reported by Hibbard [33]. The results showed that $\langle 111 \rangle$ is a dominating texture in FCC materials [34]. The fiber texture effect on the mechanical properties of the drawn wire is shown in Figure 1.4.

Figure 1.4: Fiber texture effect on mechanical properties of the drawn wire subjected to varying strain [35].

1.3 Modeling Texture and its Evolution

The experimental texture studies which revealed inhomogeneity of the microstructure based on drawing strain paved the way for modeling the same using crystal plasticity based models. Crystal plasticity is a method developed to study material's heterogeneous plastic deformation based on modeling plastic slip on different slip systems within the crystal. This idea originated from the pioneering work of Taylor and his co-workers [36–40]. The method of crystal plasticity works well

for solving problems of heterogeneous mechanical behavior, and was extensively developed to study heterogeneous plastic deformation, lattice rotation and texture evolution when metals are subjected to large deformation, or to solve related practical problems seen in manufacturing processes like metal rolling and forming [41, 42].

Cold drawn gold bonding wire was studied by Cho *et al* [35]. In this study, the drawn wire texture was experimentally studied and compared with a simulation using a rate dependent crystal plasticity material model *i.e. all slip systems (both active and inactive)* always slip at a rate which depends on the current stress state and slip system deformation resistance. The slip occurs based on only the shear stress component of the slip system. The interaction of dislocations was also neglected. In another study, Mathur and Dawson [43] investigated the surface textures of the wire using a rate dependent crystal plasticity model. Complex textures were not effectively accounted in their modeling.

The grain orientation depicts the characteristic anisotropic feature of a material. Mechanical properties are estimated based on this anisotropic response. The anisotropic texture is based on the cumulative plastic shear strain, which is obtained from selective active slip systems. Thus, plastic deformation is largely heterogeneous for polycrystals. Therefore, it is worthwhile to study the deformation process using a rate independent crystal plasticity where only active slip systems are selected for the plastic flow in different crystallographic grain orientations. The multiplane yield condition is assumed and interaction between slip systems is accounted in the analysis.

1.4 Objectives

The major objectives of the current dissertation are as follows:

1. To understand the material texture and thereby mechanical properties of cold drawn micrometer sized gold/copper wire used in interconnects. The drawing

process parameters is also understood based on the texture evolution.

2. The bonding process experiments involving free air ball (FAB) is also studied and analysed based on the effect of texture.

1.5 Scope

1. Simulate wire drawing deformation process to analyze the effect of area reduction (RA), die angle ' α ' and coefficient of friction ' μ ' at the interface of the die - work piece. Axial residual stresses from the drawing are investigated to study deformation behavior and strain variations. Use simulated indentation tests to study hardness variation based on axial residual stress across the transverse cross section of a drawn wire. Macro-mechanical properties of the wire is understood. Texture or grain orientation based modeling is developed to understand the anisotropy and thereby microstructure of the drawing process.
2. Develop a rate independent crystal plasticity model with finite strain and its implementation as a user routine in commercial finite element package ABAQUS.
3. Predict the tensile and nanoindentation response of single crystal copper to understand the anisotropy effect of different crystallographic orientations. This forms the basis for validating the crystal plasticity model.
4. Apply the texture based model to study drawn polycrystalline wires. Simulate both single step and multiple step drawing process based on the rate independent crystal plasticity model to understand the complex texture evolution. Surface textures are also investigated and analysed.
5. The effect of free air ball crystallographic texture during the bond pad cratering is further investigated.

1.6 Thesis Outline

Chapter 2 provides an overview of pertinent literature available in this area. The theoretical and finite element modeling approaches along with experimental works reported on the wire drawing process are described. The need for the microstructure sensitive design and crystal plasticity modeling framework is reviewed.

In Chapter 3, finite element (FE) simulations of wire drawing are performed with process parameters similar to practical industry conditions, for analyzing the residual stress in the transverse cross section of cold multistage drawn wire. The process parameters varying the die angles ' α ', coefficient of friction ' μ ' at the interface of the die - work piece and area reduction (RA) are analyzed. Single as well as multi stage (two stage) drawing process is simulated varying the process parameters and the post drawn wire is analyzed for mechanical response by simulated indentation tests. This paved the way for modeling the wire based on texture based models

Chapter 4 presents a rate independent crystal plasticity finite element framework adopted for development of a three dimensional (3D) CPFE model in this work. A time integration scheme for implementing the model in the commercially available FEM package ABAQUS is also presented.

The developed CPFE framework is implemented to study the nanoindentation response of single crystal copper in various crystallographic orientations to ascertain the effect of texture. The anisotropic response of the single crystal is analysed, based on the heterogeneous plastic deformation, observed from the load-displacement curves, mean pressure and pile up which is explained in Chapter 5.

The study of microstructure evolution on drawn polycrystalline copper wires using the rate independent crystal plasticity finite element framework is explained in Chapter 6. The fiber texture evolution and complex surface texture of the drawn wire by two different schemes are analysed during the manufacturing.

Chapter 7 presents the effect of free air ball texture on the soft aluminum

metallization pad during the impact stage of the copper bonding process. The flow stress of the ball is analyzed based on the crystallographic texture.

Chapter 8 draws conclusions from this research study. The limitations of this study has been highlighted which forms the basis of future work.

Chapter 2

Literature Review

2.1 Effect of Process Parameters on Wire Drawing Process

Wire drawing is one of the most commonly used processes for obtaining metallic rods and wires used in mechanical applications such as: riveting, joining, welding, wire bonding etc [44–47]. The process is to be designed such that a wire drawing machine (consisting of the a several tandem dies, wire feeding mechanism and other controls) as shown in Figure 2.1 should consume as little power as possible and at the same time provide wire of desired quality with good surface finish and minimal residual stress effects. A load versus stroke diagram of a low carbon iron wire drawing process reported by Avitzur [48] is shown in Figure 2.2. Wire drawing through one of the tandem conical converging dies is shown in Figure 2.3.

Figure 2.1: A typical wire drawing set-up

Figure 2.2: Drawing load Vs stroke of a low carbon iron wire [48].

Figure 2.3: A schematic of wire drawing process[48]

Designing the wire drawing processes means understanding the effects of and optimising a number of process parameters to be controlled [49, 50], in order to

obtain the correct plastic strain and tolerance values required for the wire. Experimental studies have been reported to analyze the effect of process parameters such as die angle α , coefficient of friction μ at the interface of the die - work piece and area reduction (RA) on the deformation behavior of the wire [48]. A classic study of the wire drawing process was reported by Wistreich in 1955 [51]; many literature reports often refer to this classic work due to Wistreich's detailed experiments undertaken with precision. The wires considered for this experiments were thin copper wires, less than 0.5 mm in diameter. Drawing stress σ_d with die angle α is plotted in Figure 2.4a for various reductions in area (RA).

The total drawing force was also reported by Wistreich for die angles equal to: 2.29° , 8.02° and 15.47° . These experimental results are shown in Figure 2.4b together with the theory. The wire was reduced from initial radius $R_i = 1.35$ mm to a final radius of $R_f = 1.27$ mm at a speed of $v_f = 33$ mm/sec.

Figure 2.4: Normalised drawing stress with die angle and area reductions (symbols — experimental data, solid line — theory) [51].

The effect of process parameters on the drawing experiments was also investigated by Cristescu [52, 53] for copper wires of diameter $2R_i = 0.94$ mm and steel

wires of $2R_i = 1.02$ mm, tested slowly. The drawing stress increase with reduction and become large for very thin wires as seen in Figure 2.5. Another comparison of the drawing force with respect to die angles was recently reported by Vega *et al* [54]. They also concluded that, drawing force increase with reduction in area. These studies describe the correlations between drawing stresses σ_d developed in the wire and the main influencing drawing parameters, especially the drawing die angle and reduction in area.

Figure 2.5: Drawing stresses of copper wires (symbols — experimental data, solid line — theory) [52, 53].

Avitzur [48] conducted studies to optimise the die angle during wire drawing experiments through a conical die. A range of cone angles were analysed in his study and it was concluded that lower die angles consume less energy and produce high quality wires. The drawing stress with respect to effect of die angle is shown in Figure 2.6. Therefore, it is evident that the effect of process parameters is very important to understand.

Figure 2.6: Variation of drawing stress with die angles [55].

Process parameters also have an effect on drawn wire materials properties *i.e.* strength, yield stress, ductility, ductile–brittle transition temperature, microstructure and fracture behavior. Experimental studies have shown that, various types of fracture such as ductile fracture, transgranular or cleavage fracture and intergranular fractures occur mainly due to drawing process variations [48, 56]. The three zones of deformation in a wire during a drawing process is shown in Figure 2.7. A critical zone where central bursts occurs in the wire is noted.

Figure 2.7: Central burst zone in a drawn wire [48].

During the drawing process, the wire undergoes severe plastic deformation that significantly changes its microstructure. The residual stress induced in the wire during the cold drawing process leads to its breakage or fracture as shown in Figure 2.8. Residual stresses in the wire have been studied using X-ray and neutron diffraction techniques by Phellipeau *et al* [46]. The heterogeneous plastic strain distribution at the microstructural level produces local high stress concentrations that might explain the tendency of wires to develop longitudinal intergranular cracks. Therefore, stress localization at grain boundaries and residual stresses are of utmost high importance. This is, by far, the least understood fracture

mechanism that occurs during the cold drawing of wires. The process parameters influencing wire and its material properties after drawing are listed in Table 2.1.

Figure 2.8: Central bursting type of fracture observed in the wire [57].

Table 2.1: Process parameters influencing wire drawing [14].

Machine type	Tools	Process	Material properties
Single Pass	Type of dies	Wire temperature	Yield strength
Duplex /triple	Cemented carbides	Drawing speed	Ultimate tensile strength
Multiple	Single crystalline diamond	Reduction in area per pass	Fracture strength
	Poly crystalline diamond	True strain of drawing	Fracture toughness
	Geometry of dies	Drawing stress	Elongation /ductility
	Entrance angle	Back pull stress	Ductile–brittle transition
	Bearing length	Friction stress	Temperature (DBTT)
	Transition angles	Inter-mediate anneals	Polygonization temperature
	Polish	Die temperature	Texture
	Drawing drum	Die series	Residual stresses
	Lubrication		Stress gradients, Microstructure

Microstructural behavior on drawn wire based on texture, anisotropy etc.. have recently attracted keen attention. ETP copper wires are widely used as motor coil

windings and low spring back for optimum motor performance is desired. High elastic modulus and low yield strength are needed in the application to achieve good retention when coiled. ETP copper wires produced by cold drawing were investigated for texture evolution by Kraft *et al* [58]. Inherent anisotropy of copper was studied based on drawing die angles. Their results showed that a die angle of 8° produces less complex textures compared to 16° and 24° . The volume fraction reported from their study is shown in Table 2.3.

Table 2.3: As drawn fiber texture of ETP copper wire [58].

Die angle, α	Volume fraction		
	(111)	(200)	random
8°	0.41	0.19	0.39
16°	0.34	0.22	0.44
24°	0.20	0.15	0.65

Tungsten wires used in bulb filaments produced by successive drawing stages was investigated by Ripoll *et al* [59, 60]. The results show that, wires develop a strong (011) fiber texture during this plastic deformation and the grains exhibit curling. This phenomenon affects the hardening of the wire in the macroscopic level thereby leading to tension-compression asymmetry as shown in Figure 2.9. The wire split phenomenon that occurs in tungsten was studied based on this.

Figure 2.9: Tungsten wire uniaxial tests a. Tension and b. Compression [59].

Drawing of eutectoid steel wires were studied by Yang *et al* [61]. The fiber texture evolution based on the plastic deformation was analysed to understand the fatigue and fracture behavior. Wires of gold and copper produced by forward and reverse drawing was investigated by Cho *et al* [25] based on cumulative strain. Their results showed decrease in complex textures of the wire. The mechanical properties based on this texture patterns showed a distinct variation. Park *et al* [62, 63] have investigated the effect of drawing pass on the copper wire texture. Their results showed that, in axisymmetrically deformed FCC materials, the local circular texture develops due to the effect of transverse shear strain. Circular texture components such as $\{112\} \langle 111 \rangle$, $\{111\} \langle 112 \rangle$ and $\{110\} \langle 001 \rangle$ have been observed in the drawn wire periphery where deformation compared to plastic extension, shear dominates.

Hence, the optimization of drawing process parameters for quality wires requires the knowledge of material behavior at the microstructural level. Predicting the parameters effect on the material behavior would be useful and is addressed next.

2.2 Modeling of wire drawing process using continuum plasticity

Analytical methods such as: homogeneous deformation method, slab method (SM), upper bound method (UM) and numerical method such as finite element method (FEM) can be used to calculate wire drawing force. The advantages and disadvantages of each method have been reported in the literature [64, 65]. The homogeneous deformation method is the simplest one, but it has several drawbacks. It considers material receiving the same amount of energy per unit of volume and neither friction, nor the distortion energy is taken into account. The slab method considers friction, does not take into account distortion energy. The slip line field method can only be used for plane strain problems with rigid constitutive plastic behavior. Another method which improves the previous methods is the upper bound analysis. However, it is difficult to consider strain hardening using this formulation. Numerical methods such as the finite element is not only one of the popular methods but the dominating method for metal forming simulations, because it is able to accurately predict deformation and stress values. An analytical expression however for the parameters studied is not possible, which is the main disadvantage. The normalised drawing stress obtained for area reduction of 35% for die angles 12° , 14° , 16° and 18° is compared with experimental results in Figure 2.10. As can be observed, the upper bound method and the FEM results provide similar trend as that of experiments [66], whereas the slab method does not. On the other hand, the upper bound method provide stress values greater than FEM, but both of them show similar trends, that is, the drawing stress increases when the angle of the die is increased. The effect of process parameters on a macroscale plastic deformation can be reasonably studied by these types of modeling. However, these methods are not able to model anisotropic plastic behavior observed in experiments, particularly effect of texture, stress gradients and microstructure.

Figure 2.10: Comparison between slab, FEM and upper bound method Vs experimental drawing stress values [67].

2.3 Microstructure Modeling

Most materials used in engineering applications are polycrystalline in nature. Their properties depend not only on the properties of the individual crystals but also on parameters, like the crystallographic orientation, that characterize the polycrystal. During a deformation process, crystallographic slip and reorientation of crystals (lattice rotation) can be assumed to be the primary mechanisms of plastic deformation in a limited regime of processing conditions. These occur in an ordered manner so that a preferential orientation or texture develops [68]. The developed texture characterizes the mechanical, optical and magnetic behavior of the material. For example, earring during deep drawing of cups/cans along with variations in thickness of the cups/cans is attributed to anisotropy [69]. Anisotropy has many advantages, as preferred textures block the crack propagation or properties such as magnetic/optical can be enhanced in specific directions. The vastness of fields wherein texture affects properties makes it an interesting, challenging and industrially important problem [70, 71]. The development of this field is greatly indebted to

H.J.Bunge [70]. This development led to an exciting new concept focused on micro structural sensitive design combining texture effects with crystal plasticity based finite element modeling (FEM) pioneered by Kalidindi *et al* [72–75]. Anisotropy is observed as a common phenomena in metal forming which decides the properties of a final product [68]. Anisotropy can be taken advantage of, therefore it makes sense to control and design the texture of the material in various metal forming process to meet with the design needs.

The current practice in engineering design does not pay adequate attention to the internal structure of the material as a continuous design variable. The design effort is often focused on the optimization of the geometric parameters using robust numerical simulations tools, while material selection is typically relegated to a relatively small database. Furthermore, material properties are usually assumed to be isotropic, and this significantly reduces the design space. Since the majority of commercially available metals used in structural applications are polycrystalline and often possess a non-random distribution of crystal lattice orientations (as a consequence of complex thermo-mechanical loading history experienced in their manufacture), they are expected to exhibit anisotropic properties [76]. Texture analysis on materials has found a great impact in recent times [77–81]. Many examples exist of materials engineered to have a specific texture in order to optimize performance *e.g. single crystal turbine blades, transformer steel, magnetic thin films etc.* The control of texture is achievable through control of processing which plays an important role in the microstructure but many challenges remain. In metal forming, process plays an important role on the final texture which decides the properties. In this microstructure sensitive design (MSD) rigorous mathematical framework has been developed to facilitate the consideration of microstructure as a continuous variable in engineering design and optimization. The application of MSD in a FEM environment is described in Figure 2.11

Figure 2.11: Modern finite element approaches for realistic metal-forming simulation typically require input data about strain hardening, forming limits, and anisotropy [82].

2.3.1 Crystal Plasticity Models

The initial framework for single crystal deformation was put forward by Schmid [83], which formed the basis for all polycrystalline plasticity models. The deformation of the single crystal is shown in Figure 2.12. When a crystal is stressed, slip starts, when the shear stress on the slip systems reaches its critical value τ_c also called as critical resolved shear stress. Plastic deformation occurs when there are slips on certain active crystallographic planes in specific crystallographic directions lying in the plane. Crystallographic planes are those planes with closest atomic packing and the crystallographic directions are the closest packed directions on the slip planes. Generally, in face centered cubic (FCC) crystal, there are four (4) slip planes and each slip plane has three (3) slip directions. The combination of any of the slip planes and any one of the slip directions lying in that plane constitute a slip system. Thus, there are twelve possible slip systems for a FCC crystal.

In most of the crystals, slip can occur with equal ease in forward and backward direction. Mathematically, the condition for slip in terms of critically resolved shear stress is represented as

$$\tau = \pm \tau_c \quad (2.1)$$

where, τ is the resolved shear stress on slip plane with normal direction m and slip direction s . For a uniaxial tension along the x direction, the resolved shear stress can be expressed as

$$\tau = \sigma_{xx} \cos \phi \cos \lambda = \sigma_{xx} l_{mx} l_{sx} = \sigma_{xx} m_x \quad (2.2)$$

where, σ_{xx} is the tensile stress in x direction, λ is the angle between the loading axis and the slip direction and ϕ is the angle between the loading axis and slip plane normal direction. Here, l_{mx} and l_{sx} are the direction cosines of the slip plane normal direction m and slip direction s with respect to the loading axis and m_x is called as the Schmid factor.

Figure 2.12: Single crystal subjected to tensile stress in x direction [83].

Based on Schmid's formulation, Taylor and Elam [36] and Taylor [37, 38, 40] formulated crystallographic slip based on plastic deformation. The modern continuum mechanics framework of constitutive equations for elastoplastic behavior of single crystal material was derived by Mandel [84] and Hill [85, 86] and later extended to the finite strain formulation, by Pierce and Asaro [41, 42]. The finite strain crystal plasticity accounts crystal structure, mechanism of plastic slip, theory of dislocation and finite strain kinematics and constitutive behavior.

The crystal plasticity formulations have been divided in to rate independent and rate dependent schemes. The pioneering work of Mandel [84] assumed a rate independent crystal plasticity framework to model the elastoplastic behavior at low temperatures. The dislocation motions which leads to hardening are modeled based on critical shear stress of the slip system as given by Schmid's law. In general, for any shape change there is multiple slip *i.e.* more than one slip systems are active during plastic deformation. Due to the accumulation of dislocations, two kinds of hardening takes place. Work hardening of the active slip system due to the slips on the same slip system is called as self hardening. Hardening of slip systems due to the slips on the other slip systems, no matter whether they themselves are active or not, is called latent hardening. The objective of the time independent scheme was to predict the unique active slip systems, which these modeling approaches could not satisfy. Due to this discrepancy in modeling, Asaro and Needleman [87] proposed a classical rate dependent theory where all slip systems are always active and slip at a rate which depends on the resolved shear stress and slip system deformation resistance. No yield surface was defined. The constitutive laws proposed, could not predict stage I to stage II transition in hardening as shown in Figure 2.13. The orientation dependence on single crystal stress-strain response was ignored. Busso *et al* [88] have compared rate dependent and rate independent models. The uniqueness of selecting active slip systems was discussed under complex loading conditions. Kumar *et al* [89] proposed a stack model for rate independent polycrystals and compared with the Taylor model.

Figure 2.13: Single crystal shear stress - strain response showing three stages of hardening [90].

Wu *et al* [90] put forth a model to capture the self and latent hardening using the rate independent frame work. Their experimental work on virgin crystals of copper showed the latent hardening due to interaction of single slip orientations as seen in Figure 2.14.

Figure 2.14: Shear stress (τ) - strain (γ) curve from latent hardening experiment on virgin copper crystals [90]. l / W represents length to width ratio and P_1 , P_2 represents test samples.

Based on this Anand *et al* [91] and Miehe *et al* [92] have formulated algorithms using the crystal plasticity frame work. Anand *et al* [91] have observed that, the hardening is the least well characterised in the constitutive equations of the crystal elasto-plasticity implemented in a rate dependent framework. The stage I and II hardening were captured effectively in their approach. Stage I depends on the initial orientation of the crystal and it is also called as an easy glide stage whereas stage II is very critical as dislocations starts to pile up and a steep hardening curve is observed. The solution approach for yield functions proposed have been solved by Schroder *et al* [93], which is employed in this study.

Recent research on crystal plasticity modeling pertinent to wire drawing highlights the limitations of the rate dependent models. Rate dependent crystal plasticity model by Ocenasek *et al* [94] was applied on tungsten wire drawing process to predict the texture evolution. The finite element modeling assumed cubic grain structure with ten random grains in an unit cell and ideal drawing conditions were applied. Ripoll and Ocenasek [60] implemented viscoplastic self consistent model assuming large number of grains for the wire drawing process and compared the texture evolution with the crystal plasticity model. A sharp $\langle 011 \rangle$ fiber texture

with curling was reported from their simulations. The complex textures from the heterogeneous plastic deformation of the wire was ignored. The computational framework of the domain restricted them to account for unique active slip systems which was the limitation in their study. Surface texture of the wire was also not analysed. Taylor and Sachs models were applied to study the wire drawing process by Gambin *et al* [95]. The global stress field on all the grains are considered uniform and kinematics of the grain interactions is ignored.

2.3.1.1 Euler - Bunge angles

Generally, in metals, crystals are oriented in random direction. To represent these crystal orientations with respect to a fixed co-ordinate system. Euler angles are used.

The sample reference coordinate system has been denoted by (x^s, y^s, z^s) and the crystal coordinate system as (x^c, y^c, z^c) . One can obtain (x^c, y^c, z^c) from (x^s, y^s, z^s) by three successive rotations. The three angles of rotation are called as Euler angles. These angles are as follows: Initially, consider a coordinate system e_1, e_2, e_3 which is aligned with the sample reference coordinate system. Rotating e_1, e_2, e_3 through an angle φ_1 about e_3 . The new coordinate system is identified as e'_1, e'_2, e'_3 . Rotating e'_1, e'_2, e'_3 through angle Φ about e'_1 . The new coordinate system is e''_1, e''_2, e''_3 . Finally, rotate e''_1, e''_2, e''_3 through an angle φ_2 about e''_3 . The new coordinate system is e'''_1, e'''_2, e'''_3 . The Euler angles $(\varphi_1, \Phi, \varphi_2)$ are chosen such that it matches with crystal coordinate system *i.e.* (x^c, y^c, z^c) . These angles are called Euler-Bunge angles after the representation was identified by H.J.Bunge [70]. Figure 2.15 shows the representation of Euler angles. The total rotation of the crystal co ordinate system with respect to the sample reference coordinate system can be represented by the following matrix as shown in equation (2.3).

$$Q(\varphi_1, \Phi, \varphi_2) = \begin{bmatrix} \cos \varphi_1 \cos \varphi_2 - \sin \varphi_1 \sin \varphi_2 \cos \Phi & -\cos \varphi_1 \sin \varphi_2 - \sin \varphi_1 \cos \varphi_2 \cos \Phi & \sin \varphi_1 \sin \Phi \\ \sin \varphi_1 \cos \varphi_2 + \cos \varphi_1 \sin \varphi_2 \cos \Phi & -\sin \varphi_1 \sin \varphi_2 + \cos \varphi_1 \cos \varphi_2 \cos \Phi & -\cos \varphi_1 \sin \Phi \\ \sin \Phi \sin \varphi_2 & \sin \Phi \cos \varphi_2 & \cos \Phi \end{bmatrix} \quad (2.3)$$

Figure 2.15: Definition of the Euler angles according to the Bunge notations. The set of three Euler angles $(\varphi_1, \Phi, \varphi_2)$ uniquely determines the correspondence between the sample reference (x^s, y^s, z^s) and the crystal reference frame (x^c, y^c, z^c) [70].

2.3.1.2 Representation of Texture

Pole figures are used for representing the orientation of crystals in a 2D plane. These pole figures are constructed based on the stereographic projections of crystal faces. Generally, crystallographic planes are represented by its normal.

The unit cell of a FCC material is a cube. It is common and convenient to represent an orientation of a crystallographic plane by the stereographic projection. The construction of the stereographic projection is shown in Figure 2.16a. The procedure can be explained as:

- The unit cube is located at the origin of the coordinate system and is surrounded by a unit sphere.
- Then, a plane is passed through the center of the sphere which is parallel to the x-y plane. This plane is called as Equatorial plane
- Next, the points of intersection of the normal vectors of the crystallographic planes with the surface of the unit sphere are determined. Only the intersections P_1, P_2, P_3, P_4 on the northern hemisphere are taken into account.
- Next, the intersection points (P_1, P_2, P_3, P_4) are connected to the south pole by 4 lines.
- Finally, the intersection points (P'_1, P'_2, P'_3, P'_4) of these 4 lines with the equatorial plane are obtained. They are called poles of the respective crystallographic planes. A typical pole figure is shown in Figure 2.16b.

Figure 2.16: Pole figure representation [70].

2.3.1.3 Updating the texture [87]

The plastic spin tensor W^p in kinematics of crystal deformation describes the rotation of crystallographic axes with respect to fixed axes. This rotation is different from grain to grain.

The current crystal orientation, $[Q_N]$ is governed by the following relation

$$[\dot{Q}]_N = [W^p] [Q_N] \quad (2.4)$$

For getting the crystal orientation, equation (2.4) is to be integrated over a time increment Δt . This leads to

$$[Q_N] = [Q] \exp([W^p] \Delta t) \quad (2.5)$$

where, $[Q]$ is the initial orientation as given by equation (2.3). Here, it is assumed that the spin tensor $[W^p]$ remains constant during the time increment Δt .

2.4 Summary

1. The wire drawing process is comprehensively reviewed and the effect of process parameters on the drawing process is outlined. The macro plastic deformation of the wire is understood based on the drawing stress. There is a clear variation of drawing stress with respect to die angle and area reduction.
2. The drawing induces residual stresses in the wire, thereby inhomogeneous stress distribution occurs leading to fracture. The local deformation of the drawn wire has been studied for heterogeneous plastic deformation by diffraction measurements.
3. The microstructural properties such as texture and fiber texture evolution are strongly affected by die angles, area reduction and drawing pass.

4. The importance of microstructural sensitive design is emphasized. Microstructural design helps in understanding and optimizing the drawing process parameters for good quality wires with better mechanical properties which is essential.
5. The modern finite element framework which incorporates microstructural properties in the finite element framework is crystal plasticity based modeling, which was discussed. The theory of crystal plasticity from a single crystal to polycrystal established in the literature was analysed.
6. The rate independent and rate dependent models available in the literature are discussed. The importance of hardening in the texture evolution is seen from the models discussed.

Chapter 3

Effect of Cold Work on the Mechanical Response of Drawn Ultra-Fine Gold Wire*

3.1 Introduction

This chapter discusses on the strain inhomogeneity and gives outline of anisotropic properties of wire using indentation simulations conducted on the transverse wire cross section which lays a platform for the need to develop and implement texture based crystal plasticity models for the wire drawing process [58]. The metal forming industry uses effective strains on a formed product to predict the inhomogeneity using hardness values from analytical expressions [15]. However, an indentation test done by simulation can be comprehensive, since it can provide a better understanding of the indentation depth and work of indentation that can be used to analyze the inhomogeneous stress fields. Analysis of this kind has also been found suitable for low strain hardening materials that exhibits significant pile up at the indenter edges [96, 97]. Spherical indentation simulations for residual stress effects is also found to be effective in elastic-plastic transition deformation regimes [98, 99]. In addition, indentation tests have other uses. The mechanical properties of bulk and small volume materials such as Young's modulus (E), hardness, plastic properties measured with instrumented and simulated indentation tests has gained

*Karthic.R.Narayanan, I.Sridhar and S.Subbiah, in Computational Materials Science 49 (2010) S119 – S125

prominence [100–105]. One of the parameters used to detect inhomogeneity in flow stress is hardness variation that gives a direct measure of the material strength. Hardness can be determined indirectly from strains induced in the work material or directly using indentation tests, which can be done via simulations or via experiments. Experimented indentation tests have been conducted on a drawn wire to study the transverse cross sectional strain variations [16].

3.2 Numerical Modeling

3.2.1 Finite Element Implementation

A rigid conical die is used to reduce the cross sectional area of a gold wire 40 μm in diameter and 140 μm long by 10%, 20% and 30% in area using axi-symmetric finite element (FE) drawing simulations. Both single stage and two stage reduction processes are analysed. For the two stage process the area reduction is achieved as follows: 10% by two stages of 5% and 5%, 20% by two stages of 10% and 10%, and 30% in two stages of 20% and 10%. Semi-die angles of 4°, 5° and 6° were simulated. The die angles were kept the same within the two stages of a multi-stage drawing simulation. The coefficient of friction μ between the die and the gold wire was kept constant at a value of 0.05 for all the drawing simulations conducted. The constitutive behavior of the gold wire at the room temperature is obtained from the experimental work of Liu *et al* [1]. The plastic stress - strain behavior of the wire is modeled in the power law form $\sigma = K\varepsilon^n$, where K (291.2 MPa) is the strength coefficient and n (0.0535) is the strain-hardening exponent. Figure 3.1 shows the comparison between the experimentally measured stress - strain response and the fitted power law. The Young's modulus (E) and Poisson's ratio (ν) of the wire are 80 GPa and 0.42 respectively. A finite strain version of the J₂ flow theory is used to simulate the drawing process. The FE simulations are carried out using the commercial software ABAQUS using the explicit formulation. The wire is modeled using axisymmetric boundary conditions such that the wire is allowed to deform

in the axial direction and one end of the wire is fixed as shown in Figure 3.2a. Wire drawing is simulated by moving the die, which is given the drawing speed of 1 mm/sec causing it to traverse the wire from one end to the other.

The wire drawing simulation was conducted as the first analysis step followed by relaxation of the wire from all the external boundary conditions until the wire reaches steady state as shown in Figure 3.2b. The macroscopic stress-strain variations across the wire radial-section and over the longitudinal section were taken after this relaxation step. Therefore, the drawn wire was in a completely external load-free condition and the stresses considered for the microindentation simulation studies were all residual effects. Then, to analyse mechanical property variation across the wire cross-section, frictionless indentations were performed. Frictionless conditions were assumed since experimental evidence concluding no significant effects in spherical indentation is reported in the literature [106, 107]. The indentations are performed with a spherical indenter of $3\mu\text{m}$ radius (R), with the load controlled at a value of $30\text{mN}\pm 1$ was conducted in the next step at three different points (P_1 , P_2 , P_3) across the wire cross-section as shown in Figure 3.2c. Two-dimensional axisymmetric model was used to conduct the indentations at the center (P_1) as shown in Figure 3.2d and three-dimensional wire model was used for the off-center points (P_2 and P_3) as in Figure 3.2e. At a time, only one point on the wire cross section was indented and the simulations utilised adaptive meshing with mass scaling to minimise element distortions and to speed up the simulations respectively. The boundary conditions of the three-dimensional model for all the simulations were same as the two-dimensional axisymmetric model. Owing to the radial symmetry of the spherical indenter, only one quarter of the three-dimensional model was simulated.

Figure 3.1: Power law fit to the stress-strain of gold wire at room temperature.

Figure 3.2: Finite element modeling procedure.

3.2.2 Dimensional analysis for mechanical response

Dimensional analysis based on the energy method proposed by Ni *et al* [108] is used to analyze the indentation response of cold drawn gold wire. During the loading stage the indentation force (F_l) and the total penetration depth by including material pile-up (h_c) as shown in Figure 3.3a are functions of the material properties Young's modulus (E), Poisson's ratio (ν), yield strength (Y), n , indenter displacement (h) and indenter radius (R). Implementing the Π theorem [109] in dimensional analysis yields

$$F_l = ER^2\Pi_\alpha\left(\frac{Y}{E}, \nu, n, \frac{h}{R}\right) \quad (3.1)$$

$$h_c = R\Pi_\beta\left(\frac{Y}{E}, \nu, n, \frac{h}{R}\right) \quad (3.2)$$

where $\Pi_\alpha = F_l/ER^2$ and $\Pi_\beta = h_c/R$ are the non-dimensional load and penetration depth, respectively. The unloading force (F_u), in addition to the above parameters, depends upon the actual indentation depth at maximum load (h_{max}). Applying the Π theorem for unloading stage, we have

$$F_u = ER^2\Pi_\gamma\left(\frac{Y}{E}, \nu, n, \frac{h}{R}, \frac{h_{max}}{R}\right) \quad (3.3)$$

Equations 3.1 and 3.3 can be integrated with respect to the displacement to obtain the total work (W_t) and reversible work (W_u) defined by the areas under the loading and unloading curves as shown in Figure 3.3b. Extensive FE simulations of spherical indentations was conducted on the drawn wire to analyse the residual axial stress effect by relating h_c/h_{max} (pile up or sink in), h_{max}/R (indentation depth) as a function of material properties (Y/E , n and ν). Similarly $(W_t - W_u)/W_t$ and h_f/h_{max} (elastic recovery parameter) were investigated and calculated.

At small indentation depths (where elastic regime prevails) the indentation response is governed by Hertzian elastic behavior and is not effected by the magnitude

of residual stresses. Similarly, at large indentation depths, wherein, the fully-plastic state develops underneath the indenter, the indentation response is governed by the yield strength of the material. In the intermediate regime of indentation depths, the residual stresses control the indentation behavior by the parameters involving effective modulus $E_e = E/(1-\nu^2)$, Y , contact radius (a) $= \sqrt{A/\pi}$, mean contact pressure (p_m) and geometrical strain [110]. The indentation load-displacement curves as well as the contact area A are obtained directly from the FE simulations. The elastic recovery parameter is obtained from the load-displacement curve, and by integrating the area under the simulated loading-unloading curve the total work (W_t) and reversible work (W_u) are calculated.

Figure 3.3: a. Spherical indentation Schematic and b. definition of irreversible work ($W_t - W_u$) and reversible work (W_u).

3.3 Results and Discussion

The drawing stress results and the axial residual stress distribution obtained from the simulations are presented followed by the results obtained from the micro indentation simulations to compare the mechanical response. The indentation simulations were conducted on the relaxed wire transverse cross section.

3.3.1 Validation of the model using slab analysis

In FE simulation, the drawing stress is calculated by dividing the maximum contact force on the reference point of the rigid-die with the wire cross-sectional area. Using upper bound technique such as slab method (SM) [111], the drawing stress σ_d can be expressed as

$$\sigma_d = \bar{\sigma}_y \left(\frac{1+B}{B} \right) (1 - \exp^{-(B\varepsilon_h)}) \quad (3.4)$$

$$B = \mu \cot \alpha \quad (3.5)$$

$$\varepsilon_h = \ln\left(\frac{1}{1-r_a}\right) \quad (3.6)$$

where, $\bar{\sigma}_y$ is the mean yield stress of the gold wire, μ is the coefficient of friction between the die and wire interface, α is die semi angle, ε_h is the homogeneous plastic strain for the imposed reduction ratio r_a . The drawability limit was analyzed by plotting the normalized drawing stress with the area reduction as shown in Figure 3.4. The results indicate that the drawing stress increases with increasing reduction ratio and for a given RA the drawing stress value increases with decreasing die angle. The drawing stresses calculated from the FE are higher than that of the slab method and the difference between them increases with increasing RA. The plastic strain obtained from FEM for each area reduction is shown in Figure 3.5.

It was also noted that for particular area reduction the drawing stress values

was not considerably affected by the die semi-angles as predicted by both FEM and SM. This difference is due to the simplified homogeneous deformation that has been assumed in the slab method: the distortion energy is not considered. The FE method predicted normalised drawing stress values are in close agreement with the experimental investigations conducted on copper wires [54]. The experimental measurements are superimposed with filled markers in Figure 3.4.

Figure 3.4: Variation of normalised drawing stress with area reduction: FE predictions are compared with slab method values and published experiments [54].

(a) Reduction area 10%

(b) Reduction area 20%

(c) Reduction area 30%

Figure 3.5: Equivalent plastic strain (PEEQ) obtained at the end of drawing step from FEM.

3.3.2 Effect of area reduction (RA) and die angle (α) on the axial stresses

The axial stress (σ_{22}) variation across the cross-section of the drawn wire obtained from the FE simulations for different RA and die angle α are shown in Figures 3.6a, 3.6b and 3.6c. The figure shows that the central section remains in compression and the outer section (closer to the surface of the wire) is in tension. The regimes marked as P_1 , P_2 , P_3 in Figure 3.6a indicate the nature of the stress in each region. With increasing RA, the residual compressive stresses increases at the centre of the wire and the residual tensile stresses decreases at the outer edge of the wire, which may be due to the effect of the frictional shear stresses rendering plastic strain homogeneity at higher reduction [112, 16]. For an equivalent area reduction, the single stage drawing process predicted higher compressive stress at the centre of the wire and lower tensile stress at the outer surface of the wire than the multi stage process. The effect of work hardening induced in the first step has an effect on the following step during the multi stage drawing process. By way of an example for 10% reduction ratio, the difference in compressive stress between a single stage and a multi stage is approximately 20% and the tensile stress differed by 18% respectively. The stress variation between the single stage and multi stage drawing process decreases with increasing reduction ratio: in the particular case of 30% reduction the axial stress determined from single stage drawing within numerical scatter matches to that of the multi-stage drawing process. This is due to the strain homogeneity at higher reductions.

The effect of die-angle was found to be insignificant on the drawn wire residual stress distribution obtained from both the single stage as well as multi stage process. Smaller die angles used in the drawing dies have been found to have negligible effect on the residual axial, radial and circumferential stress distribution [112].

(a)

(b)

(c)

Figure 3.6: Axial residual stress (σ_{22}) distribution on drawn wire for area reductions (RA) a. 10%, b. 20% and c. 30%.

3.3.3 Influence of residual stress on $h_c/h_{\max}$, $(W_t - W_u)/W_t$ and p_m

The results from spherical indentation simulations performed at cross sectional points P_1 , P_2 and P_3 were analyzed. Only the area reduction effects were considered for the indentation simulations as it was shown earlier that the narrow die angle variations (*i.e.* 4° to 6°) considered in this study has negligible effect on the residual stress distribution. The plastic strain obtained from FEM simulations during the indentation and unloading is shown in Figure 3.7 to map the pile up. The pile up is evident and the distinct variations in the three area reductions are seen. The influence of residual stresses on $h_c/h_{\max}$ with respect to $h_{\max}/R$ was used to evaluate the degree of pile-up for the single stage and multi stage process as illustrated in Figures 3.8a and 3.8b respectively. The $h_c/h_{\max}$ values as a function of $h_{\max}/R$ are plotted for Y/E and n respectively. It is noted that for materials with small value of Y/E and n , such as the gold material used here, the pile-up is expected at large indentation depths. The variation in $h_c/h_{\max}$ with respect to $h_{\max}/R$ values clearly shows the influence of residual axial stress on the pile up at the different stress regions of compressive (P_1), transition from compression to tension region (P_2) and tensile region (P_3). In the compression region (P_1) low values of $h_c/h_{\max}$ are observed compared to that at points P_2 and P_3 . Higher area reduction (30%) results in higher compressive stress at P_1 and this leads to a lower $h_c/h_{\max}$ value. A small increase in $h_c/h_{\max}$ value is observed when the compressive stresses decrease with lower reduction ratios. In the transition region (P_2) an increase in $h_c/h_{\max}$ compared to P_1 was observed. However, in this region the variation in RA was not significant because the residual axial stresses were close to zero. In the tensile stress region (P_3) higher $h_c/h_{\max}$ values were seen especially at the lowest area reduction of 10% where $h_c/h_{\max}$ was the highest. Similar observations were seen for both single and multiple stage simulations. At all the stress regions lower values of $h_c/h_{\max}$ were observed for single stage drawing compared to multistage drawing. The trends in $h_c/h_{\max}$ can be explained as follows:

indentation in a compressive stress region results in less plastic deformation, while indentation in a tensile stress region produces higher plastic flow. Also, as observed from Figures 3.6a, 3.6b and 3.6c multistage drawing resulted in lower compressive residual stresses and hence higher h_c/h_{max} values.

Figure 3.7: Equivalent plastic strain (PEEQ) during indentation loading and unloading to map the pile up.

The representative load-displacement curve obtained from the finite element

simulations were analyzed to obtain the relationship for $(W_t - W_u)/W_t$ and $h_f/h_{\max}$ as shown in Figures 3.8c and 3.8d. The $(W_t - W_u)/W_t$ versus $h_f/h_{\max}$ values are found to be increasing in the different stress regions of compressive (P_1), transition from compression to tension region (P_2) and tensile region (P_3). The 30% RA at compressive region (P_1) had the lowest $(W_t - W_u)/W_t$ value and the elastic recovery parameter ($h_f/h_{\max}$) at the same location was also observed to be the lowest. This is attributed to the higher compressive residual stresses in these regions which resists the plastic flow. The transition region (P_2) showed an increase in $(W_t - W_u)/W_t$ values compared to the compressive region (P_1) but the effect of area reduction was insignificant as seen during $h_c/h_{\max}$ variations. For the case of 10% RA, in the tensile region (P_3), highest $(W_t - W_u)/W_t$ and highest $h_f/h_{\max}$ values were observed, because of the higher tensile residual stresses. The values found for $(W_t - W_u)/W_t$ versus $h_f/h_{\max}$ from single stage drawing were found to be lower than the multistage process. A similar trend has been observed in these regions during $h_c/h_{\max}$ analysis. As discussed earlier, the reason is due to single stage drawing yielding higher compressive stress at the centre and lower tensile stresses at the edge compared to multistage. The variation of $(W_t - W_u)/W_t$ with respect to $h_f/h_{\max}$ for single stage and multi stage drawing was seen to be linear. In all the indentation simulations, the loading and unloading curve were seen to be almost linear. This linear trend has also been reported in experiments in several different materials [108].

Figures 3.8e and 3.8f show that the variation of normalized mean pressure (p_m/Y) with normalized strain (E_{ea}/YR) is affected by the residual stress variation across the wire cross section. The mean contact pressure p_m for RA 30% at compressive region (P_1) was found to be the highest and for RA 10% at tensile region (P_3) was lowest. The mean contact pressure p_m at the transition region (P_2) was lower compared to the compressive region (P_1) but higher than the tensile region (P_3). Tensile stresses observed at P_3 region are found to reduce the p_m as it promotes yielding and plastic flow by increasing the local mises stress,

whereas the compressive stress observed at P_1 tend to have an opposite effect. Swadener *et al* [98] have carried out spherical indentation tests on prestressed (tensile/compressive) 2024 aluminum substrate. Their measurement of normalised contact pressure at several strain values are superimposed (R_c / R_T) in Figures 3.8e and 3.8f. The measurements compare well with the numerical analysis within the experimental scatter. Also these effect of axial residual stress variation on the mechanical response, observed by the indentation simulations, agrees well with the experimental nano indentation test results on a drawn steel wire as reported [16]. Due to higher compressive stress and lower tensile stress values for single stage, the mean contact pressure (p_m) was found to be higher compared to the multistage.

Figure 3.8: Influence of residual stress on h_c/h_{max} (pile-up) Vs h_{max}/R (indentation depth) a. single stage drawing, b. multi stage drawing, $(W_t - W_u)/W_t$ Vs h_f/h_{max} (elastic recovery parameter) c. single stage drawing, d. multi stage drawing and p_m/Y Vs $E_e a/YR$ e. single stage drawing, f. multi stage drawing.

3.4 Summary

The influence of process parameters in the cold drawn wire for the residual stress effects was investigated and analyzed by finite element simulations. The major conclusions from this work are as summarized below:

1. The residual axial stresses across the transverse section of the drawn wire were beneficially influenced by the area reduction while insignificant change was observed for the range of die angles used for this study. As area reduction increased the compressive stress increased in the centre of the wire while at the outer section the tensile stresses reduced. Single stage drawing of the equivalent area reduction had higher compressive stresses at the center and lower tensile stress at the edge compared to multi stage drawn wire
2. The mechanical response analyzed on the drawn wire cross section showed the influence of residual stresses on the micro hardness variation. The residual axial tensile stresses were found to promote yielding thereby leading to larger penetration depths while the compressive stresses resulted in smaller indentations indicating resistance to yielding which was also reflected in variation of the pile-up, indentation work and mean contact pressure distributions. The elastic recovery parameter h_f/h_{max} increased when the residual stress regions shifted from compression to tension and linear trend was observed between the indentation work and elastic recovery parameter relation. The mean contact pressure on the indenter was higher at compressive stress regions and decreased as it moved to the tensile regions of the drawn wire.
3. Both the single stage and multi stage simulations show the same effect of residual axial stress namely: that at a given indentation load, the total depth of penetration h_{max} is much greater for regions of residual stresses in tension (P_3) as compared to compression (P_1) and near zero residual stress (P_2).

Chapter 4

Computational Framework of 3D rate independent crystal plasticity

The theoretical formulations of Pierce *et al* [41, 42] for the kinematics and constitutive relations of the single crystal plasticity is introduced in this chapter. Hardening evolution equations for the rate independent crystal plasticity method are coupled with the crystal kinematics. The crystal plasticity framework implemented as a user subroutine in commercial FEM package ABAQUS using an explicit time integration procedure is also explained.

4.1 Kinematics of deformation

When a crystal is subjected to stresses, it gets deformed. The whole mechanism of crystal deformation can be divided into parts. Plastic slip occur in specific crystallographic directions on slip planes. since the plastic slips occur in the integral multiples of crystal lattice spacing, crystalline nature of the metal is preserved and the lattice orientation remains unchanged. Apart from the plastic slips mentioned above, the material particles deform elastically without the relative movement between the material properties and the lattice as shown in Figure 4.1. Stretching or shortening, distortion and rigid body rotation are responsible for elastic deformation of the crystal lattice.

Figure 4.1: Kinematics of deformation in crystalline material[68]

In the light of the above mentioned phenomena, during crystal deformation, total deformation gradient tensor F can be decomposed into plastic deformation gradient tensor F^p , corresponding to plastic slips along slip planes of the crystal lattice and elastic deformation gradient tensor F^e corresponding to stretching or shortening, distortion and rigid body rotation. The multiplicative decomposition is:

$$F = F^e F^p \quad (4.1)$$

If L is the velocity gradient tensor, then it is related to the deformation gradient tensor by the relation

$$L = \dot{F} F^{-1} \quad (4.2)$$

substituting for F from equation (4.1) and simplifying equation (4.2) becomes

$$\begin{aligned} L &= \dot{F}^e (F^e)^{-1} + F^e \dot{F}^p (F^p)^{-1} (F^e)^{-1} \\ &= L^e + F^e L^p (F^e)^{-1} \end{aligned} \quad (4.3)$$

where L^e and L^p are the elastic and plastic velocity gradient tensors respectively. The tensor L can also be decomposed into the symmetric and antisymmetric parts as

$$L = \dot{\varepsilon} + W \quad (4.4)$$

where $\dot{\varepsilon}$ and W are called strain rate tensor and spin tensor respectively. Further, both $\dot{\varepsilon}$ and W can be decomposed into the plastic and elastic parts as

$$\dot{\varepsilon} = \dot{\varepsilon}^p + \dot{\varepsilon}^e \quad (4.5)$$

$$W = W^p + W^e \quad (4.6)$$

Elastic deformation is assumed as small and negligible

($F^e \simeq 1$, $L^e \simeq 0$, $\dot{\varepsilon}^e \simeq 0$, $W^e \simeq 0$) compared to the plastic deformation.

Then equations (4.3 - 4.6) reduces to

$$L \simeq L^p = \dot{\varepsilon}^p + W^p \quad (4.7)$$

Plastic slip occurs on the specific crystallographic planes in the specific crystallographic directions. So for a multiple slip, L^p can be expressed as

$$L^p = \sum_{\alpha=1}^N \dot{\gamma}^{(\alpha)} \left(s^{(\alpha)} \otimes m^{(\alpha)} \right) \quad (4.8)$$

where, $s^{(\alpha)}$ and $m^{(\alpha)}$ denote direction cosines of the slip direction and slip plane normal direction respectively of the α slip system of the current crystal orientation.

The quantity $\dot{\gamma}^{(\alpha)}$ denotes the shear strain rate caused by the plastic slip on the α slip system and N is the number of slip systems. Decomposing equation (4.8) into the symmetric and antisymmetric parts, and comparing it with equation (4.7), we get

$$\dot{\varepsilon}^p = \sum_{\alpha=1}^N \frac{1}{2} \left(s^{(\alpha)} \otimes m^{(\alpha)} + m^{(\alpha)} \otimes s^{(\alpha)} \right) \dot{\gamma}^{(\alpha)} \quad (4.9)$$

$$W^p = \sum_{\alpha=1}^N \frac{1}{2} \left(s^{(\alpha)} \otimes m^{(\alpha)} - m^{(\alpha)} \otimes s^{(\alpha)} \right) \dot{\gamma}^{(\alpha)} \quad (4.10)$$

4.2 Algorithm

Kinematics of crystal plasticity deformation is based on finite strain theory of Pierce *et al* [41, 42] as given in the section 4.1. The algorithm of solving crystal plasticity with finite element method and solution approach for the yield function is discussed in this section. The true stress state and update of the solution dependent variables are also solved.

4.2.1 Constitutive model for copper single crystal

The plastic deformation in a face centered cubic (FCC) copper (Cu) crystal considered here is confined to preferred (dense) crystal planes and directions, known as slip systems α . The FCC lattice deforms on the slip systems defined by the $\{1\ 1\ 1\}$ family of slip planes m^α in the $\langle 1\ 1\ 0 \rangle$ family of slip directions s^α . There are twelve combination of slip systems which govern the macroscopic plastic deformation of a FCC single crystal. The slip plane direction and normal for this single crystal are shown in Figure 4.2. A slip system is represented by $[u\ v\ w]\ (h\ k\ l)$ where $[u\ v\ w]$ represents the slip direction and $(h\ k\ l)$ denotes the relevant slip plane. Wu *et al* [90] described the octahedral slip systems in terms of primary, conjugate, cross glide and critical respectively as shown in Table 4.1.

Figure 4.2: Stereographic projection from $[100]$ orientation showing the 24 standard triangles for FCC single crystal.

Table 4.1: Classification of FCC slip systems.

Primary system	1	B5	$(11\bar{1})$	$[011]$
	2	B4	$(11\bar{1})$	$[101]$
	3	B2	$(11\bar{1})$	$[\bar{1}10]$
Conjugate system	4	C5	$(1\bar{1}1)$	$[011]$
	5	C1	$(1\bar{1}1)$	$[110]$
	6	C3	$(1\bar{1}1)$	$[10\bar{1}]$
Cross-glide system	7	D4	$(\bar{1}11)$	$[101]$
	8	D1	$(\bar{1}11)$	$[110]$
	9	D6	$(\bar{1}11)$	$[0\bar{1}1]$
Critical system	10	A6	(111)	$[0\bar{1}1]$
	11	A3	(111)	$[10\bar{1}]$
	12	A2	(111)	$[\bar{1}10]$

The displacement field is considered for the deformed body $u : D \rightarrow R^3$ in the finite element domain. The elastic energy as given in equation (4.11) for the computation is derived from the elastic strain component ε^e of the total strain.

$$E(\varepsilon^e) = \frac{1}{2} \varepsilon^e : E^e : \varepsilon^e \quad (4.11)$$

The stress tensor for the elastic strain is shown in equation (4.12).

$$\sigma = \frac{\partial E(\varepsilon^e)}{\partial \varepsilon^e} = E^e : \varepsilon^e \quad (4.12)$$

Here E^e is the fourth order elastic modulus tensor derived from the unit vectors as given in equation (4.13).

$$E^e = E^{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l \quad (4.13)$$

The total strain $\dot{\varepsilon}$ can be divided into elastic and plastic components and is related to the deformation gradient F as follows:

$$\dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^p \quad (4.14)$$

$$\dot{\varepsilon} = \frac{1}{2} [F^T F - I] \quad (4.15)$$

where I is the identity tensor. The deformation gradient F is calculated for each load step or increment by the ABAQUS FE programme. The Cauchy stress for finite deformation and the logarithmic strain, calculated as an integral of the symmetric part of velocity gradient with respect to time is implemented. A trial strain as in equation (4.16) is calculated assuming plastic strain $\varepsilon^p = 0$ before yield occurs. Forward Euler integration is used with small incremental time steps to solve for the plastic strain increments in each step.

$$\Delta \varepsilon_{n+1} = \Delta \varepsilon_{n+1}^e + \Delta \varepsilon_{n+1}^p \quad (4.16)$$

The external stress increment $\Delta \sigma$ for the corresponding trial strain increment

is calculated using the following equation (4.17).

$$\Delta\sigma_{n+1} = E^e : \Delta\varepsilon_{n+1} \quad (4.17)$$

A cubic elastic anisotropic tensor E^e is used for the computation of the external stress applied on a single crystal in the elastic regime. The moduli values used in this simulation are $E_{11} = 145 \text{ GPa}$, $E_{12} = 127.4 \text{ GPa}$ and $E_{44} = 75.4 \text{ GPa}$ [91].

When a crystal is subjected to an external stress σ , the resolution of this stress on to the preferred slip system is called the Schmid stress τ . When the Schmid stress is higher than the slip system resistance to yield, plastic deformation takes place. The Schmid stress increment $\Delta\tau$ on a specific slip system α is given by the following equation (4.18).

$$\Delta\tau_{n+1}^\alpha = \Delta\sigma_{n+1} : P_n^\alpha \quad (4.18)$$

where P^α is a symmetric space spanned by slip direction s^α and slip plane normal m^α as defined by the following equation (4.19) .

$$P^\alpha = \frac{1}{2} (s^\alpha \otimes m^\alpha + m^\alpha \otimes s^\alpha) \quad (4.19)$$

The slip direction and normal are subjected to co-ordinate transformation at the beginning of each incremental step. The Schmid stress is computed as shown in equation 4.20

$$\begin{aligned}\tau &= \sigma_{xx}^s l_{mx} l_{sx} + \sigma_{yy}^s l_{my} l_{sy} + \dots + \sigma_{xz}^s (l_{mx} l_{sz} + l_{mz} l_{sx}) \\ &= \sigma^s : (s \otimes m)\end{aligned}\tag{4.20}$$

where σ^s is the symmetric part of Cauchy stress tensor σ . By decomposing $(s \otimes m)$ into the symmetric and antisymmetric parts and using the symmetry of σ^s , the above equation can be simplified as follows.

$$\begin{aligned}\tau &= \sigma^s : \frac{1}{2} (s \otimes m + m \otimes s) + \sigma^s : \frac{1}{2} (s \otimes m - m \otimes s) \\ &= \sigma^s : \frac{1}{2} (s \otimes m + m \otimes s)\end{aligned}$$

since

$$\sigma^s : \frac{1}{2} (s \otimes m - m \otimes s) = 0\tag{4.21}$$

Equation 4.21 represents the resolved shear stress for a single slip system.

$$\tau^\alpha = \sigma_{ki}^s \left(\frac{1}{2} \right) (s_k^\alpha m_i^\alpha + s_i^\alpha m_k^\alpha)\tag{4.22}$$

where, τ^α is the resolved shear stress on α system, σ_{ki}^s are the components of σ^s , s_k^α and m_k^α are the direction cosines of the slip direction and the slip plane normal direction on α slip system with respect to the crystal coordinate system. Since the slip direction should lie in the slip plane, the slip plane normal direction and the slip direction are always perpendicular to each other.

The yield criteria as defined by the equation (4.23) is validated for each of the slip system.

$$\Phi_{n+1}^\alpha = \left(\tau_n^\alpha + \Delta \tau_{n+1}^\alpha \right) - \tau_0^\alpha - g_{n+1}^\alpha\tag{4.23}$$

The hardening variable, $g^\alpha = \tau_0$, is the initial critically resolved shear stress and its value used in this simulation is 34.8 MPa for copper single crystals [91]. A

typical shear stress-strain response for Cu on (111) plane is shown in Figure 4.3 along with the three stages of hardening mechanisms; stage II hardening is noted.

Figure 4.3: Shear stress - strain response of Cu (111)plane.

The flow rule governing the plastic strain increment is given by the equation (4.24). The plastic strain increment is computed based on the shear strain γ of each active slip system $\alpha \in A$, *activated*. A rate independent crystal plasticity case is considered here where the determination of active slip systems is based on Kuhn-Tucker criteria [92] as defined by the equations (4.25, 4.26 and 4.27). The slip systems with shear strain $\gamma^\alpha < 0$ are not considered for the yield function validation during that particular time step since they do not contribute to the plastic strain increment in the flow rule. The first incremental step assumes $A=0$ *i.e.* no slip systems are active.

$$\Delta \varepsilon_{n+1}^p = \sum_{\alpha \in A} \gamma^\alpha \frac{\tau_n^\alpha}{|\tau_n^\alpha|} P_n^\alpha \quad (4.24)$$

$$\gamma^\alpha \geq 0 \quad (4.25)$$

$$\Phi_{n+1}^\alpha \leq 0 \quad (4.26)$$

$$\gamma^\alpha \Phi_{n+1}^\alpha = 0 \quad (4.27)$$

To compare the simulated numerical behavior with experimental response of nanoindentation measurements, the interaction of dislocations are taken into account by the hardening law g^α . The anisotropic hardening behavior of copper (Cu) as given by the equation (4.28) is applied on the activated slip systems. The hardening behavior accounts for both self hardening $h_{\alpha\alpha}$ and latent hardening $h_{\alpha\beta}$ for each slip system. The parameter q representing the ratio of latent over self hardening is taken to be 1.4 from the experimental results [91].

$$g_{n+1}^\alpha = g_n^\alpha + \sum_{\beta \in A} h_n^{\alpha\beta} \gamma^\beta \quad (4.28)$$

$$h_n^{\alpha\alpha} = \frac{\Delta \sigma_n^\alpha}{\Delta \varepsilon_n^\alpha} \quad (4.29)$$

$$h_n^{\alpha\beta} = h_n^{\alpha\alpha} [q + (1 - q) \delta^{\alpha\beta}] \quad (4.30)$$

Yield function is solved by substituting all the obtained trial stress and trial shear stress in equation 4.23. The twelve yield functions for the slip systems are computed. The step is assumed to be purely elastic if, the yield function is less than zero and a global momentum balance is performed until it reaches the equilibrium condition.

$$\sum_{\beta \in A} (P_n^\alpha : E^e : P_n^\beta + h_n^{\alpha\beta}) \gamma^\beta = P_n^\alpha : E^e : (\varepsilon_n^e + \Delta \varepsilon_{n+1}) - g_n^\alpha - \tau_0^\alpha \quad (4.31)$$

The slip system shear strain rate γ^β is solved based on the Kuhn-Tucker criteria and consistency conditions. The elastic and plastic strain variables for the activated slip system after each time step is updated in ABAQUS. The incremental step is defined as $n + 1$ and plastic strain is given by equation 4.32.

$$\varepsilon_{n+1}^P = \varepsilon_n^P + \sum_{\alpha \in A} \gamma^\alpha \frac{\tau_n^\alpha}{|\tau_n^\alpha|} P_n^\alpha \quad (4.32)$$

Incremental elastic strain is derived from the trial state as shown in equation 4.33.

$$\varepsilon_{n+1}^e = \varepsilon_{n+1}^{trial} - \sum_{\alpha \in A} \gamma^\alpha \frac{\tau_n^\alpha}{|\tau_n^\alpha|} P_n^\alpha \quad (4.33)$$

The stress update on the activated slip systems are deduced from equation 4.34.

$$\sigma_{n+1} = \sigma_n + E^e : (\Delta \varepsilon_{n+1} - \Delta \varepsilon_{n+1}^p) \quad (4.34)$$

For every time increment, the updated stress values are substituted in the yield function to satisfy the global equilibrium and thereby convergence. A flow chart is shown in Figure 4.4 to illustrate the algorithm of the crystal plasticity model with the finite element method.

Figure 4.4: Flow chart of crystal plasticity model with finite element method implemented in ABAQUS.

Chapter 5

Indentation Response of Single Crystal Copper Using Rate Independent Crystal Plasticity*

5.1 Introduction

In recent years, several engineering devices such as micro electro mechanical sensors (MEMS) and thin films with micrometer and nanometer features need to be manufactured. The materials used to fabricate/process these devices can be characterised for their mechanical behavior using an instrumented indentation test. Indentation experiments are popular because of their ease of operation and non-destructive nature. The mechanical response of the indented materials are often evaluated based on contact mechanics principles of indenting solids, which are predominantly assumed to have an elastic-plastic behavior at low temperatures for engineering alloys. These assumptions fail to capture the anisotropic nature of some crystalline materials such as copper (Cu), silver (Ag) and magnesium oxide (MgO) at small length scales when only a few grains are present. Spherical and Vickers indentation experiments on single crystal MgO were investigated by Khan *et al* [113] in three different crystallographic orientations (100), (011) and (111) respectively. The differences in deformation behavior and hardness showed the effect of crystal orientation. microindentation experiments conducted to study pile-up

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and sink-in effects on single crystal tungsten(W) and molybdenum (Mo) in three different crystallographic orientations (100), (011) and (111) revealed orientation dependent response [114]. The anisotropy of materials revealed by these studies paved the way for modeling the same. Molecular dynamics indentation simulations at few angstroms depth on FCC single crystals using different size and shape of indenters provided crystal orientation dependent hardness values and predicted the material flow around the indenters [115, 116]. However, due to the restricted computational domain size the molecular dynamics results are not comparable to laboratory scale measurements to a good degree of accuracy. Crystal plasticity finite element method have also been used to study indentation of single crystals [117–119]. The models used for these studies were rate dependent. The orientation dependent properties of single crystal copper depends on heterogeneous behavior of the active slip systems. In this context, the single crystal plastic zone feature and contact anisotropy using a rate independent 3D crystal plasticity model, which accounts for only active slip systems in different crystallographic orientations is analyzed. The crystal plane anisotropy is explored by studying the load displacement response and plastic flow underneath the indenter. The indent in these cases is confined to a single grain, leading to anisotropy associated with the slip system orientations. Anisotropic behavior obtained from this type of constitutive modeling is related to single crystals but paves for understanding the indentation response of polycrystalline material influenced by texture and grain orientation.

5.2 Finite element simulations

The single crystal plasticity constitutive model as described in chapter 4 is implemented to study indentation response of single crystal copper by spherical indenters of radii (R) $3.4\ \mu m$ and $10\ \mu m$. The anisotropic deformation of single crystal copper observed from nanoindentation experiments were conducted with a diamond spherical indenter. In the simulation, the indenter made of diamond is consid-

ered rigid. This is justified as diamond has a modulus of 1000 GPa, an order of magnitude higher than that of Cu, which has a range of moduli from 110 GPa to 150 GPa. All the finite element calculations were carried out using ABAQUS software with a user sub-routine implemented for the constitutive model. The geometry of the computational domain is a cylindrical specimen of 30 μm radius and 15 μm height. Due to the radial symmetry of the spherical indenter and specimen geometry, only a quarter of the three dimensional model is considered for the simulation. The discretized geometry along with boundary conditions for the indentation simulations is shown in Figure 5.1. It is to be noted that the dimensions of the computational domain are smaller when compared to the actual experimental measurements, yet much larger than the maximum indentation depth thus minimising any edge or boundary effects. The specimen is discretized with 4588 eight noded 3D elements, with reduced integration (C3D8R) and enhanced hour glass control. The mesh selection is usually a compromise between solution accuracy and computational cost. The strain gradients beneath the indenter are the highest, so a very fine mesh is used in the indentation regime and coarser mesh is used in other regions. The mesh size on the numerical solution accuracy was investigated by benchmarking an element size of 160 nm. The indentation simulation was performed on a (100) oriented single crystal and obtained load-displacement curve was compared with experimental results in the literature. The numerical results were in good agreement with a 4.6% maximum deviation. Two additional mesh sizes of 280 nm and 200 nm were tested. In the case of 280 nm, increased oscillations were observed and the results of the simulation showed a 18% deviation with the benchmark curve whereas the 200nm mesh size showed a deviation of only 6.8%. Based on this sensitivity analysis, it was concluded that, the simulation results with element size of 200nm have converged with respect to the benchmark mesh size. To compare the experimental pile up profile of the crystal plane, a friction coefficient was used. Coulomb coefficient of friction of 0.4 for (100) plane, 0.3 for (011) plane and 0.2 for (111) plane were considered at the indenter and

copper interface to analyse the pile-up patterns. The friction coefficient effect on the load displacement curve for different crystal orientations have been found to be negligible [120]. The simulation steps consist of both loading and unloading stages. All the indentation simulations were done under load control with small increment steps to allow for the solution convergence and to avoid the instability usually observed in indentation simulations.

Figure 5.1: Finite element discretization of the computational domain

5.3 Results and discussion

Finite element simulations of nanoindentation with a spherical indenter of radius $3.4\ \mu\text{m}$ and $10\ \mu\text{m}$ were conducted on a copper single crystal in three crystallographic orientations [(100), (011) and (111)] at various indentation depths. The published nanoindentation experimental load-displacement response, and mean effective pressure p_m , underneath the loading spherical punch are compared with the simulation results. Then, the material behavior beneath the indenter is analysed from the shear stress, shear strain and pile up profiles of the single crystal copper.

5.3.1 Elastic-plastic contact response

Numerically simulated load displacement curve for $3.4\ \mu\text{m}$ and $10\ \mu\text{m}$ radius indenter is compared with the experimental [121] measurements conducted on Cu crystals in Figure 5.2. The load displacement curves obtained from simulation are superimposed over the experimental curves. For the purpose of comparison, the indentation loading and unloading steps in the simulation are similar to that in the experimental measurements. The maximum indentation load for $3.4\ \mu\text{m}$ indenter is restricted to 5 mN, whereas for $10\ \mu\text{m}$ indenter it was set to 35 mN.

The loading contact response exhibits the anisotropic properties of different crystallographic planes when indenting. The triaxial stress fields underneath the indenter facilitates the activation of admissible slip systems during the elastic-plastic contact response in the oriented surface. The contact response is particularly complex when the fully plastic zone develops close to the indentation zone.

From the loading curve, for the $3.4\ \mu\text{m}$ radius indenter at an indentation depth of 200 nanometer, (111) orientation displayed the highest load of 3.10mN, followed by (011) at, 2.97 mN and (100) at, 2.86 mN displayed the lowest. A similar trend was observed from the loading curve of the $10\ \mu\text{m}$ radius indenter. At 500 nanometer depth, (111) orientation had the highest load of 21.97 mN followed by

(011) at, 21.76 mN and (100), orientation displayed the lowest with 20.84 mN. The simulation and experimental loading curves of the 3.4 μm and 10 μm radius indenter compared reasonably well within the experimental scatter. From the simulated response, the ratio between the applied loading P in the (111) plane and (100) plane, P_{111}/P_{100} was seen to be, 1.13 for 3.4 μm and 1.05 for the 10 μm radius indenter. The corresponding experimentally measured load P ratio are 1.23 for 3.4 μm and 1.06 for 10 μm radius indenter respectively. The contact regime beneath the spherical indenter evolves as the plastic deformation increases with the penetration depth. The relative compliance of the different indented planes does not remain constant. As the indentation proceeds, the corresponding indentation loading rate increases at different rates depending on the indented plane of the crystal. The degree of anisotropy inferred from the indentation loading curve on the indented surfaces at low loads are found to be higher compared to that at higher loads. This shows that anisotropic response is due to primary glide alone in $\{1\ 1\ 1\}\langle 1\ 1\ 0\rangle$ family of slip systems as might be expected from materials having four independent primary slip systems.

Negligible elastic recovery is observed from the indented unloading curve in the (100), (011) and (111) oriented surfaces for the 3.4 μm radius indenter at low loads. The radius of the residual impression beneath the indenter at shallow indentation depths is two orders of magnitude smaller which is the cause for steep elastic recovery. An anomalous elastic recovery is observed for 10 μm indentation at deeper impressions. The indenter penetrates sufficiently leading to a proportional increase in the diameter of the impression with depth which, agrees well with the experimental results of Foss and Brumfield [122]. The slope of unloading contact response is determined as a measure of the elastic properties *i.e.* mainly Young's modulus, E of the crystals. The Young's moduli ratio obtained from the initial slope of the unloading curve are, $E_{111} (190.1_{R=3.4\mu m}, 189.2_{R=10\mu m}) / E_{100} (66.93_{R=3.4\mu m}, 65.92_{R=10\mu m}) = 2.84$ for 3.4 μm and 2.87 for 10 μm radius indenter. The corresponding experimentally measured Young's moduli ratio are 2.91 for 3.4 μm and 2.88 for 10 μm radius inden-

ter respectively. The elastic and elastic-plastic anisotropic contact response when indenting, bulk copper single crystal with sharp indenters have shown that (111) plane is the stiffest [123]. The Hertz elastic solution using spherical indentation have produced similar results [124].

Figure 5.2: Load displacement curves of single crystal copper in three crystallographic orientations.

The mean effective pressure p_m *i.e.*, hardness from the indentation simulations of 3.4 μm and 10 μm radius indenter were also compared with experimental data to determine the mechanical behavior of single crystal in three different orientations.

Figure 5.3 shows the variation of p_m with the geometric strain, defined as the ratio of the indent radius (a) to indenter tip radius (R). For completeness the experimental measurements are compared with the numerical simulations. The simulation results of mean effective pressure p_m was calculated by dividing the indentation load with the projected area of contact. The contact area beneath the indenter was directly obtained from ABAQUS. The mean effective pressure was found to be highest for (111) plane and lowest in (100) plane, as referred by the load-displacement response. The mean effective pressure p_m for $3.4\ \mu m$ radius indenter showed orientation effects whereas the results of $10\ \mu m$ indenter in the indented planes were all similar which overall agrees with the experimental observation [125, 27]. A gradual increase in mean pressure or Meyer hardness, p_m with a/R has been reported, which is observed from the present investigation. It was also concluded that, p_m versus a/R for indenters of radii $30\ \mu m$, $200\ \mu m$, and $500\ \mu m$ all fall on the same curve, but for indenter $7\ \mu m$, the p_m values were slightly higher than for the larger indenters ($30\ \mu m$, $200\ \mu m$, and $500\ \mu m$). Thus, it can be verified that, the scaling effect is negligible which agrees well with the current simulation results.

(a) $R = 3.4 \mu m$

(b) $R = 10 \mu m$

Figure 5.3: Variation of mean effective pressure p_m as a function of geometric strain a/R in three different orientations of single crystal copper.

5.3.2 Plastic zone size variation beneath the indenter

The plastic zone variation is studied based on the shear stress, shear strain and material pile-up profiles of the copper single crystal. With the y-axis as the indentation direction in the global coordinate system under load, the three different orientations are analysed. The simulation results for only the $3.4\ \mu\text{m}$ radius indenter at low loads, where orientation effects are present are discussed here, since the scaling effect using the $10\ \mu\text{m}$ radius indenter at high loads, are found to be negligible with respect to the crystal orientations as seen from the load-displacement curves and meyer hardness values.

The shear stress, shear strain distribution underneath the indenter is shown in Figure 5.4. The shear strain γ is calculated as the summation of absolute values of shear strains in all the active slip systems. The plastic zone assessment is critical in terms of contact anisotropy as it is largely influenced by the indented crystallographic plane. Even though the spherical indenter is radially symmetric, the distribution and magnitude of the shear stresses are not symmetric indicating a strong crystal anisotropy. The shear stress reaches a maximum value of 105.23 MPa on (1 1 1), 97.27 on (0 1 1) and 48.35 on (1 0 0) planes respectively. The magnitude of shear strain distribution γ calculated for (111) plane is 0.74 which is the highest, indicating a close packed plane for single crystal copper and (100) plane is seen to have the lowest value of 0.59. The plastic deformation is largely heterogeneous and concentrated on only active slip system directions. The (100) plane exhibited a more localized plastic zone beneath the indenter compared to the (111) plane which has a wider deformation gradient. The experimentally observed plastic deformation zone around the indenter ranges in size from 1-7 μm as reported by Bahr *et al* [126] which was quantified using a atomic force microscope (AFM). The simulated results predict a value of $\sim 2\text{-}6\ \mu\text{m}$ which reasonably agree with the experimental measurements. The understanding of deformation zone size to analyse the yield surface of single and poly crystalline materials is essential.

Shear stress (MPa)

Shear strain

(a) 100 Surface

(b) 011 Surface

(c) 111 Surface

Figure 5.4: Shear stress and strain distribution in the copper single crystal in three different orientations

The material pile-up around the indenter is shown in Figure 5.5. The pile up profile around the indentation showed orientation effects as (100) plane had a maximum pile up and (111) plane had the least. All the admissible slip systems were observed to be active for the (100) oriented surface. The (111) plane exhibited a maximum resistance to slip because of the presence of primary independent slip systems of the material, thus, leading to a lower pile up region around the indenter. The plastic deformation zone from the simulation exhibited a four-fold, two fold and three fold symmetry for the (1 0 0), (0 1 1) and (1 1 1) planes.

For all the orientations considered, exhibited pile-up patterns rather than a sink-in effect which is expected. The F.C.C crystals strain harden in stage II proportional to the shear moduli. This phenomenon has been explained on the basis of crystal kinematics and the flow dynamics associated with the plastic slip. The number of slip systems activated for planes (100), (011) and (111) are eight, four and six. The active slip systems undergo a strong rotational component compared to a translation. This phenomenon has also been observed in the experimental indentation studies by Wang et. al on single crystal copper [127]. The primary slip systems activated for each orientation leads to a local strain hardening rate around the indents. This locally dominating plastic slip rate leads to pile-up patterns. The distribution of shear stresses, shear strain and plastic zone information obtained around the indent indicates the effect of strong crystal orientation effects.

(a) 100 Surface

(b) 011 Surface

(c) 111 Surface

Figure 5.5: Pile up profile on single crystal copper

5.4 Summary

Nanoindentation simulations using a spherical indenter (radius of $3.4\ \mu\text{m}$ and $10\ \mu\text{m}$) on single crystal copper of three crystallographic orientations, i.e., $(1\ 0\ 0)$, $(0\ 1\ 1)$ and $(1\ 1\ 1)$ were carried out using a commercial software (ABAQUS) incorporating a rate independent crystal plasticity constitutive law. Experimental measurements of nanoindentation obtained from the literature are compared with the simulated load displacement curves, mean effective pressure and pile up profiles. For a spherical nanoindentation, distributions in three crystallographic orientations, $(1\ 0\ 0)$, $(0\ 1\ 1)$, and $(1\ 1\ 1)$ showed pile-ups with a topographical pattern of four-fold, two-fold, and three-fold symmetry, respectively similar to that seen in experimental data from the literature. The magnitude of the in-plane shear stresses and the total shear strains are compared in single crystal copper under nanoindentation on the three surfaces to determine the orientation effects. The material behavior of single crystal copper, including the topographical characteristics, the shear stress distribution and the hardness obtained using a $3.4\ \mu\text{m}$ radius spherical indenter depends strongly on the crystal orientation which agrees reasonably with the experimental data in the literature.

Chapter 6

Experimental and Numerical Investigations of the Texture Evolution in Copper Wire Drawing*

6.1 Introduction

The wire bonding industry is exploring the options of using copper because of its cost [6]. The price of copper has been estimated to be 10-40% of the gold (Au) and it is not subject to sudden market fluctuations. Copper wire is much cheaper compared to gold wire in the present scenario considering the volume used in the IC chip fabrication. The current market price of gold wire, diameter $20\mu m$ 500m spool, is approximately 200 USD, which is 1000% higher than the comparable copper wire [7]. The selection of copper stands vindicated not only based on cost alone, but owing to specific mechanical properties which are found superior to gold. The copper wires have better electrical and thermal properties than gold wires. Copper is approximately 25% more conductive than gold, accounting for increased power rating and better heat dissipation. Higher electrical conductivity results in lowering the IC delay and less power loss [128]. Copper wires have higher tensile strength, lower wire sag and better loop stability is obtained during encapsulation [129, 130]. Copper wires are found to have excellent ball neck strength after the

*Karthic.R.Narayanan, I.Sridhar and S.Subbiah , in Applied Physics A: Materials Science & Processing Volume 107, Number 2, 485-495

ball formation [131]. Compared to gold wires, the higher stiffness of copper wires is more suitable to fine pitch bonding, leading to better looping control and less wire sagging for ultra-fine-pitch wire bonding [5]. Using copper wire can be a solution to the wire short problem caused by small wire sizes, besides other solutions such as using insulated wire and having varying loop heights. High stiffness and high loop stability of Cu wire lead to better wire sweep performance during encapsulation or molding for fine-pitch devices, and can help to achieve longer/lower loop profiles [6]. Both gold and copper possess a face centered cubic (FCC) lattice but their mechanical, thermal and electrical properties are widely different [132–134]. A direct replacement to gold is not feasible which is the reason for the keen interest of the semiconductor industry in this material.

6.2 Experimental procedures

6.2.1 Materials and methods

The copper wire of initial diameter $\phi 1.6mm$ was bought from a supplier. The original copper wire of $\phi 1.6mm$ was drawn to $\phi 1.3mm$ in two drawing schemes *i.e.* a single step and multiple step for the area reduction (RA) of $\sim 33\%$. In the single step drawing, the original wire of $\phi 1.6mm$ was drawn to $\phi 1.3mm$ in a single draw whereas in the multiple step, the wire was reduced to $\phi 1.5mm$, $\phi 1.4mm$ and then finally to $\phi 1.3mm$. The wire was drawn through tungsten carbide dies attached in a drawing plate in order to achieve the area reduction. The die angle α and the bearing length of the drawing die are $4.5^\circ \pm 0.5$ and $1.4 \pm 0.2mm$ respectively as specified by the die manufacturer. A solid lubricant of graphite is used to minimize the effect of friction μ during the drawing process. A controlled drawing velocity of $25mm/sec$ was used and the strain rate was kept constant for both the drawing schemes. The total drawing strain was ~ 0.40 from the initial as received wire to the final wire.

6.2.2 Mechanical testing

The tensile strength of as received and drawn copper wires were measured from room temperature tensile tests using Instron testing machine. The testing was performed based on ASTM standard F219-96, which is for testing fine round and flat wire for electron device and lamps. Each type of three specimens were tested for consistency and reliable data. To determine the tensile strength, yield strength and elongation at room temperature, all the samples had a gauge length of 254 mm. A minimum sufficient load was applied to the specimen to keep the wire straight. The tests were performed at a strain rate of 25.4 mm/min. The failure of the specimen near the clamps are not acceptable and those test were repeated.

6.2.3 Scanning Electron microscopy

Microstructural characterizations were carried out on a JEOL SEM with energy and wavelength dispersive spectrometers. The operating voltage was set to 20KV. The purity of the as received copper wire was characterized using a energy dispersive spectroscopy (EDS) and found to be more than 99.99% . The microstructure of the failed tensile test samples were also recorded and analyzed.

6.2.4 X-ray diffraction measurement

Experimental measurements of the texture of the as received copper wire and drawn copper wire were obtained by X-ray diffraction method with $Cu K_\alpha$ radiation using a Bruker D8 diffractometer. Incomplete pole figures were generated on $\{111\}$, $\{200\}$, $\{220\}$ and $\{311\}$ crystallographic planes. The irradiated surfaces were measured along the longitudinal section of the wire and the area was $\sim 0.8 \times 2.5 \text{ mm}$. The average grain diameter of the as received copper wire was about $60\mu m$, a typical irradiated surface samples about 764 grain orientations. The incomplete pole figures in its raw form is uncorrected and is in the form of discretized intensities as a function of goniometer position angles. The raw data

was processed using MULTEX, a built - in package with Bruker D8 X-ray diffraction. Each measured pole figure was corrected for background and defocusing. All pole figures are equal area projections of the specified crystallographic planes. In order to obtain complete information of a texture, orientation distribution function (ODF) is considered for the representation since a large amount of technically relevant information required for qualitative analysis of textures can be obtained from such a representation. ODF was calculated from the experimental pole figures using orthorhombic sample and cubic crystal symmetry. The symmetry requires the elementary three dimensional Euler space defined by $0^\circ \leq \varphi_1 \leq 360^\circ$, $0^\circ \leq \phi \leq 90^\circ$ and $0^\circ \leq \varphi_2 \leq 90^\circ$.

6.2.5 Finite element analysis

The algorithm of the crystal plasticity constitutive model as described in chapter 4 is implemented to study the wire drawing experiments. A rate independent 3D crystal plasticity model incorporating finite strain theory employed in commercial code ABAQUS is applied to simulate the drawing process and study the anisotropic response in the polycrystalline copper wire. The finite element (FE) simulations was used to understand the deformation during the two drawing schemes with process parameters similar to experimental conditions.

For the wire fabrication, a drawing plate with several individual dies were used to achieve the area reduction. For consistency, the wire was drawn in the same direction through each die such that the axis is parallel to the subsequent drawing direction. In single step, the die imparted a total drawing strain of ~ 0.40 whereas in multiple step, controlled drawing strains of ~ 0.12 , 0.13 and 0.14 were achieved. The final bonding wires with $1.3mm$ were achieved from the drawing schemes.

The finite element modeling characterize the essential features of the deformation imposed in the wire drawing experiments. Using the symmetry of the experimental set up, an axi-symmetric analysis was carried out. A rigid conical die is used to reduce the cross sectional area of a copper wire $0.8mm$ in diame-

ter and 2.5mm long by $\sim 33\%$ using axi-symmetric finite element (FE) drawing simulations as shown in Figure 6.1. The FEM workpiece consisted of 2272 four noded axi-symmetric elements, with reduced integration (CAX4R) and enhanced hour glass control. The pole figures processed from the uncorrected raw data was superimposed on the FE workpiece. The initial texture of the FE model have 568 unweighted discrete grain orientations which corresponds to the experimental crystallographic texture of the as received wire, as shown in Figure 6.2. A simple tension on an aggregate of 568 unweighted grain orientations representing a polycrystalline copper material was simulated. The tension test parameters for the simulated study depicts the experiments in terms of loading and boundary conditions but for failure and necking criteria as shown in Figure 6.3a. The experimental measurements and simulation for the stress-strain response of the as received copper wire are in good agreement as shown in Figure 6.3b. In this paper, a texture component designated by $\{hkl\} \langle uvw \rangle$ means that the $\{hkl\}$ plane normal is parallel to the radial direction (RD) and $\langle uvw \rangle$ is parallel to the drawing or axial direction (AD). With four axi-symmetric elements representing each grain orientation in the finite element model, the simulation was conducted. The die angle α and the bearing length of the die are $4.5^\circ \pm 0.5$ and $1.4 \pm 0.2\text{mm}$ respectively, which is the same with the experimental drawing conditions. The die angles were kept the same for both the drawing schemes in the simulation. The coefficient of friction between the die and the copper wire was kept constant at a value of 0.05 for all the drawing simulations conducted. The friction in diamond die has been considered to be negligible during modeling by Cho *et al* [25] and Park *et al* [62, 63]. They assumed 0.001 as Coulomb coefficient of friction between the die and wire. Here, experiments were conducted in a tungsten carbide die instead of diamond, which is widely used in the industry. The friction coefficient between the tungsten carbide die and copper wire was found to be in between 0.03 – 0.11 investigated by Haddi *et al* [135]. Within numerical scatter, the obtained results were almost constant for friction coefficient values of 0.03, 0.05 and 0.07 and finally we selected 0.05 for

all the simulations. Wire drawing is simulated by moving the wire, which is given the drawing speed of 25mm/sec causing it to traverse the die from one end to the other.

Figure 6.1: Finite element schematic of wire drawing process.

Figure 6.2: Initial texture of as received copper wire : (a) experimental $\{111\}$ (equal area projection) pole figure and its (b) numerical representation by 568 grain orientations.

Figure 6.3: Comparison of stress-strain curve in tension using 568 unweighted grain orientations with experimental measurements.

6.3 Results and discussion

The mechanical properties of the wire with different drawing schemes were obtained from tensile testing. The fracture micrographs of the specimen obtained from SEM

study gives an understanding of the failure mechanisms in the macroscopic scale. A comprehensive assessment of the microstructural and textural evolution in the drawn copper wires by two drawing schemes is given here from the experimental measurements and its FE predictions. The microstructural inhomogeneities developed in the wire during deformation contributed substantially in understanding the fiber texture, which is discussed. The effect of drawing strain on the complex surface texture of the wire is analyzed.

6.3.1 Mechanical properties

The mechanical properties of the wire is analyzed from tension test results as shown in Figure 6.4. The macroscopic properties such as Young's modulus E , failure strain and ultimate tensile strength of the specimens are extracted and analyzed. The Young's modulus E of the as received wire is 96 GPa with a failure strain of 0.38 and ultimate tensile strength of 176.43 MPa. The Young's modulus of the single pass drawn wire reaches 125.61 GPa, whereas the multi pass wire has 112.18 GPa. The failure strain reaches to 0.015 and 0.023 whereas the ultimate strength reaches 278.3 MPa and 326.8 MPa for the single pass and multi pass drawn wires respectively. The wire after the drawing process has a substantial increase in Young's modulus. The failure strain of the wire reduces for both the drawing schemes compared to the as received wire. The wire drawn with multi pass drawing scheme shows a slightly higher ductility and ultimate tensile strength compared to the single pass drawn wire.

Figure 6.4: Mechanical properties of the wire.

The microstructural characterization of the fracture surface after the tensile test is analyzed. Figure 6.5, shows the fractographs obtained from SEM of as received, multi pass and single pass drawn wires respectively. The fracture surface of the as received wire as shown in Figure 6.5a has a ductile failure mode whereas the drawn wire surface has a near brittle failure as observed from Figures 6.5b and 6.5c respectively. The multi pass drawn wire showed a considerable ductile failure surface compared to the single pass drawn wire. The fracture surface clearly shows the transition from a ductile to brittle failure mechanism. The reduction of the failure strain in the drawn wires are a direct result of work hardening as observed from the fracture surfaces of the specimens.

Figure 6.5: Fracture micrographs of the wire specimen after the tensile test

6.3.2 Crystallographic texture

The longitudinal section of the as received wire of $\phi 1.6mm$ shows predominantly a mixture of weak $\langle 111 \rangle$ and $\langle 100 \rangle$ orientations with regions of more complex textures. The texture measured by X-ray diffraction in the form of pole figure of the as received wire is shown in Figure 6.2. A $\{111\}$ pole figure with AD parallel to the drawing direction shows a overall well developed $\langle 100 \rangle$ fiber texture and a random local texture. The main texture component is close to a rotated cube component $\{100\} \langle 011 \rangle$ or ideal Goss component. As the wire diameter decreases during drawing, equivalent plastic strain increases and strong single component crystallographic texture evolves near the drawing axis. The initial grain orientation of the polycrystalline wire also influences the crystallographic texture of the drawn

wires, which is seen from the presence of $\langle 100 \rangle$ texture across the wire section in both the drawing schemes.

The pole figure of the copper wire measured and predicted using FE calculation, drawn by single step area reduction, is shown in Figure 6.6. The texture of the drawn wire also exhibited similar duplex $\langle 111 \rangle$ and $\langle 100 \rangle$ components. However, the presence of $\langle 111 \rangle$ texture component increased in the single step drawing subjected to a area reduction of $\sim 33\%$. The presence of $\langle 100 \rangle$ component is very weak, but this property is inherited from the initial texture of the received wire. This variation correlates well with the moderately high stacking fault energy (SFE) ($\gamma = 21 \text{ mJ/m}^2$) of copper during deformation as reported by English and Chin [31]. The increase of $\langle 111 \rangle$ texture component is attributed to slip dependent behavior. The proportion of $\langle 100 \rangle$ texture have been argued by Calnan [136] and Bishop [137] based on latent hardening in active slip systems. The finite element prediction is based on specific slip system interaction imposed by the deformation, which is considered here. Relative amount of slip on the specific systems leads to differential hardening which is a fundamental feature in texture formation. The FE also shows a strong $\langle 111 \rangle$ texture which compares well with the experimental measurements. The $\langle 111 \rangle$ fiber texture components tends to align with the axial direction of the cold drawn wire which is clearly seen from the simulation as well as experimental measurements. A drawn wire, in the intermediate stage of a multiple step, was analyzed for the multistage drawing texture development. The experimental pole figure of the wire drawn to a strain of 0.12 and its FE prediction is shown in Figure 6.7. A strong $\langle 112 \rangle$ texture parallel to the drawing direction and a random $\langle 110 \rangle$ texture is observed. The comparison with finite element simulation shows a good agreement for strong $\langle 112 \rangle$ texture component. The pole figures show a weak drawing texture after the intermediate drawing step. This shows the heterogeneous nature of plastic deformation. At low strains, Cu shear band formation was extrapolated from the pole figures. Although, the shear bands are observed in low to high strain wires, they were aligned at 60° to the AD parallel

to the drawing direction in low strains (0.12), another interesting observation is that, the shear bands tend to closely relate with the Brass component $\{110\} \langle 112 \rangle$ with a tolerance angle of 15° from the ideal orientation. The rotation of the shear bands towards the AD (drawing) direction is shown through the multiple step drawn wire texture experimental measurement and its FE predicted pole figure, as shown in Figure 6.8. As the strains in the wire increase, the shear bands tend to rotate towards the $\langle 111 \rangle$ or $\langle 100 \rangle$ texture through $\langle 221 \rangle$ or $\langle 210 \rangle$. The $\langle 111 \rangle$ grains start to appear throughout the section as the applied strain increases in the multistage drawing process. It is inferred that, at the strain of 0.40, the $\langle 100 \rangle$ oriented grains does not change much in both the drawing schemes but the $\langle 111 \rangle$ increases monotonically in the single step drawing compared to multiple step. At high strains, the texture components are predominantly a mixture of $\langle 111 \rangle$ and $\langle 100 \rangle$ oriented grains, which is observed from both the drawing steps. The misorientation angle of the shear band in the multiple step wire lies between $10^\circ - 15^\circ$ from the drawing direction. This transformation has been observed in copper and its alloys [138, 139]. Despite the heavy deformation applied in both the drawing steps, deformation twins were not observed in the drawn wires. Deformation twins in copper and its alloys subjected to room temperature forming operations are rarely reported. This is due to presence of ample slip systems to accomodate the plastic deformation. The complex fiber texture component is decreasing with the increase in drawing strain as observed from the two drawing schemes analyzed.

Figure 6.6: Texture of drawn wire - single step: (a) experimental $\{111\}$ (equal area projection) pole figure and its (b) FE prediction.

Figure 6.7: Texture of drawn wire - Intermediate step: (a) experimental $\{111\}$ (equal area projection) pole figure and its (b) FE prediction.

Figure 6.8: Texture of drawn wire - Multiple step: (a) experimental $\{111\}$ (equal area projection) pole figure and its (b) FE prediction.

The crystallographic texture exerts significant influence on many physical and mechanical properties of the deformed materials. The analysis of fiber texture evolution in the cold drawn wire during plastic deformation helps in understanding the deformation mechanisms associated with the wire drawing. The ODF of $\langle 111 \rangle + \langle 100 \rangle$ oriented regions in the wire is systematically analyzed based on the drawing strain. The ODFs of received wire, single step, intermediate step and multiple step drawn wires are shown in Figures 6.9a to 6.9d. The ODF is extracted from the pole figure using WIMV method [140]. For a two dimensional representation, the Euler space is subdivided into cells or boxes. The two axes chosen here for the representation: sections of φ_1 with a cross section at $\varphi_2 = 45^\circ$.

The major texture component of the received wire as observed from the ODF in Figure 6.9a confirms the presence of a Goss component being predominant over the whole area followed by Copper and Brass components. The overall texture of the wire shows a cylindrical symmetry with a random local texture. In the $\langle 111 \rangle + \langle 100 \rangle$ regions of the drawn wire, exhibit $\alpha - fiber$ (*Goss - Brass*) and $\beta - fiber$ (*Brass - S - Copper*) components. The ODFs show a strong $\alpha - fiber$ and $\beta - fiber$ components during the single step drawing compared to the multiple step drawn wire. The intermediate step drawn wire has a weak $\alpha - fiber$ and $\beta - fiber$ components with the Brass component dominant which verifies the pole figure measurements. There are a still a few Copper and Goss oriented grains as observed in the $\langle 111 \rangle + \langle 100 \rangle$ region of the intermediate step drawn wire. As the drawing deformation increases, Brass component is observed to be very weak, while the Copper component becomes prevalent in the drawn wire manufactured by single step compared to multiple step drawn wires. Although the complex texture component decreases with increase in drawing strain, the S and Brass components still exists.

From the rate independent crystal plasticity theory, the inhomogeneous deformation observed from the ODFs, is due to the latent hardening applied on the specific active slip systems of the grains. The finite element takes into account het-

erogeneous slip interaction during the drawing process. The shear strain in each slip system of the grain depends on the loading rate, which causes the slip reaction between the grains. Park *et al* [62, 63] using a rate dependent crystal plasticity theory, assuming no hardening between the grains, have shown that the shear strain contribution to the metal flow behavior decreases with increasing drawing strain and remains unaffected. At high drawing strains of 0.40 obtained from both the drawing schemes, the shear strain contribution on the grain becomes relatively unaffected which is also verified from the ODFs based on the fiber texture evolution. The shear deformation at low strains of 0.12, plays a vital role in the latent hardening of the grains which contributes to the texture evolution.

Figure 6.9: ODFs ($\phi_2 = 45^\circ$) for $\langle 111 \rangle + \langle 100 \rangle$ fiber texture components of the wires.

6.3.3 Surface texture

Frictional tractions in metal forming process such as rolling, wire drawing and extrusion leads to surface textures differing from those inside the workpiece, as reported in the literature. The surface texture of rolled sheets has been investigated and found to vary with the work piece predominant texture. Shear deformation due to frictional effects in the roll was observed to play a role in the sheet texture sharpening. Therefore, it is important to pay special attention to the surface texture of the drawn wire. The surface texture of the copper wire is studied and analyzed based on FE modeling. Figure 6.10 shows inverse pole figure (IPF) maps for longitudinal sections of the wire. The projection of wire axis onto the (100) (011) (111) standard triangle is shown in Figure 6.10a, which is used to represent the die-wire interface texture. In this study, a minimum friction is applied on the die-wire interface. Shear deformation on the surface of the wire due to workpiece - tool frictional contact is not analyzed in this study. Mathur and dawson [43] have pointed out that, the influence of friction on surface texture of the drawn wire is negligible. In the drawing schemes studied with varying deformation strain applied, shear deformation on the surface was found to have contributed in the textural development.

The IPF depicting the surface texture of the received wire, single, intermediate and multiple step drawn wires is shown in Figure 6.10b - 6.10e. In the surface, the shear strain increases and deformation deviates from ideal drawing condition. The texture of the surface shows a decrease in $\langle 111 \rangle + \langle 100 \rangle$ components and an increase in complex texture components. The surface texture of the received wire shows a deviation from the drawing texture, which is also observed from the single, intermediate and multiple step drawn wires. The $\langle 111 \rangle + \langle 100 \rangle$ texture components is seen to appear marginally on the wire surface in all drawing conditions. This may be related to the minimum friction in the die-wire interface. The random texture regions are apparent in the received wire as seen in Figure 6.10b. The single step drawing shows a homogeneous surface texture as seen in

Figure 6.10c. The intensity of the complex regions increases in the intermediate step drawn wire as shown in Figure 6.10d compared to the multiple step drawn wire as in Figure 6.10e. The complex texture components is related to the shear deformation of the wire surface.

The volume fraction for the complex texture components of the received and drawn wires is shown in Figure 6.11. The initial texture of the received wire were random with a large volume fraction for complex textures as seen in Figure 6.11a. The Brass, S and Copper components increases in the center of the wire as the deformation strain. However, they were seen to decrease on the surface of the wire. The volume fraction for complex textures decreases in single step drawn wire surface, which can be seen in Figure 6.11b. The $\{112\} \langle 110 \rangle$ and $\{111\} \langle 112 \rangle$ texture volume fraction tend to increase in the complex texture region. The $\{112\} \langle 110 \rangle$ complex texture component increases significantly in the single step drawn wire compared to the received wire. The volume fraction for the $\{112\} \langle 110 \rangle$ complex texture component remains unaffected in the intermediate step, however, the $\{110\} \langle 112 \rangle$ oriented texture components increases as shown in Figure 6.11c. The multiple step drawn wire surface shows a decrease in $\{110\} \langle 112 \rangle$ component, however the $\{112\} \langle 110 \rangle$ complex texture component increases as compared to the intermediate step wire as shown in Figure 6.11d. This agrees well with the results of Rajan and Petkie [29] on the drawn copper wire surface texture.

The shear strain plays a vital role in the wire - die interface texture evolution. The shear strain at the wire surface during the single step drawing is lower compared to the intermediate and multiple step. The low shear strain at the surface leads to activation of all the available slip systems, thus leads to a more homogeneous deformation. The latent hardening on the surface grain ignores the strain hardening flow rule because of a negligible shear in the surface. In the intermediate step, the shear strain increases on the surface and the latent hardening on the individual grains is heterogeneous with selectively activated slip systems. The uneven shear strain leads to a inhomogeneous distribution of texture components

on the wire surface, which has also been observed by Cho *et al* [35]. The processing strain during the multiple drawing step increase as the shear strain on the wire surface reduces, which tend to have negligible influence on the texture evolution, thereby, the deformation is fairly homogeneous.

Figure 6.10: Inverse pole figures of drawn wire surface texture calculated from the FE calculations.

Figure 6.11: Volume fraction for complex texture components of (a). as received wire, (b). single step drawn wire, (c). intermediate step drawn wire and (d). multiple step drawn wire.

6.4 Summary

High purity polycrystalline Cu wire was drawn in a single and multiple step for the equivalent area reduction (RA) of $\sim 33\%$. The drawn wires microstructure was characterized by XRD and analyzed as a function of drawing strain. In order to understand the effect of deformation process on texture evolution, the drawing process is numerically simulated using a rate independent crystal plasticity with finite strain, which is implemented as a user routine with a commercial finite element package ABAQUS. The following major observations are made:

1. The pole figure of the received wire across the longitudinal cross section had a $\langle 100 \rangle$ texture parallel to the drawing direction and a weak random local texture. As the drawing strain increased to ~ 0.40 in the single step, $\langle 111 \rangle$ texture component increased in strength. The intermediate step drawn wire subjected to strain of ~ 0.12 exhibited strong $\langle 112 \rangle$ texture components and a weak $\langle 110 \rangle$ texture. The $\langle 112 \rangle$ texture component rotated to $\langle 111 \rangle$ texture

during the multiple step drawing. The $\langle 100 \rangle$ texture was present in the cross section during both the drawing schemes. The complex texture component decreases with the increase in drawing strain. The $\langle 111 \rangle$ texture component is observed to be unstable at low drawing strains, (see Figures 6.6 - 6.8).

2. The ODF of the received wire confirmed the presence of ideal Goss component being dominant with Copper and Brass components. The single step drawn wire exhibited strong α - *fiber* and β - *fiber* components while the Brass component was prevalent in the intermediate step drawn wire. The Copper and Goss components remnant from the received wire was also present. As the drawing strain increases, the Brass components becomes weak and a strong Copper component was observed in the multiple step drawn wire. The strength of the Copper component was relatively less compared to single step drawn wire, (see Figures 6.9a - 6.9d).
3. The IPF representing the surface texture was analyzed based on shear deformation during the drawing process, (see Figure 6.10). The surface texture of the wire deviated from the ideal drawing texture due to the the shear deformation playing a major role along the radial cross section of the wire. Complex texture components were seen on the surface of the received wire. During the single step drawing, the surface texture had an increase in strength of the $\langle 110 \rangle$ oriented grains. The $\langle 112 \rangle$ texture component strength increased on the surface during the intermediate step with complex texture prevalent. In the multiple step drawn wire, the complex texture strength reduced and $\langle 100 \rangle$ oriented grains appeared marginally.

Chapter 7

Effect of free air ball texture on copper bonding using a rate independent crystal plasticity*

7.1 Introduction

High process reliability in creating the bond is crucial to determine the overall yield of the production process. The IC manufacturing processes demands a wire with higher breaking load and stiffness both preferred during the bonding process since high drag forces, induced by the rapidly moving bond head, is encountered. As discussed earlier in Chapter 5, a copper wire has better mechanical properties than a typical gold wire. Specifically the elastic modulus and hardness are higher for a copper wire. In fact, to further optimise the needed modulus and stiffness, specific textures of copper such as (111) direction over (100) direction, is chosen during the bonding process [141]. However, when such copper wires are used in the bonding process, cratering arises due to these high mechanical properties [142] as shown in Figure 7.1. Due to this, the aluminum (Al) pad squeezing and its plastic deformation around the impacted free air ball (FAB) is a major area of concern during the wire bonding process as it can cause damage to the silicon layer underneath [143, 144]. Hence, understanding the bond pad cratering deformation is important to increase reliability.

*Karthic.R.Narayanan, A.Rajaneesh, I.Sridhar and S.Subbiah, under revision in Microelectronics Reliability

Figure 7.1: Cratering during copper wire bonding [144].

The failure mode of interfacial delamination/stress induced cratering on the Al pad was investigated by He *et al* [145]. To understand the reasons for the Al squeeze a nonlinear finite element method was adopted and the complete stress-strain behavior of the free air ball was modelled using a power law [146]. The mechanism of ball bond impact stage in the process have also been studied using elastic-plastic finite element analysis [147, 148]. However, these studies are based on conventional finite element method that fail to capture adequate local information of the free air ball with respect to the grain orientations. To understand the large plastic deformation at normal temperature and strain-rate, slip is considered to be the predominant mechanism for permanent deformation and can be viewed as the gliding of dislocations on a slip-plane [149–151].

This chapter studies the reasons for the plastic deformation in the aluminium metallization layer seen in the form of squeeze-out in actual experiments is studied in detail using a crystal plasticity based finite element (CPFEM) simulation. The deformation mechanism of the grain texture is analysed to study its effects on the flow strength of the free air ball.

7.2 Finite element model development

A finite element model is developed to characterize the essential features of the deformation imposed in the experiments. In a ball bond process, the spherical FAB is deformed on Al metallized bond pad by microforging using a controlled force. A

three dimensional (3D) rate independent crystal plasticity constitutive model for the copper ball is utilised here to study the response during cratering. The implementation scheme and algorithm is described in detail in chapter 4. All the finite element calculations were carried out using the ABAQUS finite element package with a user sub-routine for the constitutive model. Due to the radial symmetry of the capillary and copper ball, only an axi-symmetric model is considered for the simulation. The modelled geometry consists of three components: the free air copper ball, the capillary and the aluminum pad. The discretized geometry along with boundary conditions for the microforging simulations are shown in Figure 7.2a. The diameter of the free air ball is set to $70\mu m$ based on experiment measurements of Hsu *et al* [147]. In the simulation, the capillary is considered to be rigid. This is justified as the capillary is made from alumina ceramic of elastic modulus 310 GPa which is larger than that of free air copper ball. The Inverse pole figure map of the following three cases of the copper ball texture are shown in Figure 7.2b: T_1 - (100) texture, T_2 - (011) texture and T_3 - (111) texture. Microstructural study on the initial FAB exhibits predominantly these kind of textures as reported by various researchers [141, 149–151]. The aluminum metallization pad was modelled as a deformable elastic-plastic material with J_2 plasticity and isotropic hardening [34]. The Young's modulus and the Poisson's ratio are 70.3 GPa and 0.33 respectively. The plastic stress-strain region of the metallization pad follows a power law $\sigma = K\varepsilon^n$, where $K= 120\text{MPa}$ (strength component) and $n= 0.12$ (strain hardening exponent). The computational domain of the FAB is discretized with 2767 and aluminum pad with 1200 four noded axi-symmetric elements, with reduced integration (CAX4R) and enhanced hour glass control. The strain gradients beneath ball-pad interface are the highest, so a very fine mesh is used in the contact regime and coarser mesh is used in other regions. The mesh selection is usually a compromise between solution accuracy and computational cost. The frictional contact interactions between the capillary - FAB, FAB - aluminum metallization pad are modelled using a Coulomb coefficient of 0.4 [148]. All the microforging simulations

are done under load control at a value of $15gf \pm 1$ ($\sim 0.15 N$) with 12000 increment in steps to allow for the solution convergence and to avoid the instability usually observed in dynamic simulations.

Figure 7.2: Crystal plasticity finite element model of the impact stage showing a. boundary conditions, b. Inverse pole figure representing grain orientations of the FAB.

7.3 Results and discussion

The flow stress *i.e.* critical resolved shear stress of the free air copper ball with different crystallographic texture during the bond pad cratering is analyzed. The resulting dislocation pile up on the ball is understood to study the shear deformation bands. The axial stress on the aluminum metallization pad, which leads to squeeze out in the pad during the impact stage, is discussed.

7.3.1 Flow stress in the free air copper ball

The flow stress in the free air copper ball is analyzed for various crystallographic texture orientations. The ball when deformed under the capillary exhibits, crystallographic slip, which is explained with the simulations. The slip bands are formed due to lattice distortion. As the lattice distortion becomes more severe, the number

of distinct slip planes increases and these slip planes interact with one another. Due to this, the slip system becomes active, nucleation of dislocation begins and plastic deformation of the FAB is observed. The deformation bands of the copper ball obtained from the finite element simulations are shown in Figure 7.3a to 7.3c. The dotted line from A (the point where the capillary is in contact with the FAB) - B (base of the FAB) clearly illustrates the formation of the slip bands. It can be seen that, the severe stress concentration and lattice distortion happens predominantly at the base of the ball, which is clearly observed from the simulations and is compared with experimental observations. The dotted line from A-B as observed from Figure 7.3d shows the experimentally observed slip bands at the base of the ball which reasonably agrees to the numerical study. The free air ball, irrespective of the crystallographic texture slips leading to plastic deformation.

At the end of the simulation or applied load of $15gf$, the flow stress of (100) textured ball reaches the highest followed by the textured ball (011), whereas the (111) textured ball shows the least stress. The (100) ball, which has least stiffness, slips considerably due to which, less impact load is transferred to the Al metallization pad. The (011) ball also shows a slight resistance to slip which can be seen from the simulation results, but flow occurs relatively throughout the ball. It is interesting to note that, the (111) plane though, susceptible to slip because of its closed packed nature, resists slipping due to a softer metallization pad. This may be attributed to the number of slip systems activated and the way these systems interact. In FCC materials, there are 12 different slip systems that can contribute to the deformation process. The contribution of each slip systems to the plastic deformation of the FAB plays a prominent role in the slip systems activity. The number of active slip systems increases at the onset of plastic flow. While in some grain orientations, primary and secondary slip occurs during large plastic deformation, the crystal kinematics is respected that primary slip increases at the onset of plastic flow, while secondary slip is almost negligible. As expected, (100) orientation has the largest number of activated slips (eight systems) on all four slip

planes followed by the (011) orientation, which has four slips activated on three different slip planes and finally (111) in which three slip systems on two slip planes are activated. This clearly proves that the grains are locally exposed to different load levels from the external load applied on the free air ball. The flow stress of the primary slip systems from the different crystallographic grain orientations can be attributed through Schmid factors. The (100) texture is not favourably orientated to the external strain, which leads to a lower global Schmid factor than the (111) texture *i.e. the slip systems can be activated under a smaller external load*, thereby plastically deform before grains which are favourably oriented to the external strain *such as (111) grain orientations*. The (011) grain orientations are also oriented to the local loads rather than the external load, thereby displays a similar flow stress pattern of (100) crystallographic texture. The (111) grain orientations from the flow stress is shown to have higher global Schmid factors, because they are more favourably orientated to the global external strain compared to their local, internal load in the grains. The above fact can be attributed that, there is no favorable slip direction for the deformation of (111) FAB and no slip system can be directly activated. Due to this, the flow stress of the (111) crystallographic texture after the impact simulation shows that, the deformation on the FAB is not large enough to change the activated primary slip systems in some dead regions as shown in Figure 7.3c. The (100) orientation exhibits the highest symmetry among all orientations with four possible $\{111\}$ slip planes that have identical Schmid factor of 0.4082, which leads to immediate work hardening [141]. The (011) orientation also exhibits symmetry with three possible slip planes that have Schmid factor of 0.4082. The (1 1 1) orientation has the lowest symmetry among these three orientations with two possible slip planes. The flow stress of the FAB starts from the onset of capillary impact which is a common phenomenon observed in all the texture cases. The deformation zone obtained from the flow stress pattern in the free air ball through the crystal plasticity finite element (CPFEM) simulations is in good agreement with the experimental observation. The slip band initiation and the flow stress

concentration are well mapped in the simulations.

Figure 7.3: Flow stress in the free air ball with different crystallographic texture a. 100, b. 011, c. 111 and d. Slip bands from SEM observation [2].

The slip system shear strain γ as shown in Figure 7.4 of the free air ball with various crystallographic textures provides a clear understanding of the plastic flow of the grain orientations. Consequently, γ is an index that represents the interaction of dislocations from the effect of hardening in the FAB for different crystallographic textures. As for the magnitude of total shear strain from all the activated slip systems, it is largest for the (100) and smallest for the (111) oriented free air copper ball. Under the loading considered here, strain localization and shear banding are

the common phenomenon observed in the free air copper ball [149]. Furthermore, these plots show that the dislocations are very sensitive to crystal orientation. The accumulated slip calculated by the CPFEM model for the impact stage after each increment is defined as the sum of all shear strains on all active slip systems which indicates the deformation energy stored in the material. The deformed shape of the impacted ball shows the formation of bands of localized strain in the regions where the dislocations are very high. This suggests that the activities of fast moving dislocations accompanied by energy dissipation, can be considered as sources for localized deformation. The interaction of latent slip systems has been able to explain this. The overall hardening in the grain has been attributed to different strength of dislocations in the various slip systems. The high hardening rate of the FAB in stage II is a direct consequence of dislocations in the secondary slip systems. The selectively active slip systems hardens at a faster rate due to the interactions of the dislocations *i.e. latent hardening*. Figure 7.4a clearly shows the formation of band-like dislocation cells coincident with the slip planes. In the (100) crystallographic texture, at the edges of the FAB where the bulk shear bands are initiated, shear strains between 0.35 and 0.4 occur, whereas shear strains are slightly lower in between 0.25 and 0.3 in the (011). The (111) textured FAB shows the smallest shear strain of between 0.17 and 0.21. At the base of the (100) FAB, the shear strain increases to a value between 0.4 and 0.5. When the dislocations are activated by the stress field, the lattice distortion is inevitable and the deformation energy will increase. The deformation shows quite a homogeneous distribution at the base of the FAB. The (011) textured FAB exhibits a lower shear strain at the FAB base, where it measures between 0.19 and 0.24 whereas the (111) textured FAB exhibits a least deformation shear strain value between 0.03 and 0.07. Although the main features of these bands do not seem to change with crystal orientation, the dislocation pile up in these bands differ from one orientation to another. As observed from slip activation discussion, (100) orientation shows multiple bands running on the primary activated slip planes. On the other hand

(011) orientation shows bands crossing each other suggesting the activation of dislocations on three slip planes and (1 1 1) orientation shows weak bands running on two primary slip planes.

Figure 7.4: Accumulated plastic slip of the FAB with different crystallographic texture a. 100, b. 011 and c. 111

7.3.2 Aluminum squeeze in the pad

The axial stresses σ_{22} in the y direction of the aluminum metallization pad after the cratering simulation with (100), (011) and (111) crystallographic oriented free air ball is shown in Figures 7.5a to 7.5c and compared with the experimental mea-

surements as shown in Figure 7.5d. The experimental cratering process clearly shows squeeze out from the aluminum metallization pad. The deformation of the pad and the aluminum squeeze agrees well with the simulation results. When a spherical free air copper ball smashes the aluminum layer, an axial stress is generated purely due to the impact on the copper surface which travels radially outside, away from the center. This contributes to shearing the aluminum layer when the shear strength of the aluminum layer is exceeded. The causes of plasticity produced in the aluminum metallization leading to squeeze-out in actual experiments can be analyzed by simulations. The aluminum squeeze out with different crystallographic textured FAB is measured from the simulations as shown in Figure 7.6. The anisotropic crystallographic properties of the ball is responsible for the deformation characteristics of the pad.

The axial stresses generated in the softer aluminum metallization pad is a result of resistance to deformation, when different crystallographically textured FAB impacts the pad. A higher compressive stress of 28.30 MPa is generated in the surface when a (100) crystallographic oriented ball impacts, compared to 6.20 MPa in (011) and a tensile stress of 9.20 MPa in the (111) FAB. The (100) ball shows a homogeneous plastic deformation leading to less squeeze out compared to the other free air balls. The aluminum surface shows a compressive stress when smashed with the (011) ball whereas a transition from compressive to tensile stress is observed in the surface during the impact of (111) ball. This is due to the increase in resistance to deformation in the aluminum pad impacted with (011) and (111) ball. The results showed a higher squeeze out of $3.52\mu m$ from the pad when impacted with a (111) oriented ball displaying a large resistance to plastic flow. The aluminum surface impacted with (011) ball also showed a slight increase in the squeeze out value to $2.37\mu m$ compared to the (100) FAB which showed the least squeeze out at $1.19\mu m$. The ball deformation directly affects the softer aluminum pad. The (100) ball had a large plastic deformation and the load was equally dissipated to the aluminum pad, whereas the FAB with higher elastic stiffness *i.e* (011) and

(111) FAB transferred the load to the pad thereby deforming the pad to a greater extent.

Figure 7.5: axial stress σ_{22} in the pad during the cratering with different free air ball texture a. 100, b. 011, c. 111 and d. Aluminum pad squeeze out [151].

Figure 7.6: Aluminum pad squeeze

7.4 Summary

Microforging simulation of polycrystalline free air copper ball of three crystallographic orientations, i.e., (1 0 0), (0 1 1) and (1 1 1) were carried out using a commercial finite element software (ABAQUS) incorporating a rate independent crystal plasticity constitutive law. The crystallographic texture effect of FAB on

the slip band formation is discussed in detail and compared with experimental measurements. The aluminum metallization pad squeeze from the simulations is also analyzed to understand the flow stress of the FAB. From the slip system activity, the flow stress was studied and analyzed. The shear strain patterns gave an overview of the deformation energy in the crystallographically oriented FAB. The effect of the flow stress and dislocations observed, directly replicates the plastic flow of the softer aluminum pad. The following observations are made:

1. The crystallographic texture of FAB plays a major role in the bonding process. The flow stress of the FAB depends on the grain orientations from where the slip occurs. The (100) grain orientation FAB slips appreciably compared to the (011) and (111) texture. The (111) texture exhibits dead regions and resists slip. The shear strain pattern based on the slip system activity confirmed these results.
2. The aluminum metallization pad is softer and the impact load is transferred. The (100) FAB which impacts the aluminum pad shows a low squeeze out. The deformation is relatively homogeneous due to the considerable load absorbed by the FAB. The aluminum pad when impacted with (011) and (111) texture exhibits a large squeeze out patterns. The FAB resist to flow under load, thereby causing less deformation to the ball. The ball in turn transfers the load to the softer bond pad which in this case is aluminum.
3. The bond pad cratering is a reliability issue in the process. Large squeeze out of aluminum leads to the pad failure. The (111) texture of the wire which is preferred for the bonding process due to its high strength and stiffness can cause considerable damage to the bond pad leading to the failure. This remains a challenge how these contradictory properties can be optimised for better reliability during the bonding process.

Chapter 8

Conclusions and Recommendations

This chapter focuses on the major contributions of this thesis. A concluding summary of the work is discussed. Some general recommendations for further investigation is given.

8.1 Conclusions

Thin wires used in interconnect technology is produced by cold wire drawing process. The properties of the wire plays a major role in the reliable performance of the chip. This work primarily focuses on analysing the drawn wire mechanical properties affected by microstructure using crystal plasticity based computational framework for the constitutive modeling. Also, further interest is on the bond pad cratering. The major conclusions from this thesis are as follows:

- Single and multistage drawing simulations based on industrial process parameters such as die angle and area reduction were simulated to using classical flow theory of plasticity. From the simulations, the residual stresses in the wire as a function of drawing stages are obtained. The drawn wire transverse cross-section was analyzed for stress inhomogeneity by simulated microindentation tests. The results showed that, lower die angles *i.e.* 4° to 6° used in this study does not influence the drawing stress, which was seen from finite element calculations, slab method and experimental measurements. Also, the residual stress distribution was seen to be negligible. The area reduction had

significant effect on the drawing stress as well as residual stresses of the wire (Figures 3.4 and 3.6a - 3.6c). The center and surface of the wire obtained from single stage drawing have higher compressive and lower tensile residual stresses compared to multistage for the equivalent area reduction. The tensile stress regions of the wire promotes yielding leading to larger indentation depths compared to the compressive regions. This was seen from the profiles of pile up (h_c/h_{max}), elastic recovery parameter (h_f/h_{max}) and mean contact pressure distribution p_m . The (h_c/h_{max}), (h_f/h_{max}) values increased when the residual stress region shifted from compressive to tensile whereas the p_m values decreased (Figures 3.8a - 3.8f). The stress inhomogeneity across the transverse cross section of the wire was clearly seen from this study.

- The initial study provided the reasoning to understand the microstructural behavior of the wire. The constitutive modeling of the material based on crystal plasticity framework for microstructural behavior has been implemented based on a rate independent theory. Rate independent theory incorporating self and latent hardening to account for dislocations is studied. A multi-yield surface condition is solved for the active slip systems based on Kuhn-Tucker criteria and the slip systems interactions is accounted. Complex texture based on heterogeneous plastic deformation in the active slip systems is analyzed. A hardening response (Figure 4.3) showing three stages of hardening in a single crystal copper of (111) orientation validates the interaction of active slip systems
- The nanoindentation simulation of single crystal copper in different crystallographic orientations was studied based on implemented rate independent crystal plasticity theory. The interaction of active slip systems was analyzed to understand the single crystal behavior. The heterogeneous plastic deformation of different crystallographic orientations was studied based on load - displacement and mean effective pressure curves (Figures 5.2 and 5.3). The shear stress and strain in the active slip systems showed the anisotropic stress

fields in different crystallographic orientations (Figure 5.4). The analysis confirmed the effect of crystallographic orientation on the mechanical properties of the material.

- The resulting microstructure of the polycrystalline copper wire from the drawing process was studied based on crystal plasticity theory to understand the fiber texture in the center and complex texture at the surface. The wire drawing was simulated to understand the deformation processing involved. Experiments of the wire drawing process was conducted to study the texture evolution. The wires were drawn in single as well as multistage for a given equivalent area reduction. The initial wire exhibited a random texture with $\langle 100 \rangle$ along the longitudinal section. As the drawing strains increased, the $\langle 111 \rangle$ texture increased in strength (Figures 6.9b - 6.9d). The complex textures also decreased with increase in drawing strain. The single stage drawn wire had high $\langle 111 \rangle$ texture component with less complex textures. The fiber texture also exhibited strong α and β components. The Goss and Copper components were also present remnant from the initial wire microstructure. The multistage drawn wire also exhibited Copper and Brass components. The surface texture of the drawn wire showed prevalent complex texture components for both the drawing schemes studied (Figure 6.10).
- The effect of the free air ball crystallographic texture on the copper bonding is analysed. The bond pad impact stage is simulated to study the cratering which plays a vital role in the reliability of the process. The microstructure of the free air ball was superimposed from experimental studies reported in the literature (Figure 7.2b). The impact stage simulation results showed that, free air ball with (111) crystallographic texture resists to slip thereby resulting in large squeeze out from the aluminum metallization pad. The shear strain of the active slip systems also verified these observations (Figure 7.4c). The slip occurs predominantly at the base of the ball for all the

crystallographic orientations studied. The high stiffness wire is desired for the bonding applications where it has to withstand high loop stability and drag forces but considerable damage to the soft metallization pad is also an area of concern.

8.2 Suggestions for future work

Further research pertinent to this related area is as follows:

- The finite element modeling of the wire drawing process using the rate independent crystal plasticity is limited to account only active crystallographic slip and grain orientations *i.e.* texture during the deformation process. Size of grains and the dislocations such as statistically stored (SSDs), geometric necessary (GNDs) associated along the grain boundaries are ignored. This can be included empirically to the numerical framework when studying texture evolution.
- The aim of the wire drawing industry is to reduce the residual stresses in the wire. Recent studies using skin pass die has attracted considerable attention. Drawing experiments and simulations can be conducted based on this die set-up and mechanical response can be analysed. Some of the preliminary simulation results analysed from our study can be found in Appendix A.
- The crystal plasticity modeling has serious limitations with respect to the computational time and domain. Even though relative amount of microstructural information is obtained, the computational cost is expensive. For applications related to fatigue, the anisotropic criteria is relatively useful. Phenomenological anisotropic yield surface can be developed based on crystal plasticity modeling and implemented in finite element framework. Understanding the fatigue of the drawn wire based on anisotropic constitutive modeling will help in analysing the mechanical properties at the macroscale.

- Drawn wire is coiled onto a circular drum for storage. The properties of the drawn wire has always been an area of interest and are being studied. However, there lies a gap in literature related to mechanical properties of the drawn wire when it is coiled. The mechanical properties of the wire after it undergoes a coiling and uncoiling is quite an interesting research to explore which will provide useful information to the wire bonder. Appendix B shows some initial results of finite element simulations obtained.
- During the bond pad cratering, temperature rise of the free air ball and its effect on texture can be accounted. This will lead to modeling the softening of the free air ball during the wire bonding process.

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Finite element simulation results of the drawn wire using a stepped die

Diagram illustrating a mechanical system for a moving wire. A vertical wire is shown, labeled "Deformable wire". A horizontal force r is applied at the top. The wire is supported by a rigid die and a moving die. The moving die is labeled "Die moving @ $V=1\text{mm/sec}$ ". The angle of the wire is labeled α_2 . The boundary condition $U_r = 0$ is indicated on the left.

134

(a) RA 10%

(b) RA 20%

(c) RA 30%

Figure A.2: Axial residual stress distribution on drawn wire for area reductions (RA) a. 10%, b. 20% and c. 30%

(a)

(b)

(c)

Figure A.3: Influence of residual stress on a. $h_c/h_{\max}$ (pile-up) versus $h_{\max}/R$ (indentation depth) , b. $(W_t - W_u)/W_t$ versus $h_f/h_{\max}$ (elastic recovery parameter) and c. p_m/Y versus $E_e a/YR$

Appendix B

Simulations of texture evolution in the drawn wire after coiling-uncoiling

The drawn wires are coiled and uncoiled from a circular drum. To replicate the experimental conditions in the finite element simulation, the coiling was simulated by applying a displacement at the end of the wire and was wrapped on a circular drum of radius 100 mm. The displacement unloading reasonably resembles uncoiling. Limited number of grain orientations *i.e.* 80 was considered for these simulations. The as received copper wire, single stage and multistage drawn wire were studied for texture evolution after these simulations. Some results from this analysis are shown in Figure B.1.

(a) as received wire

(b) Single stage drawn wire

(c) Multistage drawn wire

Figure B.1: Texture evolution of the wire after coiling - uncoiling simulations.