

Stress Field Effects on Phonon Properties in Spatially Confined Semiconductor Nanostructures

L.L. Zhu^{1,2,3} and X.J. Zheng^{1,2}

Abstract: The phonon properties of spatially confined nanofilms under the pre-existing stress fields are investigated theoretically by accounting for the confinement effects and acoustoelastic effects. Due to the spatial confinement in low-dimensional structures, the phonon dispersion relations, phonon group velocities as well as the phonon density of states are of significant difference with the ones in bulk structures. Here, the continuum elasticity theory is made use of to determine the phonon dispersion relations of shear modes (SH), dilatational modes (SA) and the flexural modes (AS), thus to analyze the contribution of stress fields on the phonon performance of confined nanofilms. Our numerical calculations indicate that the phonon properties can be modified by the preexisting stress fields significantly. The influence of the stress field on the phonon energy, phonon group velocity and the phonon density of states are sensitive to the strength and the direction of stress fields. The results in this paper can offer an alternative and applicable approach for phonon engineering to control the phonon properties in semiconductor nanostructures.

Keywords: spatially confined nanofilms, phonon engineering, continuum elasticity theory, acoustoelastic effects, phonon dispersion relation, phonon group velocity, phonon density of states.

1 Introduction

In recent decades, rapid progress in the area of scientific and technical research has created promising the great potential applications in modern industry for the

¹ Key Laboratory of Mechanics on Western Disaster and Environment, Ministry of Education, P.R. China, and Department of Mechanics and Engineering Science, College of Civil Engineering and Mechanics, Lanzhou University, Lanzhou, Gansu 730000, P.R. China.

² Corresponding Author. Tel: +86-931- 8912112, Fax: +86-931-8625576. Email: zhulinl03@lzu.cn (Linli Zhu), xjzheng@lzu.edu.cn (Xiaojing zheng)

³ Present address: Department of Mechanical Engineering, The Hong Kong Polytechnic University, Hong Kong, P.R. China. Email: mmlzhu@polyu.edu.hk (Linli Zhu)

nanostructures due to their novel or enhanced electric, magnetic, optical and mechanical properties with respect to the corresponding bulk materials [Wharam et al (1988); Lee et al (1995); Huang et al (2001); Gudikson, Wang and Lieber (2002); Bauer, Birenbaum and Meyer(2004); McGary et al (2006)]. The semiconductor nanostructures have been playing a vital role in the potential future devices such as the nanoelectronic or nanomechanical devices. Many of the current research efforts identified that the acoustic phonon properties of such nanostructures exhibit great contributions on the electronic, thermal and optical performance of materials. For example, the confined phonon properties of nanostructures lead to the modification of the phonon-electron interaction in nanodevices [Banov, Aristov and Mitin (1995); Grosse and Zimmermann (2007)], and the phonon properties of nanostructures can alter the thermal transport in thermoelectric materials significantly [Balandin, Pokatilov and Nika (2007); Cahill et al (2003)]. Therefore, the phonon engineering in the semiconductor nanostructures, including the control and manipulation of acoustic reflectivity, phonon group velocity, density of states, polarization, etc., has been providing the effective method in the control of the electric, thermal and optical properties in nanodevices [Balandin (2005); Balandin, Pokatilov and Nika (2007); Hepplestone and Srivastava (2010)].

For the sake of better application of the phonons in nanostructures, researchers have been focusing on seeking the effective ways, such as designing different structural geometric size or components, to tailor the properties of phonons such as the phonon dispersion relations, the phonon density of states and the group velocity etc [Balandin, Pokatilov and Nika (2007); Lanzillotti-Kimura et al (2007a,b)]. Pokaitilov et al. (2004) made use of the continuum model to study the modification of the acoustic phonon spectrum in the cladding and core layers of semiconductor heterostructures, and demonstrated the phonon quantization by tuning the thickness of the structures. Moreover, the influence of the elastically dissimilar barriers was also investigated on the acoustic phonon spectra and phonon propagation in rectangular coated nanowires, which could be used for reengineering the properties of phonons in nanodevices [Pokatilov, Nika and Balandin (2005a,b)]. Based on the point of view of phonon engineering, the thermal properties of semiconductor nanostructures are theoretically studied by considering the spatial confinement, which can be modified by tuning the phonon dispersion relations [Zincenco et al (2007); Zou, Lang and Richardson (2006)]. For the impact of the phonon engineering on electric properties, Nika et al (2008) revealed that the phonon spectrum modification in the silicon/diamond heterostructure can enhance the electron mobility in the ultrathin Si layer which is benefited in the applications of electronic nanodevices. Simultaneously, the phonon engineering through tailoring phonons properties has been extensively used in the design of the THz phonon devices, the

creation and control of the phononic band gaps and the adjustment of the electron-phonon interaction. For instance, the properties of the acoustic phonons such as the phonon dispersion and spectra were investigated in theory and in experiments for the nanocavities and the multilayer acoustic nanowave devices [Lanzillotti-Kimura et al (2006); Lanzillotti-Kimura et al (2007a,b)].

On account of the existence of the surface/interface scattering and the spatial confinement of the phonons, the properties of the phonon in nanostructures such as the phonon dispersion relations are distinct to the one of the corresponding bulk materials remarkably. Thereby, the comprehensive knowledge of the phonon performance in nanostructures is required to provide a useful favor for the wide use of semiconductor nanostructures in nanodevices. The phonon properties in the low-dimensional semiconductors, e.g., semiconductor superlattice films, quantum wells, quantum wires and nanowires, have been studied using several different methods in the last decade [Kanellis, Morhange and Balkanski (1980); Strosio and Dutta (2001); Mingo and Yang (2003); Hepplestone and Srivastava (2006); Balandin, Pokatilov and Nika (2007); Saib et al (2009); Lang et al (2009); Rino et al (2009)]. In general, the elastic continuum models are employed to investigate the effects of space confinement on the properties of phonons in nanostructures [Bannov, Aristov and Mitin (1995); Pokatilov, Nika and Balandin (2003); Zou, Lang and Richardson (2006); Peng, Chen and Zou (2007); Saib et al (2009); Lang et al (2009)]. This approach provides an adequate description of the properties of acoustic phonons in nanostructures. Besides, the lattice dynamical models with different forms are always utilized to discuss the acoustic phonon dispersion relations of nanostructures [Hu and Zi (2002); Mingo and Yang (2003); Hepplestone and Srivastava (2006)]. Moreover, scalar model based on elasticity theory was adopted to study the ballistic thermal transport in nanostructures with low temperature [Santamore and Cross (2001); Li et al (2004)].

Despite some efforts being carried out to understand the interaction between the phonons and the strain/stress fields [Bhowmick and Shenoy (2006); Trubitsin and Dolgusheva (2007); Saib et al (2008); Pham and Cagin (2010)], it is still very scarce to give an insight into the influence of the stress field on the properties of phonons in nanostructures. Rouvaen et al (1977) analyzed the nonlinear elastic interaction between acoustic bulk and surface wave when the thin film is subjected to the surface stress with possible applications in the nonlinear scanning and signal processing. Osetrov et al (2000) studied the acoustoelastic effects for the layered heterostructures by the transfer-matrix method and suggested that the acoustic wave propagation could be modified notably by the residual stress and third-order stiffness constants. Gross and Zimmermann (2007) investigated the electron-phonon interaction in embedded semiconductor nanostructures by accounting for the strain

within the continuum elasticity, which can change the phonon characteristics in the structures. Motivated by this point, the analysis of the relationship between the stress fields and the properties of phonons can provide an alternative approach for the phonon engineering in semiconductor nanostructures. In addition, it is worth to notice that the considerably higher stresses can occur in the practical applications of nanodevices and the preparation process for the nanostructures. Consequently, the theoretical study for the performance of phonons in stressed nanostructures is essential and of significant importance not only in the fabrication and design of nanodevices but also in the measurement of physical properties of semiconductor nanostructures.

This work employs the continuum elastic model to describe the properties of phonons in nanostructures, which involves the effects of the strain/stress fields on the phonon characteristics such as the phonon dispersion relation, group velocity and the state density in semiconductor nanofilms. The quantitative results are addressed to illuminate the fact that the stress fields can impact the phonon performance of different phonon modes in nanofilms significantly. The effects of the stress fields on phonon properties are associated with the direction of the stress and the type of phonon modes. Following this introduction, section 2 presents the theoretical description of the phonons in stressed nanofilms. In section 3, the analytical expressions of the phonon dispersion, group velocity and the state density are addressed. The numerical results for the properties of phonons with three different modes in stressed nanofilms and the conclusions are drawn respectively in section 4 and section 5.

2 Elastic continuum model for acoustic phonons

The continuum elasticity theory has been, in general, utilized to characterize the acoustic phonon properties of spatially confined nanostructures. The acoustic phonon of free-standing nanofilms is often given as an example to monitor the features of phonon modes in confined nanostructures. In the acoustoelastic theory, the acoustic propagation under residual stresses is commonly explored in a prestressed body, in which the original state free of stress and strain is denoted to the natural state. After the wave motion superposed to the initial state, the structure is deformed to the final state. In the following, the continuum description of the acoustoelastic effects is addressed for the semiconductor nanofilm with the existence of prestress fields.

Consider a nanofilm subjected to the lateral stress, which is biaxial and equal in both directions. Suppose the film as the isotropic material in the natural state, the initial stress of the nanofilm can follow

$$\sigma_{11}^0 = \sigma_{22}^0 = \sigma_0, \sigma_{3i}^0 = 0. \quad (1)$$

Here, σ_{ij}^0 is the static stress tensor, the subscript 1 and 2 denotes the in-plane direc-

tions, and subscript 3 is the transverse direction. Based on the stress-strain constitutive in elasticity theory, the initial strain can be yielded as

$$u_{11}^0 = \frac{s_{22} - s_{12}}{s_{11}s_{22} - s_{12}^2} \sigma^0, u_{22}^0 = \frac{s_{11} - s_{12}}{s_{11}s_{22} - s_{12}^2} \sigma^0, u_{33}^0 = -\frac{c_{13}}{c_{33}} u_{11}^0 - \frac{c_{23}}{c_{33}} u_{22}^0, \quad (2)$$

in which $s_{11} = c_{11} - c_{13}^2/c_{33}$, $s_{12} = c_{12} - c_{13}c_{23}/c_{33}$, $s_{22} = c_{22} - c_{23}^2/c_{33}$, u_{ij}^0 is the static strain tensor, c_{ij} is the elastic modulus tensor. Because of the existence of the biaxial stress in the nanofilm, the second elastic modulus is modified as well as the equation of motion for elastic vibration, which is addressed to describe the phonons in nanostructures as follow

$$\rho^{new} \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial x_j} (\bar{C}_{ijkl} \frac{\partial u_k}{\partial x_l}) + \sigma_0 \frac{\partial^2 u_i}{\partial x_1^2}. \quad (3)$$

Here, u_i is the displacement vector, $\rho^{new} \approx \rho(1 - \Delta u^0)$ is the density after static strains, in which ρ is the density of the natural state and $\Delta u^0 = u_{11}^0 + u_{22}^0 + u_{33}^0$. The effective elastic modulus \bar{C}_{ijkl} is expressed as

$$\bar{C}_{ijkl} = c_{ijkl}(1 + u_{ii}^0 + u_{jj}^0 + u_{kk}^0 + u_{ll}^0 - u_{11}^0 - u_{22}^0 - u_{33}^0) + c_{ijklmn} u_{mn}^0, \quad (4)$$

where c_{ijkl} and c_{ijklmn} are the natural second- and third-order elastic modulus tensors. The non-zeroed components of the effective elastic modulus can be written explicitly as

$$\begin{aligned} \bar{C}_{11} &= c_{11}(1 + 2u_{11}^0 - u_{33}^0) + (c_{111} + c_{112})u_{11}^0 + c_{112}u_{33}^0 \\ \bar{C}_{33} &= c_{11}(1 + 2u_{11}^0 - u_{33}^0) + 2c_{112}u_{11}^0 + c_{111}u_{33}^0 \\ \bar{C}_{13} &= c_{12}(1 + u_{33}^0) + (c_{123} + c_{112})u_{11}^0 + c_{112}u_{33}^0, \\ \bar{C}_{12} &= c_{12}(1 + u_{33}^0) + 2c_{112}u_{11}^0 + c_{123}u_{33}^0 \\ \bar{C}_{44} &= c_{44}(1 + u_{33}^0) + (c_{144} + c_{155})u_{11}^0 + c_{155}u_{33}^0 \end{aligned} \quad (5)$$

in which $\bar{C}_{11} = \bar{C}_{22}$, $\bar{C}_{23} = \bar{C}_{13}$, $\bar{C}_{55} = \bar{C}_{44}$, $\bar{C}_{66} = (\bar{C}_{11} - \bar{C}_{12})/2$. Consequently, the equation of motion for elastic vibration in nanofilms with biaxial stresses can be given by

$$\left\{ \begin{aligned} &(\bar{C}_{11} + \sigma^0)u_{1,11} + \bar{C}_{66}u_{1,22} + \bar{C}_{44}u_{1,33} + (\bar{C}_{12} + \bar{C}_{66})u_{2,12} + (\bar{C}_{13} + \bar{C}_{44})u_{3,13} \\ &= \rho^{new} \frac{\partial^2 u_1}{\partial t^2} \\ &(\bar{C}_{66} + \sigma^0)u_{1,11} + \bar{C}_{11}u_{1,22} + \bar{C}_{44}u_{1,33} + (\bar{C}_{12} + \bar{C}_{66})u_{1,12} + (\bar{C}_{13} + \bar{C}_{44})u_{3,23} \\ &= \rho^{new} \frac{\partial^2 u_2}{\partial t^2} \\ &(\bar{C}_{44} + \sigma^0)u_{3,11} + \bar{C}_{44}u_{3,22} + \bar{C}_{33}u_{3,33} + (\bar{C}_{13} + \bar{C}_{44})u_{1,13} + (\bar{C}_{13} + \bar{C}_{44})u_{2,32} \\ &= \rho^{new} \frac{\partial^2 u_3}{\partial t^2} \end{aligned} \right.$$

(6)

Here, $u_{i,jk} = \partial^2 u_i / \partial x_j \partial x_k$. When the thermal energy or the acoustic waves propagate along the x_1 direction, the displacements of the nanofilms are the functions of x_1 and x_3 and one can look for the solution of the Eq.(6) in the form of $\mathbf{u} = \bar{\mathbf{u}}(x_3) \exp[i(\omega t - q_0 \cdot x_1)]$, in which ω is the frequency and q_0 is the wave vector. By substituting these forms into the equation of motion, the eigenvalue equation can be obtained as

$$\mathbf{D}\bar{\mathbf{u}}(x_3) = -\rho^{new} \omega^2 \bar{\mathbf{u}}(x_3), \quad (7)$$

where

$$\mathbf{D} = \begin{bmatrix} \bar{C}_{44} \frac{d^2}{dx_3^2} - (\bar{C}_{11} + \sigma_0) q_0^2 & 0 & -iq_0(\bar{C}_{13} + \bar{C}_{44}) \frac{d}{dx_3} \\ 0 & \bar{C}_{44} \frac{\partial^2}{\partial x_3^2} - (\bar{C}_{66} + \sigma_0) q_0^2 & 0 \\ -iq_0(\bar{C}_{13} + \bar{C}_{44}) \frac{d}{dx_3} & 0 & \bar{C}_{33} \frac{d^2}{dx_3^2} - (\bar{C}_{44} + \sigma_0) q_0^2 \end{bmatrix}. \quad (8)$$

(a) For the shear modes (SH) in nanofilms, one can get $\mathbf{u} = (0, u_2, 0)$. Substituting it into Eq.(7), the eigenvalue equation is simplified as

$$\bar{C}_{44} \frac{d^2 \bar{u}_2}{dx_3^2} + [\rho^{new} \omega^2 - (\bar{C}_{66} + \sigma^0) q_0^2] \bar{u}_2 = 0 \quad (9)$$

Then, the dispersion relation of SH mode can be obtained as

$$\rho^{new} \omega^2 = \bar{C}_{44} q_{x_3}^2 + (\bar{C}_{66} + \sigma^0) q_0^2. \quad (10)$$

(b) For dilatational modes (SA) and the flexural modes(AS), the solutions of the displacement in x_2 direction is disappeared, resulting in the eigenvalue equation given as

$$\begin{cases} \bar{C}_{44} \frac{d^2 \bar{u}_1}{dx_3^2} - iq_0(\bar{C}_{13} + \bar{C}_{44}) \frac{d\bar{u}_3}{dx_3} + [\rho^{new} \omega^2 - (\bar{C}_{11} + \sigma^0) q_0^2] \bar{u}_1 = 0 \\ \bar{C}_{33} \frac{d^2 \bar{u}_3}{dx_3^2} - iq_0(\bar{C}_{13} + \bar{C}_{44}) \frac{d\bar{u}_1}{dx_3} + [\rho^{new} \omega^2 - (\bar{C}_{44} + \sigma^0) q_0^2] \bar{u}_3 = 0 \end{cases} \quad (11)$$

In this case, the dispersion relation of SA mode and AS mode must be solved by the numerical method. Combining with the boundary condition of nanofilm,

$$\sigma_{33} = -iq_0 \bar{C}_{13} \bar{u}_1 + \bar{C}_{33} \frac{\partial \bar{u}_3}{\partial x_3} = 0; \sigma_{13} = \frac{\partial \bar{u}_1}{\partial x_3} - iq_0 \bar{u} = 0; \sigma_{23} = \frac{\partial \bar{u}_2}{\partial x_3} = 0, \quad (12)$$

three independent vibrational polarizations can be turned out by using numerical method, leading to the determination of the phonon dispersion relations with the shear modes(SH), dilatational modes(SA) and the flexural modes(AS) of nanofilms [Bannov, Aristov and Mitin (1995)]. It is worth to note that the dispersion relations of these modes are all relevant to the stress field because of the presence of the initial stress in the effective elastic modulus and vibrational equations of the acoustic phonons.

3 The dispersion relations of confined phonons in prestressed nanofilms

For the macroscopic characteristics of semiconductor nanostructures, such as thermal conductivity, heat capacity etc., it is required to determine the phonon properties, e.g., the phonon group velocity, the phonon density of states etc. Based on the derivation in Sect.2, the phonon dispersion relation of SA and AS modes are solved by using the finite difference method with the phonon wave vector q_0 from interval $q_0 \in (0, \pi/\tilde{a})$ in which \tilde{a} is the lattice constant. Since this work basically focuses on the impact of the stress fields on the phonon properties of spatial confined nanostructures, we suppose the nanofilm with smooth surfaces in which the boundary scattering does not contribute to the phonon performance. From the determined vibrational spectrum of nanofilms, the phonon group velocity of three modes can be given by a numerical differentiation

$$v_n^{SA,AS,SH}(q) = d\omega_n^{SA,AS,SH}(q)/dq, \quad (13)$$

in which q and ω are the phonon wave vector and the honon frequency, respectively. Herein, the subscript n is the quantum number of the modes. With a given polarization, n equals to the ratio $H/2\tilde{a}$, where H is the thickness of the film. The average phonon group velocity thus can be reached by the following formula

$$\bar{V} = \left\{ \sum_{N=1}^{M(\omega)} [v_s^{SA,AS,SH}(\omega)]^{-1} / M(\omega) \right\}^{-1}. \quad (14)$$

in which M is the total number of phonon branches. In a 2D nanostructure [Zou, Lang and Richadson (2006)], the phonon density of states of each branch can be defined by

$$f_n^{SA,AS,SH}(\omega) = [q_n^{SA,AS,SH}(\omega) / v_n^{SA,AS,SH}(\omega)] / 2\pi H. \quad (15)$$

where q_n is the wave vector of the phonon branch n . Thus, the total density of states for all polarizations is obtained by a summation over all n ,

$$F^{SA,AS,SH}(\omega) = \sum f_n^{SA,AS,SH}(\omega). \quad (16)$$

Note that due to the presence of stress which alters the effective elastic modulus and the density of deformed state, the phonon dispersion relations for SH, SA and AS modes will depend on the stress field, leading to the change of the phonon group velocity and the total density of states.

4 Numerical results and discussion

In order to quantitatively characterize the phonon of confined semiconductor nanofilms in the stress fields, we perform numerical calculation based on silicon nanofilms with the thickness as 5.42nm to study the corresponding properties of phonons. The bulk elastic parameters c_{ijkl} and c_{ijklmn} of semiconductors are obtained from Ref. [Hearmon (1979)]. First, we consider phonon models of the shear polarization for which the effects of quantization and the stress field are performed in more pronounced way than those in SA and SA polarizations. Figure 1 shows the dispersion relation with the presence of positive and negative stress for a set of shear modes. One can see from the figure that the phonon modes are quantized in the region nearby the Brillouin zone center for spatially confined nanofilm and the cut-off phonon energy ($q=0$) is independent on the preexisting stress field. However, the slope of each dispersion curve for shear modes is sensitive to the stress field as well as the characteristic line L which is approximately equal to the transverse wave velocity of the film. The results display that the negative stress makes the phonon energy increased whereas the positive one weakens the phonon energy. It must be pointed out that the influence of the negative stress on the phonon energy of shear modes is more significant than the one of positive stress.

Figure 2 depicts the group velocity of SH modes varied with wave vector under stress fields. Note that the preexisting stress can alter the group velocity remarkably. In the Brillouin zone center the slope of the linear phonon group velocity with respect to the wave vector is changed on account of the existence of the stress fields, that is, the positive stress makes the slope lower down and the negative one enhances the slope of the phonon group velocity. With increasing the wave vector the slopes of all curves of phonon group velocity decrease and then reach a limit as the transverse wave velocity of the film, which is associated with the magnitudes and direction of the stress field. We also present the phonon density of states as a function of the phonon energy (seen in figure 3). It can be noticeable to find that there exists the oscillatory behavior of the density of states which can be interpreted by the manifestation of the phonon mode quantization in the confined nanofilms. Each step in the density of states refers to the onsets of new phonon branches when their cut-off energy is approached. It is interesting to note that the preexisting stress fields have no contributions on the range of phonon energy for the oscillatory behavior. This is because of the fact that the cut-off energy is independent on the

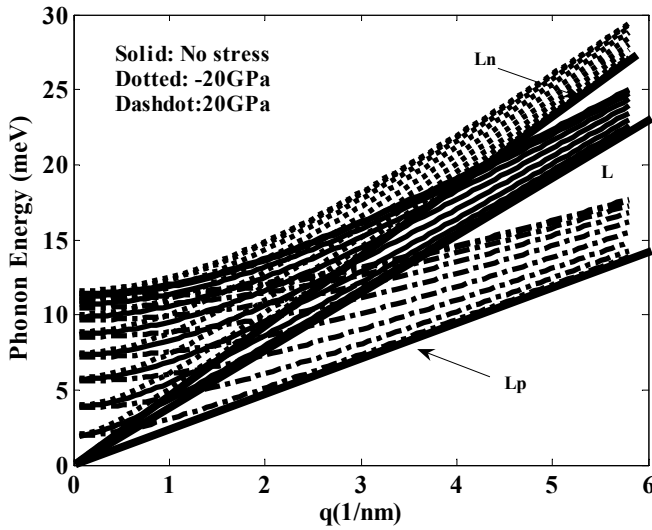


Figure 1: Phonon energy of SH modes as a function of the wave vector with the positive and negative stresses

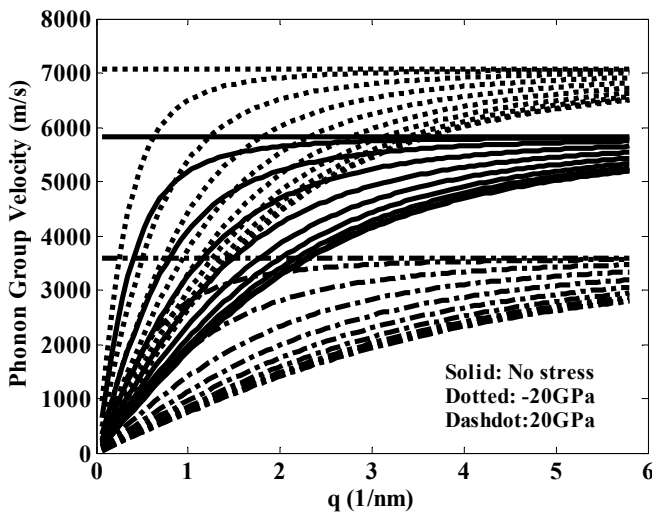


Figure 2: The phonon group velocity varied with the wave vector under positive and negative stress field

stress fields as shown in figure 1. In addition, we can also observe that the positive stress increases the density of states while the negative stress makes the decrement of the density. The trend of the density of states varied with stress field is contrary with the ones of the phonon energy or the group velocity as the functions of stress fields, that is because the phonon density of states is inversely proportional to the phonon velocity as shown in Eq.(15).

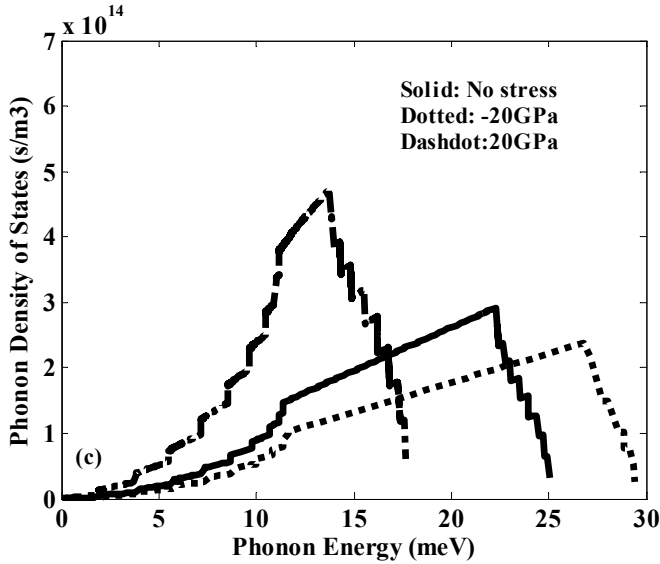
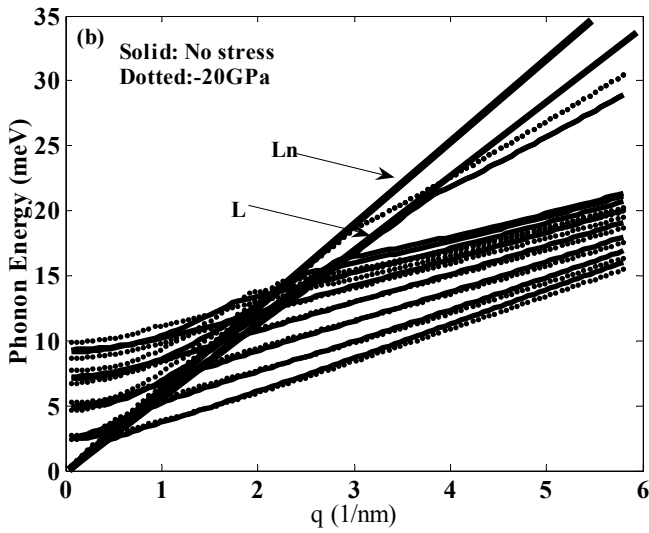
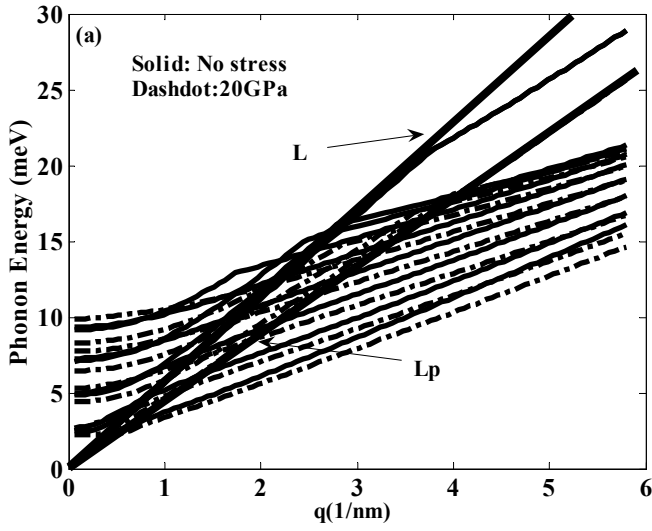


Figure 3: The phonon density of states as a function of phonon energy with different stress fields

Owing to the presence of the stress fields in spatially confined nanofilms, the analytical expressions of the dispersion relations for SA modes and AS modes can not be addressed exactly, resulting in that the numerical method must be adopted to solve Eq.(11) combining with the boundary conditions in Eq.(12). Through numerical calculation, the curves of phonon energy for SA modes and AS modes are given in figure 4 as the functions of wave vector under different stress fields. One can see from the figure that the cut-off energy for the lower-order modes is irrespective to the stress fields, while with increasing the orders of modes, the corresponding cut-off energy are relevant to the preexisting stresses. Similarly, the negative/positive stress can induce the phonon energy increase/decrease for SA modes and AS modes, but the effects of stress fields on the phonon energy for SA modes and AS modes are weaker than the ones for SH modes. It also can be found that the stress field can modify the slope of the characteristic line L which is the velocity of



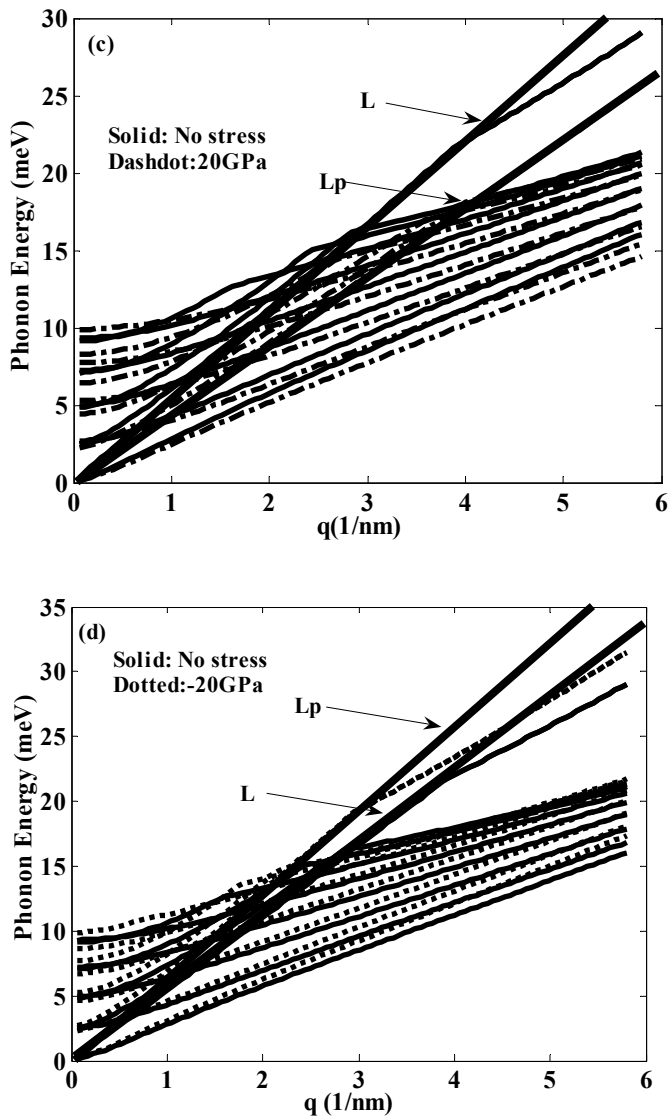


Figure 4: The phonon energy of SA modes and AS modes varied with wave vectors under different stress fields. a)SA modes with positive stress; b)SA modes with negative stress; c)AS modes with positive stress and d) AS modes with negative stress.

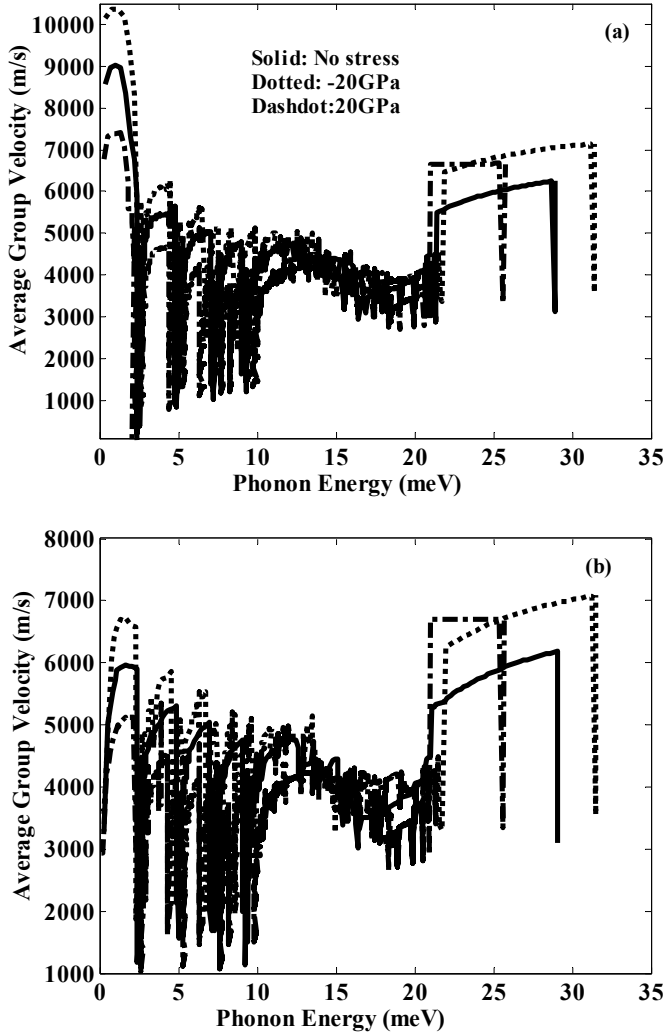
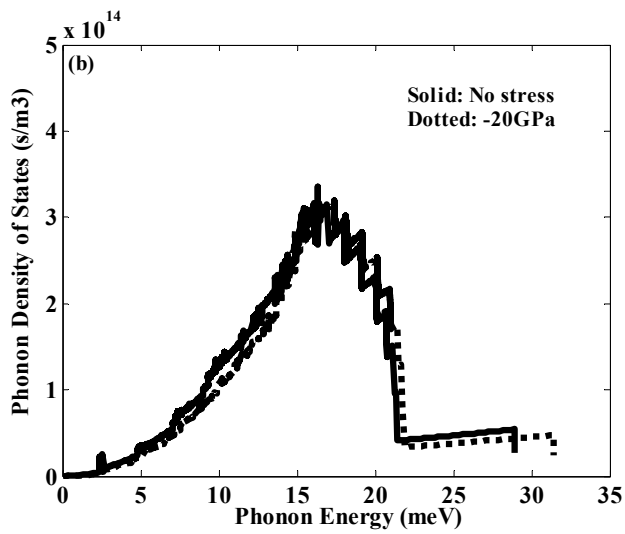
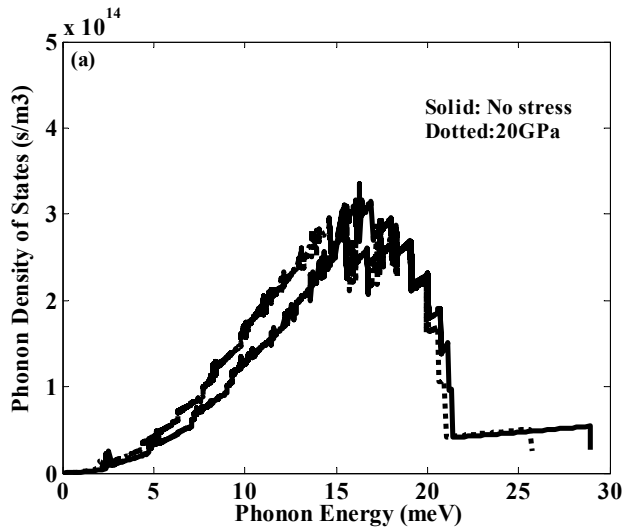


Figure 5: The average phonon group velocity of SA modes and AS modes as the functions of phonon energy with different stress fields

longitudinal wave in films. The velocity becomes greater when the nanofilm is under negative stress and it is fallen down for the positive stress. Moreover, the slopes of energy curves for high-orders modes under stress fields are all greater than the ones without preexisting stress field in the range of the large value of wave vector.

With the aid of the determined dispersion relations of SA modes and AS modes, the consequent average phonon group velocity and average phonon density of states



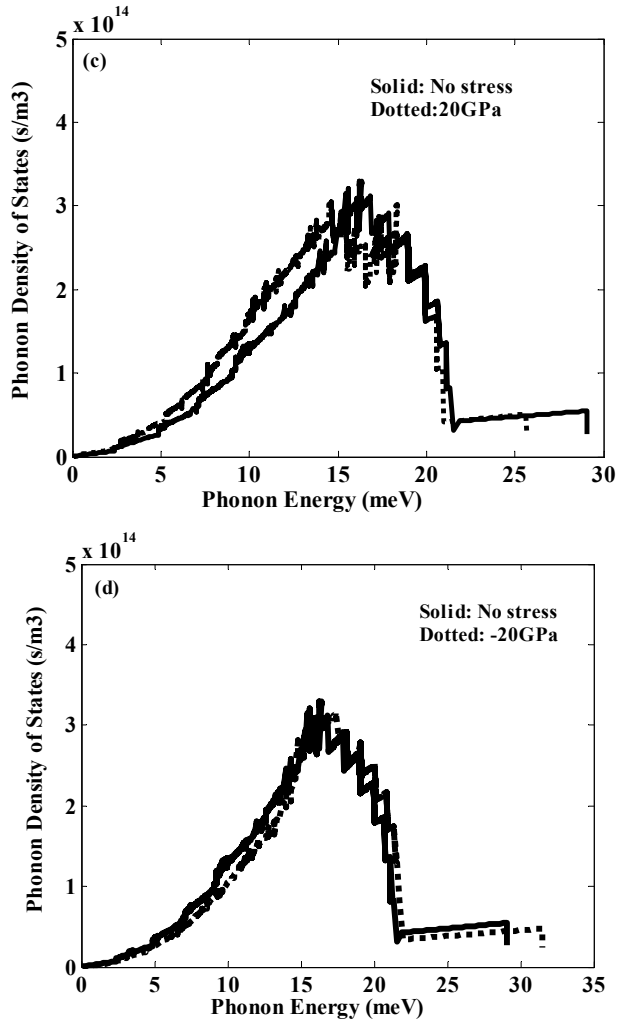


Figure 6: The average phonon density of states of SA modes and AS modes varied with phonon energy under different stress fields. a)SA modes with positive stress; b)SA modes with negative stress; c)AS modes with positive stress and d) AS modes with negative stress.

can be scraped according to Eqs.(14) and (16), as shown in figures 5 and 6 respectively. It can be noticed from figure 5 that the group velocities of SA modes and AS modes exhibit the oscillatory behaviors with variation of phonon energy. In the limit of the phonon energy with oscillatory, the negative stress leads to increasing the average group velocities and the positive one decreases the average group velocities. Whereas, in the range of the large phonon energy, e.g. greater than 20 meV, the group velocities with the preexisting stress fields are greater than the ones in the absence of the stresses, which are independent on the direction of the stress fields. This can be explained by the fact that, in the case of the existence of stress fields, the slopes of curves for the phonon energy in dispersion relation (seen in figure 4) are all greater than the ones without stress fields in the limit of the large phonon energy. Figure 6 shows the phonon density of states for SA modes and AS modes varied with the phonon energy. Similarly, the effects of stress on the density of states for SA modes and AS modes are in accordance with the ones for SH modes when the density of states increases with the increment of the phonon energy. However, when the density of states decreases with increasing the phonon energy, the negative stress enhances the densities and the positive one makes the densities decrease. On the other hand, one can notice from figures 3 and 6 that the influences of stress fields on the density of states for SH modes are more apparent than the ones for AS modes and SA modes. In addition, it is valuable to point out from figure 1 to figure 6 that the positive stress influences the phonon properties of nanofilms more remarkably than the negative one does.

5 Conclusion

In summary, the phonon properties of spatially confined semiconductor nanostructures have been studied under the preexisting stress fields with the aid of the continuum elasticity theory which are usually utilized to describe the confinement effects of the semiconductor nanostructures. Taken into account the acoustoelastic effects stemmed from the presence of stress fields, the phonon dispersion relations for SH modes, SA modes and AS modes in semiconductor nanofilms are calculated to investigate the impacts of the stress fields on the phonon energy, phonon group velocity as well as the density of states in different modes. Numerical results reveal that, for these three polarization modes in nanofilms, the stress field effects on the phonon properties are related to the strength and the direction of stress fields. The negative stress enhances the phonon energy and the phonon group velocity while weakens the density of states. When the nanofilms are subjected to the positive stress, the phonon energy and the phonon group velocity are decreased and the density of states turns greater. With the same magnitude for the stresses, the positive ones have more contributions on the phonon performance than the negative

ones have. Moreover, the influences of stress fields on the phonon properties for SA modes and AS modes is weaker than the ones for SH modes. The results presented in this paper can provide an alternative methodology to tune the phonon properties so as to enhance the performance of various semiconductor-based nanoelectronic devices by controlling the preexisting stress fields.

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