MODELING OF THE ELASTIC MODULUS OF CRYSTALLINE SILICON BASED ON A LATTICE DYNAMICS APPROACH

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ABSTRACT

An augmented continuum theory, based on lattice dynamics theories, is developed to examine the elasticity of three-dimensional crystalline Si materials. The second-order elastic constants of Si can be expressed as the function of the force constants, with the modified Keating model. The phonon dispersion relations have been calculated by using the density functional perturbation (DFP) theory, from which the force constants can be extracted. Then the elastic modulus in any crystallographic directions can be calculated. The average deviation of Young's modulus from experiment is less than 3.8%. This approach is expected to be used in the design of silicon-based MEMS.

KEYWORDS

Elastic modulus, crystalline silicon, lattice dynamics

INTRODUCTION

Crystalline silicon revolutionized the way we think about electronics. Besides the fact that silicon is an excellent electronic material used in most integrated circuits, it also has excellent mechanical properties: high elasticity, stiffness, fracture, thermal conductivity, thermal stability. Consequently, silicon is widely used in MEMS fabrication and NEMS fabrication, both as a substrate for compatibility with semiconductor processing equipment and as a structural material for MEMS and NEMS device [1-3]. The elastic modulus of a material is a key parameter for mechanical engineering design. Elasticity in semiconductors, especially in Si, is a topic of some technological as well as scientific interests.

In the past two decades, the measurement of the elastic constants of bulk silicon material is best performed using the technique of acoustic wave propagation measurements in the solid. These measurement methods are described in detail elsewhere[4-5]. The values for the elastic constants c_{11}, c_{12}, and c_{44} are 165.6 GPa, 63.9 GPa, and 79.5 GPa respectively. In [6], Sharpe shows a lot of measurements of the Young's modulus of silicon for MEMS application. As expected, the results converge on the values calculated from acoustic wave propagation in bulk samples[7].

The effective design and use of MEMS and NEMS require the development of predictive capabilities for their properties. Models have been developed. The elastic theories of diamond-type crystals start with a classic paper by M. Born and K. Huang. They proposed a model with nearest-neighbor central and noncentral force constants[8]. This model agrees well with experiments in the condition of long wavelengths, but deviates from the experiments at short wavelengths. Obviously, the number of force constants is too few to characterize the elasticity exactly. So a large number of researchers are interested in modifying the model by increasing the force constants, even to the 25 nearest-neighbor [9]. But with the increase of force constants, the complicity of model will be exponentially increased.

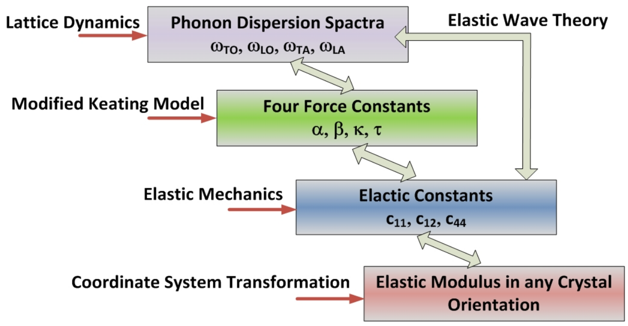

Figure 1: The process of calculating elastic modulus in the model and the corresponding theory in each part of the model .

In this paper, an augmented continuum technique based on the lattice dynamics theory is developed for the elasticity of three-dimensional Si materials. The elasticity of cantilevers in the micron level can be analyzed in the atom level. The process of calculating elastic modulus in this model is shown in Figure 1. It also depicts the theory used in each part of the model. The second-order elastic constants of Si can be expressed as the function of the force constants. A modified Keating model, as the interactional potential, includes four interactions, and needs four corresponding force constants. The phonon dispersion relations have been calculated by using the density functional perturbation theory, from which the force constants can be extracted and optimized. Combining the modified Keating model with the phonon dispersion relations, the analytic expressions for certain high-symmetry k points phonon frequencies and the elastic constants of Si can be obtained. Then the Young's modulus in any crystallographic directions can be calculated. This approach is expected to be used in the design of silicon-based MEMS.

THEORY

Lattice Dynamics

The classic calculation of the elasticity of diamond-type crystals by using the lattice dynamics start with a classic paper by M. Born and K. Huang. In the view of their method, the force on a atom is calculated in terms of the force constants and atomic displacements.

Keating model has been widely used to study elastic and static properties of covalent semiconductors. Calculation of the phonon dispersion with this model gives a good description of LO, TO, and LA modes in covalent semiconductors, but it does not reproduce the flatness of the TA mode dispersion. Consequently, further interactions with neighboring atoms are needed[10]. In this paper, a modified Keating model has been used as the interactional potential.

The potential energy used by Keating takes into account only the bond-stretching and bond-bending interactions. While, the modified potential energy, including four types of interactions, the two original Keating interactions, the nearest-coplanar angle and nearest-bond interaction. Such four interactions can be plotted as Fig. 2, and α, β, τ, as well as κ are the corresponding force constants.

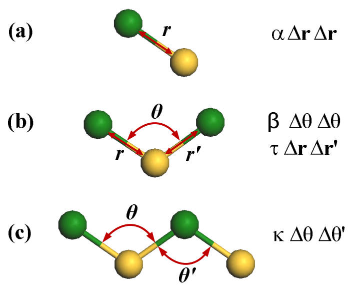

Figure 2: Schematic representation of nearest-neighbor forces: (a) two-body force, (b) three-body forces, (c) four-body force.

As shown in the Figure 2, α describes a two-body forces, and β, as well as τ represent three-body forces, whereas κ depicts a specific four-body force [10].

Phonon Dispersion Relations

The first-principles theories have been extensively applied for the calculation of lattice dynamics properties in bulk Si material and Si nanostructure. The phonon spectra of three-dimensional Si materials have been studied using the Castep package based on the first-principles theories. The calculations are performed employing density functional perturbation (DFP) theory, norm conserving pseudopotential, and General Gradient Approximate (GGA) for exchange correlation potential. The integration over the Brillouin zone is performed on a regular 8×8×8 Monkhorst-Pack mesh, which gives a rather good description for the interactions between the atoms connected by the zigzag chain along the <110> directions[11].

Elastic Constants

When a body changes in shape or in size it is said to be strained, and the deformation of the body is called strain. Hooke's law states that stress is directly proportional to strain for small strains. That is

$$T_i = \sum_{j=1}^{6} c_{ij} e_j, \quad i, j = 1,2,\ldots 6. \qquad (1)$$

Where, T_i and e_j are stresses and strains respectively. The coefficients are called the elastic constants or modulus of elasticity. In general c_{ij} should have 36 components and only 21 components are independent. When we take into account the symmetry of the crystal, the number of independent elastic constants is further greatly reduced. If the crystals have cubic symmetry, such as the silicon, the number of independent elastic constants reduces to 3. They are c_{11}, c_{12}, and c_{44} respectively.

Once c_{ij} are obtained, the elastic modulus of any crystal orientation will be extracted by using the coordinate system transformation and Hooke's generalized law.

RESULTS AND DISCUSSION

The prototype under study is three-dimensional Si materials, such as cantilevers, which are the basic structures for MEMS and NEMS. The atoms structure of crystalline Si can be depicted in Figure 3. As shown in Figure 3, there are two interpenetrating fcc Bravais lattices in the Si crystalline lattice, so it has two types of atoms, denoted as green spheres and yellow spheres. The component atoms are connected by covalent bonds and each atom is tetrahedrally bonded to four neighboring silicon atoms [12]. The movements of the atoms are determined by the laws of lattice dynamics. The vibrations of the atoms in a crystal not only determine its thermal properties but also govern phenomena of the elasticity.

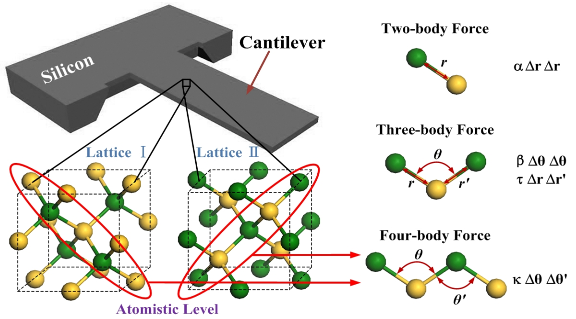

Figure 3: Two atom configurations of Si lattice in a Si cantilever, and the schematic representation of neighbor atoms interactions.

The modified Keating model are used as the interactional potential. α and β are the leading terms in a systematic expansion of the strain energy. Furthermore, it has been found that the length-length correlation τ is important for an accurate overall improvement of the fit to the Si phonon dispersion curves and the four-body force κ is needed to describe the zone-boundary softening of the transverse acoustical branch.

In the framework of elastic mechanics, the second-order macroscopic strain energy density for cubic crystals can be expressed by the function of the second-order elastic constants:

$$\frac{U_0}{V} = \frac{1}{2}C_{11}\left(e_{xx}{}^2 + e_{yy}{}^2 + e_{zz}{}^2\right) + C_{12}\left(e_{xx}e_{yy} + e_{xx}e_{zz} + e_{yy}e_{zz}\right) + \frac{1}{2}C_{44}\left(e_{xy}{}^2 + e_{xz}{}^2 + e_{yz}{}^2\right). \quad (2)$$

Comparing the static potential energy with the macroscopic energy density in equation (2) gives

$$\begin{aligned} C_{11} &= \frac{1}{a_0}(\alpha + 3\beta + 3\kappa + 3\tau), \\ C_{12} &= \frac{1}{a_0}(\alpha - \beta - \kappa + 3\tau), \\ C_{44} &= \frac{1}{a_0}\left[(1-\xi)^2\alpha + (1+\xi)^2\beta + (1+\xi)^2\kappa - \tau\right]. \end{aligned} \quad (3)$$

Where ζ is the internal strain parameter.

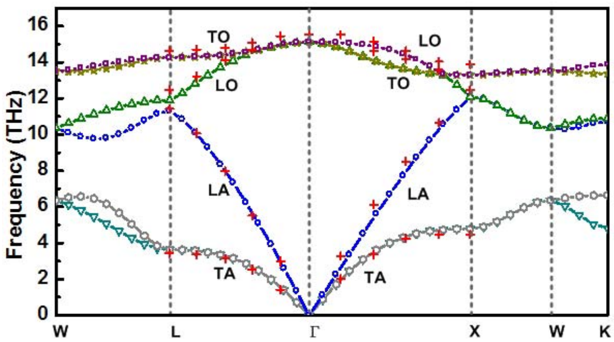

Figure 4: Phonon dispersion curves along the different directions in Si. The red color crosses depicting the experimental results from [13] .

In order to optimize the four force constants, the phonon dispersion relations of three-dimensional Si materials have been calculated using density functional perturbation theory. The obtained phonon spectra of Si are shown in Figure 4, from which the force constants can be extracted. Some experimental data [13] are also plotted, represented by cross. As shown in Figure 4, the overall dispersion relations agree well with the experimental data and the average deviation of phonon frequencies is less than 3.4%. It is worth to note that the flatness of TA phonon can be reproduced well.

Table 1. The phonon frequencies and the analytical expressions.

Frequencies	Expressions	Model	[13]
$\omega_{LO,TO}(\Gamma)$	$\left[8(\alpha+\beta+\kappa-\tau)/M\right]^{1/2}$	15.18	15.40
$\omega_{LO,LA}(\mathrm{X})$	$\left[4(\alpha+2\beta+\kappa+\tau)/M\right]^{1/2}$	12.09	12.32
$\omega_{LO}(L)$	$[(6\alpha+\beta)/M]^{1/2}$	11.90	12.42
$\omega_{TA}(L)$	$[4\beta/M]^{1/2}$	3.63	3.42

The analytic expressions for phonon frequencies are obtained by constructing and analytically diagonalizing the dynamical matrices at certain high-symmetry k points. This is done at the Γ, X, and L points, which are tabulated in table 1, and the corresponding experimental values from [13] are also listed. As shown in table 1, the calculated phonon frequencies are in good agreement with experimental data, with the relative error ranging from 1.4% to 6.1%.

By combining this analytic expressions at some high-symmetry k points with the corresponding phonon frequencies from the Figure 3, the parameters α, β, τ, and κ can be extracted. Then inserting the α, β,τ, and κ into equation (3), the second-order elastic constants will be obtained. Table 2 tabulates the results of the optimized four force constants and the second-order elastic constants. For comparison, the experimental values of second-order elastic constants from [1] are also listed.

Table 2. The force constants and the second-order elastic constants.

	α (N/m)	β	κ	τ	c_{11} (GPa)	c_{12}	c_{44}
Model	42.4	6.0	8.6	4.1	181.7	73.7	73.0
[1]					165.6	63.9	79.5

Once c_{ij} are obtained, the elastic modulus of any crystal orientation will be extracted by using the coordinate system transformation and Hooke's generalized law[14]. Figure 5 shows the transformation between arbitrary primed orthogonal axes and unprimed cube axes by the direction cosines. And Figure 6 gives the results of corresponding elastic modulus in some main crystal orientation. For instant, the Young' modulus in <100>, <110> and <111> crystallographic directions are 139.3 GPa, 168.2 GPa, and 180.7 GPa, respectively. It is obvious that the calculated Young's modulus from model are rather approximate the values of the experiment[14], compared with the other theoretical approaches[15]. The average relative errors is about 3.8%.

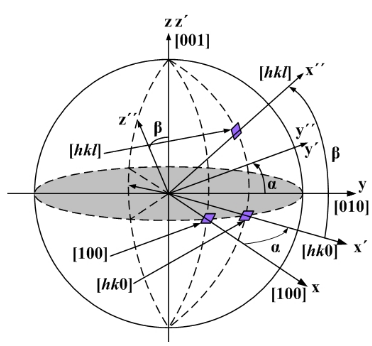

Figure 5: Illustration of coordinate system transformation, the elastic modulus in any orientation can be obtained by the coordinate system transformation.

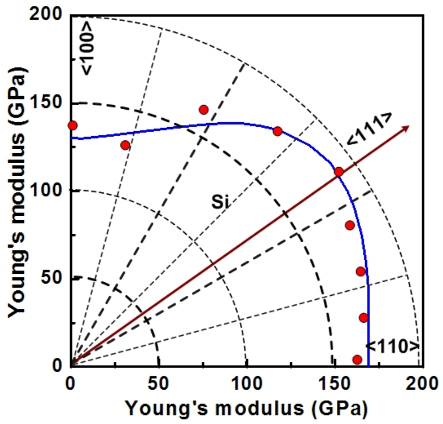

Figure 6: Young's modulus in any crystal orientation.

CONCLUSIONS

In this paper, an augmented continuum theory based on the theory of lattice dynamics is developed, which establishes the relationship between the macroscopic elasticity and the force constants of atoms. A modified Keating model has been used as the interactional potential, which includes four interactions and needs four force constants. The force constants have been calculated and optimized using the phonon dispersion relations. The calculated phonon frequencies by DFT method are in good agreement with experimental data. The analytical expressions for certain high-symmetry k points phonon frequencies and the elastic constants of Si have been obtained. Lastly, the Young's modulus in any crystallographic directions has been calculated. The results show that calculated Young's modulus agrees well with experimental results and the average deviation is less than 3.8%. Results of pre-existing theoretical and experimental works, used as benchmarks, have confirmed that our model is of reliability, accuracy, and simplicity.

Before closing, we comment on the potential of this model to analyze the nano Si structures. This technique extracts the material properties in the continuum level from the atomistic description of the underlying local environment. Similarly, it is possible to analyze the surface effects, such as the surface stress, surface absorption surface reconstruction and native oxide layers by using the same technique. Once the characteristic properties of bulk and surface are known, the overall behaviors of nano devices will be predicted. Our further work will focus on the size-effect on the elasticity of the cantilevers in NEMS.

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