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Effects of heterogeneity and prestress field on phonon properties of semiconductor nanofilms

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ABSTRACT

The phonon dispersion relation, phonon group velocity and phonon density of state in GaN-based wurtzite nanofilms under prestress fields are investigated theoretically. Considering the acoustoelastic effects and spatial confinement effects, the acoustic phonons properties in stressed AlN/GaN/AlN nanofilms are derived by using the elasticity model, comparing with those in the pure AlN nanofilm and pure GaN nanofilm. Numerical simulations demonstrate that the heterogeneity in GaN-based nanofilms can modify the phonon dispersion relations of nanofilms, leading to the change of phonon group velocity and phonon density of state. The stress field can significantly affect the phonon properties of GaN-based heterostructural nanofilms, e.g. the positive stress decreases the phonon energy and group velocity while enhances the density of state. The influence of the stress field is also sensitive to the thickness of each component in heterostructural nanofilms. The present work will be useful in tuning the phonon properties through phonon engineering and strain/stress engineering to control the thermal and electrical performance in GaN-heterostructure-based electronic devices.

1. Introduction

With the increasing development in nanomechanical and nanoelectronic devices or systems, the semiconductor materials with low-dimensional structures like nanowires and nanofilms draw more and more attentions. When the dimensions are limited to nanometer level, semiconductor nanostructures could be extremely different with the bulk materials in physical and mechanical properties such as carrier mobility, electric resistance, thermal conductivity and elastic modulus. Due to the wide applications of semiconductor nanostructures in optoelectronics [1,2], resistive switching [3,4], and biochemical sensora [5,6], the optimization and modification for their properties have made great progress. Since the nanoelectronic devices or systems are facing difficulties in heat dissipation, it is critically necessary to give an insight into the thermal properties in nanostuctured semiconductors [7–11].

Phonons as the quanta of crystal vibration, especially acoustic phonons, are dominant in transporting heat in semiconductors. Because of that the thermal and electric properties of semiconductors are sensitive to the phonon properties, it is important to study phonon performance in nanostructured semiconductors which have been widely used in micro/nano electronic devices or systems [12–15]. For instance, Balandin and his coworkers [16] theoretically simulated the phonon propagation and dispersion relations in the GaN nanostructures covered with various materials such as AlN and plastic materials. Groenen [17] made the calculations for phonon dispersion relations in Si membranes and silicon-on-insulator structures. Zou and Balandin [18] discussed the decrease of thermal conductivity under phonon confinement and boundary scattering in a silicon nanowire.

To optimize the physics properties of semiconductor materials in micro/nano devices or systems, many efforts have been carried out to investigate the properties of hetero- and nanostructured semiconductors [19–22]. For example, Royo et al. [23] reviewed the growth, properties and applications of core-multishell semiconductor nanowires. Ajay et al. [24] made experiments to study the physical properties in planar and nanowires of Ge- and Si-doped GaN/AlN heterostructures, showing great electrical and optical performance. On the other hand, one can tune the ability of material based on the strain/stress engineering and surface/interface engineering through controlling multi-field coupling effects [25–30]. Luo and Zhu [31] calculated the phonon properties

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of GaN nanofilms under surface stress and achieved the thermal conductivity variation in GaN nanofilms subjected to the surface stress. Li et al. [32] analyzed the stress/strain effects on the thermal management of nanostructured semiconductors including SWCNT and single-layer graphene. Zhu and Luo [33] simulated the thermal properties of GaN nanofilms through analyzing acoustic phonon properties under various stress fields. Shchepetov et al. [34] proposed a method to avoid buckling of released membranes by adding a strain compensating frame on ultra-thin suspended single crystalline flat silicon. However, there exist no researches how the prestress fields affect the phonon properties of nanostructured semiconductors with heterostructures.

In this work, we perform theoretical studies on the phonon properties of wurtzite (AlN/GaN/AlN) nanofilms under prestress fields. The homogeneous nanofilms with pure AlN or GaN nanofilms are also addressed for a comparison on phonon performance. The elastic model is applied to calculate the phonon dispersion relation of various structures under prestress fields, in which the acoustoelastic effects and spatial confinement effects are considered. Numerical results demonstrate that the heterogeneity can change the phonon properties in GaN-based nanofilms significantly, including the phonon dispersion relation, phonon group velocity and phonon state density. In addition, the prestress field can modify the phonon properties of the wurtzite AlN/GaN/AlN nanofilms. The theoretical model used for calculating phonon dispersion relation is presented in Section 2. The derivation for the phonon group velocity and density of state is presented in Section 3. After that, we display the outcomes of simulations in Section 4, and then draw our conclusions in Section 5.

2. Theoretical model

2.1. Confined phonons in heterostructured nanofilms

To analyze the acoustic phonon properties of heterostructures with spatial confinement effect, the continuum elasticity model which has been proved to describe the confined phonons successfully [35–40], is adopted to characterize the phonon properties in nanostructured semiconductors. The features in phonon modes of confined nanostructures could be derived with acoustic phonons of free-standing nanofilms. Let's begin with the vibration equations for an elastic solid as

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial x_j}\left(C_{ijkl}\frac{\partial u_k}{\partial x_l}\right), \tag{1}$$

where the displacement vector is defined as u_i, the three Cartesian coordinate axes are indicated with $i, j = 1, 2, 3$. ρ is, and C_{ijkl} is the four-order modulus tensor which is varied along the thickness in nanofilms with the presence of heterogeneity. There are only two independent elastic constants stated as C_{11} and C_{44} for isotropic materials when we contract the indices using the general rules: $(iijj) \to (ij)$ and $(12) \to (6)$, $(13) \to (5)$, $(23) \to (4)$. The x_3 direction is defined as the transverse direction of the thickness, as well as the hexagonal axis of the AlN and GaN crystal orientations in nanofilms. The in-plane directions are defined as x_1 and x_2. Thereby, the displacements of the nanofilm are the functions of x_1 and x_2, and the elastic modulus $C_{ij}(x_3)$ is the function of x_3. Then, we can write the displacement of Eq. (1) in the form of

$$u = \bar{u}(x_3)\exp[i(\omega t - k \cdot x_1)], \tag{2}$$

where ω is the frequency and k is the wave vector. $\bar{u}(x_3)$ is defined as the amplitude of displacement vector and i is imaginary unit. Using the solution of Eq. (2) to substitute the variables in the Eq. (1), the corresponding eigenvalue equation can be derived as

$$\text{Đ}\bar{u}(x_3) = -\rho\omega^2\bar{u}(x_3), \tag{3}$$

where

$$\text{Đ} = \begin{bmatrix} C_{44}\frac{d^2}{dx_3^2} - C_{11}k^2 + \frac{dC_{44}}{dx_3}\frac{d}{dx_3} & 0 & -ik(C_{13}+C_{44})\frac{d}{dx_3} - ik\frac{dC_{44}}{dx_3} \\ 0 & C_{44}\frac{d^2}{dx_3^2} - C_{66}k^2 + \frac{dC_{44}}{dx_3}\frac{d}{dx_3} & 0 \\ -ik(C_{13}+C_{44})\frac{d}{dx_3} - ik\frac{dC_{13}}{dx_3} & 0 & C_{33}\frac{d^2}{dx_3^2} - C_{44}k^2 + \frac{dC_{33}}{dx_3}\frac{d}{dx_3} \end{bmatrix} \tag{4}$$

We have already known that the boundary conditions are

$$\sigma_{13} = \sigma_{23} = \sigma_{33} = 0 \text{ at } x_1 = \pm a \tag{5}$$

Here, $2a$ is the thickness of nanofilms. For the shear modes (SH), the nanofilm has its displacement $\bar{u} = (0, \bar{u}_2, 0)$, leading to the dispersion relation from the eigenvalue equation as

$$C_{44}\frac{d^2\bar{u}_2}{dx_3^2} + (\rho\omega^2 - C_{66}k^2)\bar{u}_2 + \frac{dC_{44}}{dx_3}\frac{d\bar{u}_2}{dx_3} = 0 \tag{6}$$

For the dilatational modes (SA) and the flexural modes (AS), we can get the solution by using the symmetrical and anti-symmetrical properties for the Eq. (1) of u_1 and u_3. The corresponding eigenvalue equations are expressed as

$$C_{44}\frac{d^2\bar{u}_1}{dx_3^2} + (\rho\omega^2 - C_{11}k^2)\bar{u}_1 + \frac{dC_{44}}{dx_3}\frac{d\bar{u}_1}{dx_3} - ik(C_{13}+C_{44})\frac{d\bar{u}_3}{dx_3} - ik\frac{dC_{44}}{dx_3}\bar{u}_3 = 0 \tag{7a}$$

$$C_{33}\frac{d^2\bar{u}_3}{dx_3^2} + (\rho\omega^2 - C_{44}k^2)\bar{u}_3 + \frac{dC_{33}}{dx_3}\frac{d\bar{u}_3}{dx_3} - ik(C_{13}+C_{44})\frac{d\bar{u}_1}{dx_3} - ik\frac{dC_{13}}{dx_3}\bar{u}_1 = 0 \tag{7b}$$

With corresponding boundary conditions and different elastic modulus in GaN layer and AlN layer, the dispersion relations of SH, SA, AS modes can be solved numerically. In heterogeneous nanostructures, the interfaces could play a significant role in physical and mechanical performance. For convenience, it is supposed that the GaN layer and AlN layer are connected perfectly and the interface stress induced by lattice mismatch is neglected. During simulations, the displacement compatibility condition is applied in the interfaces between GaN layer and AlN layer.

Table 1
Material parameters of AlN/GaN/AlN nanofilm for calculations.

GaN	C_{11}(GPa)	C_{13}(GPa)	C_{55}(GPa)	C_{111}(GPa)	C_{123}(GPa)
	252	129	148	−1213	−253
	C_{144}(GPa)	C_{155}(GPa)	C_{112}(GPa)	C_{456}(GPa)	ρ(kg/m^3)
	−46	−606	−867	−49	6100
AlN	C_{11}(GPa)	C_{13}(GPa)	C_{55}(GPa)	C_{111}(GPa)	C_{123}(GPa)
	282	149	179	−1073	−61
	C_{144}(GPa)	C_{155}(GPa)	C_{112}(GPa)	C_{456}(GPa)	ρ(kg/m^3)
	57	−757	−965	−9	3235