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Phononic and structural response to strain in wurtzite-gallium nitride nanowires

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Gallium nitride (GaN) nanowires exist in a myriad of cross-sectional shapes. In this study, a series of classical molecular dynamics simulations is performed to investigate the strain-phononics-structure relationship in rectangular and triangular wurtzite-GaN nanowires. The thermal conductivity of the nanowires is linearly dependent on the uniaxial strain in both compressive and tensile regimes, and shows no significant dissimilitude for the same amount of strain exerted on the two types of nanowire. This is coherent with an analytical approach using the Boltzmann transport theory. However, the thermomechanical behaviour at the vertex regions shows palpable differences between the two subfamilies, relative to the non-vertex faceted regions, as the structural morphology is most disparate at the vertices. Furthermore, the degree of strain asymmetry is a strong determinant of the vibrational response and consequently thermal conductance. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4716476>]

I. INTRODUCTION

Gallium nitride (GaN) is a group-III-V wide-band-gap semiconductor with a high melting point, high carrier mobility, and high electrical breakdown field. It is typically used in high-power and high-frequency electronic applications such as Blu-ray laser diodes,¹ high electron mobility transistors (HEMTs),² and microwave power sources.³ GaN nanowires can also be used in field-effect transistors (FETs),⁴ and these devices have displayed excellent switching and conduction behaviour. However, this leap-and-bound of nanotechnology comes with an ineludible problem—with a rapid downscaling of device size to pack more devices in a unit area, more thermal energy is generated. As the performance^{5,6} and reliability⁷ of these devices degrade at high temperatures, it is imperative that thermal energy is efficiently dissipated from the device hot spots.

Thermal transport of GaN in the bulk^{8–10} and nanowire¹¹ forms is well comprehended. However, these studies are inadequate as the nanostructures often do not exist naturally in their relaxed-lattice states. Rather, structural strain is experienced due to (1) lattice strain between contacting materials, and/or (2) intrinsic strain during growth, with compression radially and tension axially.¹² The lattice strain induces microstructural changes near the interfaces, which in turn alters the vibrational properties of the nanostructures. Similarly for an intrinsic growth strain, the structure changes in dimensions and phonon transport is perturbed. In an earlier work, the effect of strain on the thermal conductance of generic solids is modelled and theoretically analyzed.¹³ As tensile strain acts on the solid and is increased in magnitude, both the sound velocity and the phonon relaxation time decrease, both of which reduce the thermal conductivity.

Along the same train of thought, Li *et al.* postulated that barring buckling effects in some nanostructures such as single-wall carbon nanotubes and single layer graphene, the continuous drop in group velocities and mode specific heat with the transition from compressive to tensile strain reduces the thermal conductivity.¹⁴ A more relevant examination of the strain-conductivity relationship in GaN nanowires¹⁵ shows that the tensile deformation reduces thermal conductance at sufficiently large diameters and below a temperature of 1495 K.

However, for a more complete investigation of the coupling of thermal and mechanical response in GaN nanostructures (i.e., thermomechanical behaviour), it is cardinal that the entire compression-tension spectrum is examined. For instance, on one hand, the lattice strain exerted on Wz-GaN (lattice constant of 3.19 Å) by a zinc-blende silicon carbide (Zb-SiC) substrate (lattice constant of 4.36 Å) is tensile, but on the other hand, a Wz-SiC substrate (lattice constant of 3.08 Å) strains GaN compressively. Moreover, there is a close relationship between the growth methodology, conditions, crystallographic symmetry, and nanostructure shape.¹⁶ The anisotropies of surface energies in the various crystallographic orientations result in different equilibrium cross-sectional shapes. Indeed, GaN exists in various shapes, such as rectangular¹⁷ and triangular¹⁸ in some nanowires, and hexagonal pyramid¹⁹ and prism²⁰ in other nanostructures. In specific, for a triangular GaN nanowire, the hydrogen-nitrogen carrier gas ratio modulates the growth velocity on the (112) and (001) facets.¹⁸ Hence the cross-sectional shape and the crystallographic orientation of the facets of GaN nanostructures are predominantly dependent on and sensitive to synthesis conditions. The multitude of possible GaN nanostructure shapes and sizes extends the potential of this material in nanotechnological applications, and this necessitates the study of its thermomechanical behaviour in its assortment of forms.

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II. OBJECTIVES

This paper surveys the transformation of microstructure and phonon dynamics of wurtzite (Wz)-gallium nitride in its nanowire form, with the application of uniaxial mechanical strain. It compares both the structural and phononic changes in two common types of GaN nanowires—one with a rectangular cross-sectional shape (rect-GaN), and the other with a triangular one (tri-GaN). Akin to the huge family of carbon nanotubes with different chiralities, GaN nanowires have an array of possible cross-sectional shapes of different crystallographic orientations.^{17–20} The particular crystallographic planes of rect-GaN and tri-GaN are chosen in this work (A) as representative nanowires with asymmetric cross-section, and (B) with considerations to minimize the difference of the structural dimensions and number of atoms between both nanowires. Essentially, the Ga-N unit cell is identical in orientation in both nanowire types, and hence is not a determinant in any dissimilitude of the structural and vibrational response observed. Ultimately, this work aims to unravel the effects of both strain and local morphology on the thermo-mechanics of GaN nanowires.

III. SIMULATION DETAILS

Classical molecular dynamics simulations were carried out in this study. Two types of wurtzite-GaN nanowires, of the rectangular and triangular cross-sectional shapes, were modelled. In the former case, 1476 atoms were contained in a 14.3 Å by 24.8 Å by 46.7 Å simulation cell, aligned with the axial faces of the crystallographic planes $\{11\bar{2}0\}$ and $\{1\bar{1}00\}$ (Figure 1(a)), while in the latter, 1296 atoms were enclosed within a 12.7 Å by 41.3 Å by 46.7 Å cell, with the facets of planes $\{11\bar{2}0\}$ and $\{1\bar{1}00\}$ and $\{1\bar{1}00\}$ (Figure 1(b)). The three orientations are defined in Figure 1. The unit cell, which comprises of 2 gallium (Ga) and 2 nitrogen (N) atoms, was aligned in the same orientation in both types of nanowires (enclosed in dotted lines in Figure 1(b)). The gallium-nitrogen covalent-ionic interactions were expressed by the Tersoff-Brenner potential,²¹ with the parameters derived and fit by Nord *et al.*²² The Newtonian velocity Verlet algorithm was adopted to predict the next atomic positions and velocities, with a timestep of 0.5 fs. The surface atoms at the extreme ends of the nanowires were fixated and the dynamics restricted by an adiabatic approximation. Nosé-Hoover^{23,24} thermostats were used at the extreme ends of the system to create a temperature difference. The cold and hot thermostat temperatures were predefined to be 290 K and 310 K, respectively, since the intent of this work is to study the structure and phonon dynamics of GaN at room temperature. Mechanical strain is applied to the nanowire by translating atoms that are approximated adiabatically in the axial direction for a certain number of time-steps. An average equilibration time of 1 ns is allowed for all simulations, before atomic data is recorded for post-analyses. A total simulation time of 2 ns is run. The local instantaneous temperatures are defined and calculated from the atomic kinetic energy as

$$T(z, t) = \frac{m}{3k_B} \left[v_x(z, t)^2 + v_y(z, t)^2 + v_z(z, t)^2 \right], \quad (1)$$

FIG. 1. Side-view schematic of wurtzite-gallium nitride nanostructure with (a) a rectangular $\{11\bar{2}0\}$ by $\{1\bar{1}00\}$ cross-section, and (b) a triangular $\{11\bar{2}0\}$ by $\{1\bar{1}00\}$ by $\{1\bar{1}00\}$ cross-section. The orange and green circles refer to the gallium and nitrogen atoms, respectively. Dashed box depicts a Ga-N unit cell, with diagonal and parallel bonds.

where k_B is the Boltzmann constant, m is the atomic mass, and the subscripts x , y , and z , refer to the 3 orientations in the simulations.

IV. DEPENDENCE OF THERMAL CONDUCTIVITY ON STRAIN

The GaN nanowires in their relaxed-lattice state recorded a thermal conductivity of about 3 W/m K (Figure 2). This is slightly smaller than experimental measurements of 10–15 W/m K in Ref. 11, mainly due to a difference in the dimensions of the nanowires. In the aforementioned work, the length and diameter are 5 μm and 100 nm, respectively, while in this work, they are around 5 nm and 3 nm, respectively. The increased surface-to-volume ratio (of about 40 times larger, by calculation) introduces more surface-phonon scattering in the nanowire, and reduces its phonon mean free path and phonon velocity. Hence these GaN nanowires conduct thermal energy less efficiently. However, it is noted that

FIG. 2. Variation of thermal conductivity with strain for both rectangular {1120} by {1100} and triangular {1120} by {1100} GaN nanostructures.

the thrust of this study is on the strain dependence of structural and vibrational properties of different forms of GaN nanowires. In this regard, a relatively qualitative approach is taken in the analyses.

With the application of tensile strain, the thermal conductivity of both types of GaN nanowires reduces. On the other hand, compressive strain increases the thermal conductivity. The change of conductivity with strain in both regimes is fairly constant—a change of 20% in the thermal conductivity with a strain of 10%. This is comparable with that of Ref. 15, where a change of 30% in the conductivity is observed with the same amount of strain, albeit only a tensile one. Moreover, the variation of thermal conductivity with strain is similar in the rect- and tri-nanowires.

By deforming the lattice structure compressively (tensilely), the axial interatomic force constants increase (decrease) in magnitude.²⁵ In the Boltzmann transport formulation, three-phonon scattering rates are derived from Fermi's golden rule²⁶ with anharmonic interatomic force constants and phonon distribution,

$$W_{\lambda\lambda'\lambda''}^{\pm} = \frac{\hbar\pi}{4N} \frac{(n_{\lambda}^0 + 1)(n_{\lambda'}^0 + 0.5 \pm 0.5)n_{\lambda''}^0}{\omega_{\lambda}\omega_{\lambda'}\omega_{\lambda''}} \times |\Phi_{\lambda\lambda'\lambda''}^{\pm}|^2 \delta(\omega_{\lambda} \pm \omega_{\lambda'} - \omega_{\lambda''}), \quad (2)$$

where $\Phi_{\lambda}^{\pm}$ are the third-order anharmonic interatomic force constants, n_{λ}^0 are the equilibrium phonon distributions, ω_{λ} are the phonon frequencies, and N is the number of unit cells. The quantum numbers are denoted together by $=(q, j)$: q is the dimensionless wavenumber with translational periodicity, and j is the phonon branch. The three-phonon matrix element is

$$\Phi_{\lambda\lambda'\lambda''}^{\pm} = \sum_{\kappa} \sum_{l'\kappa'} \sum_{l''\kappa''} \sum_{\alpha\beta\gamma} \Phi_{\alpha\beta\gamma}(0\kappa, l'\kappa', l''\kappa'') e^{i\vec{q}' \cdot \vec{r}_{l'}} e^{i\vec{q}'' \cdot \vec{r}_{l''}} \times \frac{e_{\alpha\kappa}^{\lambda} e_{\beta\kappa'}^{\lambda'} e_{\gamma\kappa''}^{\lambda''}}{\sqrt{M_{\kappa} M_{\kappa'} M_{\kappa''}}}, \quad (3)$$

where $\Phi_{\alpha\beta\gamma}(0\kappa, l'\kappa', l''\kappa'')$ are real-space anharmonic interatomic force constants, $\vec{r}_l$ is the position vector of the l th unit

cell, κ is the atom number (with mass M_{κ}) in a unit cell, and $e_{\alpha\kappa}^{\lambda}$ are the mode eigenvector. F_{λ} is a iterative solution that is dependent on the three-phonon anharmonic scattering rates $W_{\lambda\lambda'\lambda''}^{\pm}$.^{27–33}

$$F_{\lambda\alpha} = F_{\lambda\alpha}^0 + \Delta F_{\lambda\alpha}, \quad (4)$$

where

$$F_{\lambda\alpha}^0 = \frac{\hbar\omega_{\lambda} n_{\lambda}^0 (n_{\lambda}^0 + 1) v_{\lambda\alpha}}{T Q_{\lambda}}, \quad (5)$$

and

$$\Delta F_{\lambda\alpha} = \frac{1}{Q_{\lambda}} \left\{ \sum_{\lambda'\lambda''} \left[W_{\lambda\lambda'\lambda''}^{\pm} (F_{\lambda''\alpha} - F_{\lambda'\alpha}) + \frac{1}{2} W_{\lambda\lambda'\lambda''}^{-} (F_{\lambda''\alpha} + F_{\lambda'\alpha}) \right] \right\}. \quad (6)$$

with the total scattering rate

$$Q_{\lambda} = \sum_{\lambda'\lambda''} \left(W_{\lambda\lambda'\lambda''}^{\pm} + \frac{1}{2} W_{\lambda\lambda'\lambda''}^{-} \right) + \sum_{\lambda'} W_{\lambda\lambda'}^{\text{imp}} \quad (7)$$

where α is the Cartesian coordinate for the three dimensions x , y , and z . The lattice thermal conductivity is related to the mode specific heat C_{λ} , phonon velocity v , and phonon lifetime τ_{λ} by $\kappa = \frac{1}{V} \sum_{\lambda} C_{\lambda} v^2 \tau_{\lambda} = \frac{1}{V} \sum_{\lambda} \frac{C_{\lambda} \tau_{\lambda} v^2}{\hbar \omega_{\lambda} v_{\lambda}} F_{\lambda}$, and the phonon lifetime is related to $F_{\lambda z}$ as

$$\tau_{vz} = \frac{TF_{\lambda z}}{\hbar \omega_{\lambda} v_{\lambda z}} \quad (8)$$

Therefore, with compression (tension), $F_{\lambda z}$ increases (decreases) with the axial interatomic force constants, and consequently the lattice thermal conductivity increases. The strain-thermal conductivity relationship observed in this work is thus coherent with the Boltzmann transport theory.

V. STRUCTURAL CHANGES IN STRAINED GaN NANOWIRES

As noted, all nanowires modelled in this work are built up from an identical Ga-N unit cell (Figure 1(b)). Putting these building blocks together in a different way forms the rect- and tri-GaN nanowires. Three different regions are defined: (1) vertex (as represented and exemplified by the solid black lines in Figure 1), (2) non-vertex/facet surface, and (3) bulk regions. These three regions are chosen because of the morphological differences for each of these regions. The morphology varies (a) between vertex and non-vertex, and (b) more significantly at the vertices than at the non-vertex facets between both GaN nanowires (due to different internal angles of the cross-sectional shape). Naturally, this affects the structural and vibrational response to strain, and hence it is in our interest to probe these regions.

The structural deformation that accompanies the strain in the GaN nanowires is investigated. In addition to the categorization of region (vertex, non-vertex, bulk), a distinction is made between the orientation of atomic bond. A “parallel”

Ga-N bond is in the same direction/parallel to the nanowire axis, while a “diagonal” one lies at an oblique angle to the axis (Figure 1(b)). Figure 3 presents the change of mean bond length with strain in both nanowire types. The dotted line at 1.95 Å depicts the Ga-N bond length in the unstrained lattice, predefined at the start of the simulations. However at a relaxed-lattice state, only the bulk parallel bond length remains at 1.95 Å, while the bulk diagonal bonds increase in length, and all other bonds contract. Without strain, in general from the plots, the bond length (diagonal and parallel) in the bulk is largest, followed by that at the non-vertex, and then at the vertex region. This is due to the bond-order-length-strength (BOLS) mechanism,^{34–36} whereby a smaller coordination number of atoms at these regions result in a stronger and shorter bond at equilibrium. With tensile strain, all the parallel bonds increase in length, but those in the bulk region increase significantly more than those in the other region types. The reduction in cross-sectional area (of approximately 1.9% observed in the rect-nanowire at 3.40% tensile strain) with tension could be attributed to the shortening of the (A) the vertex diagonal bonds in the rectangular nanowire, and (B) the bulk diagonal bonds in the triangular nanowire. More importantly, the vertex bonds behave in a different manner from the non-vertex bonds. The morphol-

ogy plays a critical role in dictating the minimum-energy structure of GaN.

The bond energy is a measure of bond strength in a chemical bond. The mean bond energy per bond at the vertex and non-vertex faceted region of the nanowires is calculated across different amounts of strain (Figure 4). Without strain, the bonds are stronger at the vertex region than at the non-vertex region for both nanowires, with a larger mean bond energy per bond (absolute value). The lower coordination number of the vertex atoms induces a spontaneous relaxation of their bonds, which is again coherent with the BOLS model.^{34–37} When the strain transitions from the compressive to tensile regime (in the examined range of strain), bonds other than those at the vertex region in the tri-nanowire generally strengthen. The tri-vertex bonds remain relatively constant in strength, though they are around 1.5% stronger than the rect-vertex bonds in the compressive regime, and for small tensile strains. Similar to the bond length analyses, the bond energy at the vertex for both nanowires are significantly different, as compared to that at the non-vertex. This accentuates the role played by morphology in the strength of the bonds in GaN nanowires.

VI. PHONONIC CHANGES IN STRAINED GaN NANOWIRES

To extract vibrational information at different locations from the nanowire, the velocity autocorrelation function is first computed from the time history of the velocity of the atoms, after which the local vibrational density of states (LDoS) is calculated by performing a Fourier-transform on the velocity autocorrelation function at particular atomic locations. Figure 5 shows the transition of the vertex and non-vertex LDoS (averaged over data from 3 unit cells) with compressive and tensile strain. The bulk LDoS is included as a reference. The strain of $\pm 3.40\%$ (a) approximates that present in Wz-GaN/Wz-Si crystals, and (b) is sufficiently large to distort the lattice without buckling effects. A close inspection of the prominent LDoS/vibrational density of states (VDoS) peaks indicates a shift in their positions (Figure 6) with strain. However, the direction of shift is not universal—at the vertex region, some modes stiffen, while others soften with tension, and at the non-vertex region, they soften with tension.

FIG. 3. Change of mean bond length with strain for different regions in (a) rectangular and (b) triangular GaN nanostructures.

FIG. 4. Changes in bond energy with strain at vertex and non-vertex regions.

FIG. 5. Vibrational density of states for both (a) rectangular and (b) triangular GaN nanostructures at different strains.

More interestingly, some of the modes at the vertex region of the rect- and tri-GaN nanowires behave dissimilarly (V2 and V4), while they respond likewise at the non-vertex region (N1, N2, and N3). For V1, although the peak position remains relatively constant with strain, their full-width-half-maximum (FWHM) is strain-dependent. Furthermore, the vertex phonon modes of the rect-nanowire are around 2(V4)–40%(V2) stiffer than those of the tri-nanowire, with and without strain in that range, suggesting that the vertex atomic vibrations are more rigid in the rect-nanowire when there is minimal or no strain. From the above observations, the vibrational response to strain in GaN varies spatially (for vertex, non-vertex). Between nanowires with dissimilar cross-sectional shapes, they respond differently only at the vertex region and not at the non-vertex region. Succinctly, morphology is a predominant factor of the vibrational response to strain. Apparently, both structure and atomic vibration are interrelated, and morphology is pivotal to their response to strain.

Despite the disparate vibrational response at the vertex region, the conductivity-strain relationship observed in Figure 2

FIG. 6. A Comparison of VDoS peak shifts in both rectangular and triangular GaN nanostructures at different strains.

remains relatively similar for both nanowires. This is because the ratio of vertex to total number of atoms (Rect-: $\frac{4 \text{ Vertices} \times 18 \text{ Atoms/Vertex}}{1476 \text{ Total No. of Atoms}} = 4.9\%$, Tri-: $\frac{3 \text{ Vertices} \times 18 \text{ Atoms/Vertex}}{1296 \text{ Total No. of Atoms}} = 4.2\%$) is small, diluting the significance of vertex modes. Nanowires with a larger aspect ratio (i.e., cross-sectional area is smaller) have a larger {vertex atoms-total number of atoms} ratio, and they are expected to demonstrate a different conductivity-strain relationship between nanowires of dissimilar shape.

VII. TEMPERATURE DISTRIBUTION IN STRAINED GaN NANOWIRES

Using Eq. (1), the localized temperature is calculated at every atomic position in the tri-GaN nanowire, and averaged in the x-orientation. In an unstrained state, the steady-state temperature distribution determined after a simulation time of 2 ns (inclusive of equilibration) is relatively even (Figure 7(b)); the hotter regions are near the hot sink (top) and the cooler regions are near the cold sink (bottom), with a gradually varying distribution in between these regions. With compressive or tensile strain, more “island”-like thermal hotspots are observed in the profile (Figures 7(a) and 7(c)). To guide the eye, regions with temperature in the moderate range are bound by a black solid line. This bound shape is more irregular in the strained state of the nanowire than when it is unstrained.

FIG. 7. Temperature profiles of $\{11\bar{2}0\}$ face of triangular GaN nanostructure with strain (a) $\varepsilon = -3.40\%$, (b) $\varepsilon = 0$, and (c) $\varepsilon = 3.40\%$.

VIII. MODERATION EFFECT OF PHONONIC RESPONSE TO ASYMMETRY IN STRAIN

Axial tensile/compressive strain modifies the crystal structure, and induces a change in the vibrational properties of GaN nanowires (Figure 8(a)). Matter-of-factly, strain exerted on the nanowire is likely to be asymmetric across the cross-section,

FIG. 8. Schematic of (a) symmetrically strained, and (b) asymmetrically strained rectangular GaN nanostructures.

due to: substrate lattice strain on only one side of the nanowire, structures contacting off-axis at their extreme ends, and/or growth non-uniformity. Therefore, the structure deforms asymmetrically (Figure 8(b)). Consequently, it is essential to

FIG. 9. Modulation of phonon softening/stiffening in asymmetrically strained rectangular GaN nanostructures.

FIG. 10. Change of κ - ϵ relationship in asymmetrically strained rectangular GaN nanostructure.

examine the effect of strain (and hence structural) asymmetry on vibrational response in these nanowires.

Instead of translating all atoms at the extreme ends away/towards the center of the nanowire to model mechanical strain, only atoms nearer one edge are translated. The rectangular nanowire deforms to a trapezoidal structure (Figure 8(b)). To account for strain non-uniformity, a positional translation of x for symmetric strain equates a translation of $2x$ for asymmetric strain. Figure 9 compares the peak shift of the VDoS in symmetrically and asymmetrically strained rect-GaN. The phonon mode softening/stiffening is moderated by the asymmetry of the strain; the mode frequency shifts are considerably smaller than those in a symmetrically strained nanowire. Consequently the moderating behaviour extends to and distorts the macroscopic property of thermal conductance—the strain asymmetry lowers (raises) the thermal conductivity of a nanowire under compression (tension), relative to the event whereby strain is absent (Figure 10).

IX. CONCLUSION

Mechanical strain is applied to rectangular and triangular wurtzite-GaN nanowires to uncover its effects on the structural and vibrational properties. A linear strain-thermal conductivity relationship is observed across both compressive and tensile regimes, while the absolute value of conductivity in both nanowires is similar. This strain dependence of thermal conductivity is substantiated and explained by the Boltzmann transport formulation. Despite this, these two types of nanowires have demonstrated distinctly variant thermomechanical behaviour at the vertex regions, relative to that at the non-vertex faceted regions, due to morphological differences at the vertices in rect- and tri-GaN nanowires. In addition, asymmetry of strain on the nanowires moderates the vibrational response, and consequently its thermal conductance.

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- ¹M. Ikeda and S. Uchida, *Phys. Status Solidi A* **194**, 407 (2002).
- ²Y.-F. Wu, A. Saxler, M. Moore, R. P. Smith, S. Sheppard, P. M. Chavarrak, T. Wisleder, U. K. Mishra, and P. Parikh, *IEEE Electron Device Lett.* **25**, 117 (2004).
- ³H. Morkoç, *Nitride Semiconductors and Devices* (Springer-Verlag, Berlin, 1999).
- ⁴Y. Huang, X. Duan, Y. Cui, and C.M. Lieber, *Nano Lett.* **2**, 101 (2002).
- ⁵J. Piprek and S. Nakamura, *IEEE Proc.: Optoelectron.* **149**, 145 (2002).
- ⁶M. A. Huque, S. A. Eliza, T. Rahman, H. F. Huq, and S. K. Islam, *Solid-State Electron.* **53**, 341 (2009).
- ⁷G. Meneghesso, M. Meneghini, A. Tazzoli, N. Rochi, A. Stocco, A. Chini, and E. Zanoni, *Int. J. Microwave Wireless Technol.* **2**, 39 (2010).
- ⁸M. Kamano, M. Haraguchi, T. Niwaki, M. Fukui, M. Kuwahara, T. Okamoto, and T. Mukai, *Jpn. J. Appl. Phys., Part 1* **41**, 5034 (2002).
- ⁹M. D. Kamatagi, N. S. Sankeshwar, and B. G. Mulimani, *Diamond Relat. Mater.* **16**, 98 (2007).
- ¹⁰T. Kawamura, Y. Kangawa, and K. Kakimoto, *J. Cryst. Growth* **284**, 197 (2005).
- ¹¹C. Guthy, C.-Y. Nam, and J. E. Fischer, *J. Appl. Phys.* **103**, 064319 (2008).
- ¹²H. W. Seo, S. Y. Bae, J. Park, H. Yang, and K. S. Park, *J. Chem. Phys.* **116**, 9492 (2002).
- ¹³S. Bhowmick and V. B. Shenoy, *J. Chem. Phys.* **125**, 164513 (2006).
- ¹⁴X. Li, K. Maute, M. L. Dunn, and R. Yang, *Phys. Rev. B* **81**, 245318 (2010).
- ¹⁵K. Jung, M. Cho, and M. Zhou, *Appl. Phys. Lett.* **98**, 041909 (2011).
- ¹⁶V. Jindal and F. Shahedipour-Sandvik, *J. Appl. Phys.* **106**, 083115 (2009).
- ¹⁷E. P. Pokatilov, D. L. Nika, and A. A. Balandin, *Phys. Rev. B* **72**, 113311 (2005).
- ¹⁸T. Kuykendall, P. Pauzauskie, S. Lee, Y. Zhang, J. Goldberger, and P. Yang, *Nano Lett.* **3**, 1063 (2003).
- ¹⁹T. Akasaka, Y. Kobayashi, S. Ando, N. Kobayashi, and M. Kumagai, *J. Cryst. Growth* **189**, 72 (1998).
- ²⁰J. W. Cahn and W. C. Carter, *Metall. Mater. Trans. A* **27**, 1431 (1996).
- ²¹D. W. Brenner, *Phys. Rev. B* **42**, 9458 (1990).
- ²²J. Nord, K. Albe, P. Erhart, and K. Nordlund, *J. Phys.: Condens. Matter* **15**, 5649 (2003).
- ²³S. Nosé, *J. Chem. Phys.* **81**, 511 (1984).
- ²⁴W. G. Hoover, *Phys. Rev. A* **31**, 1695 (1985).
- ²⁵M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Clarendon, Oxford, United Kingdom, 1954).
- ²⁶E. Fermi, *Nuclear Physics* (University of Chicago, Chicago, USA, 1950).
- ²⁷J. Ziman, *Electrons and Phonons* (Cambridge University, Cambridge, England, 1960).
- ²⁸A. Ward, D. A. Broido, D. A. Stewart, and G. Deinzer, *Phys. Rev. B* **80**, 125203 (2009).
- ²⁹M. Omini and A. Sparavigna, *Phys. Rev. B* **53**, 9064 (1996).
- ³⁰A. Sparavigna, *Phys. Rev. B* **65**, 064305 (2002).
- ³¹A. Sparavigna, *Phys. Rev. B* **66**, 174301 (2002).
- ³²D. A. Broido, A. Ward, and N. Mingo, *Phys. Rev. B* **72**, 014308 (2005).
- ³³D. A. Broido, M. Malorny, G. Birner, N. Mingo, and D. A. Stewart, *Appl. Phys. Lett.* **91**, 231922 (2007).
- ³⁴C. Q. Sun, *Prog. Solid State Chem.* **35**, 159 (2007).
- ³⁵L. Pauling, *J. Am. Chem. Soc.* **69**, 542 (1947).
- ³⁶V. M. Goldschmidt, *Ber. Dtsch. Chem. Ges.* **60**, 1270 (1927).
- ³⁷C. Q. Sun, B. K. Tay, X. T. Zeng, S. Li, T. P. Chen, J. Zhou, H. L. Bai, and E. Y. Jiang, *J. Phys.: Condens. Matter* **14**, 7781 (2002).
- ³⁸G. C. Loh, B. K. Tay, and E. H. T. Teo, *Appl. Phys. Lett.* **97**, 121917 (2010).
- ³⁹J. Shiomi and S. Maruyama, *Phys. Rev. B* **73**, 205420 (2006).