Research Article

First-Principles Study on the Elastic Constants and Structural and Mechanical Properties of 30° Partial Dislocation in GaAs

Huili Zhang¹, Qiannan Gao,¹ Defang Lu², Yunchang Fu,³ and Lumei Tong³

¹Department of Mathematics and Physics, Hebei Petroleum University of Technology, Chengde 067500, China

²Department of Automobile Engineering, Hebei Petroleum University of Technology, Chengde 067500, China

³College of Science, Kunming University of Science and Technology, Kunming 650500, China

Correspondence should be addressed to Defang Lu; q2384@163.com

Received 10 March 2021; Accepted 7 June 2021; Published 2 July 2021

Academic Editor: Alfonso Muñoz

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The second-order elastic constants, third-order elastic constants, and the generalized-stacking-fault energy for semiconductor GaAs are investigated using the first-principles calculations. The predictions of elastic constants are obtained from the coefficients of the fitted polynomials of the energy-strain functions. It is found that the nonlinear elastic effects must be considered when the applied deformations are larger than approximately 1.5%. With the Lagrangian strains up to 6.4%, the terms included up to third order in energy expansion functions are sufficient. The elastic constants given in this work agree well with the previous results and experimental data except for C_{144} . C_{144} given by the present paper is a positive value, and the estimated 3 GPa agrees well with the experimental result of 2 GPa. The research results can provide a reference for understanding the elasticity of GaAs. The generalized-stacking-fault energy has been calculated without and with structural relaxation, respectively. The unstable stacking fault energy with structural relaxation is about two-thirds of that without relaxation. The dislocation width and Peierls stress for 30° partial in GaAs have been investigated based on the improved P - N theory. The dislocation width is very narrow (only about one-fifth of Burgers vector b), which is reasonable for covalent materials. The Peierls stress is about 4 GPa, in good agreement with the experimental result of 2~3 GPa.

1. Introduction

III–V semiconductors receive the widespread attention due to the latent application prospect, such as photo-detectors, lasers, and light-emitting diodes [1–5]. Among the III–V direct bandgap semiconductors, GaAs is one of the most promising candidates due to its high electron mobility [6, 7]. It has been widely used in many fields, such as solar cell fabrication [8], substrate materials [9, 10], and efficient photovoltaic devices [11, 12]. Recently, lots of experimental and theoretical research studies have been carried out to study the properties of GaAs. Elasticity and plasticity are two important mechanical properties of materials, and the study of these two properties plays an important role on understanding and utilization of materials. Consequently, the elastic and plastic properties of GaAs are also of particular interest. The elastic properties of solids can be well

reflected by elastic constants. For single crystals, second-order elastic constants (SOECs) and third-order elastic constants (TOECs) are both important parameters for modeling the mechanical response. In the process of plastic deformation of materials, dislocations play a key role. Therefore, the study of the elastic constants (SOECs and TOECs) and the dislocation properties of GaAs is necessary. Many experimental and theoretical research studies have been performed on the elastic constants of semiconductor GaAs. Several methods such as ultrasonic wave propagation and optical interference are used to measure the SOECs and TOECs of GaAs [13–15]. Singh et al. have calculated the TOECs of GaAs using Keating theory [16]. First-principles calculations based on density functional theory are also widely used to investigate the elastic constants of GaAs [17–19]. These results are very vital for understanding the elasticity of GaAs. However, there still

exist argument for the magnitude and sign of the TOEC C_{144} .

The most fundamental quantity related to the plasticity of the crystal is the Peierls stress of dislocation. However, the research on the Peierls stress of dislocation in GaAs is very limited, no matter from experimental or theoretical method. Suzuki et al. and Kamimura et al. have estimated the Peierls stress of dislocations in GaAs by extrapolating the critical shear stress to the absolute zero temperature; the estimated Peierls stress is about 2~3 GPa [20, 21]. The Peierls stress of the 30° partial in GaAs estimated by Kamimura et al. based on the classical *P-N* model using *ab-initio* γ -surface is about 23 GPa [22], which is one magnitude larger than the experimental result approximately [21]. Actually, the crystal has been treated as an elastic continuum body in the classical *P-N* model, while the discrete effect of lattice which is extremely important for the narrow dislocations in semiconductors is neglected [23–25]. The improved *P-N* theory which has fully considered the discrete effect of the crystal has been proposed by Wang [26–28]. The research results show that the agreement between theoretical prediction given by improved *P-N* theory and the numerical and experimental results can be significantly improved [29–31]. It has been established that the glide of dissociated dislocations on closed packed planes is responsible for the high temperature plasticity in zinc-blende crystals [21, 32]. And, the 30° partial generally possesses higher Peierls stress compared with the 90° partial and controls the deformation [33]. And, as such, the improved *P-N* theory is applied for the 30° partial in GaAs. The restoring force in the dislocation equation is generally given by the gradient of the generalized-stacking-fault energy (GSFE) as suggested by Christian and Vitek [34]. In this paper, the SOECs, TOECs, and GSFE along $(1/2)\langle 112 \rangle$ on glide set of GaAs have been calculated by the first-principles calculations. Based on the calculated SOECs and GSFE, the core width and Peierls stress of 30° partial in GaAs have been investigated by the improved *P-N* theory.

2. Determination of SOECs and TOECs

2.1. Computational Method. The finite-strain continuum elasticity theory [35–40] is widely used to obtain the TOECs; the relation between the strain energy density Φ and the elastic constants can be expressed as follows [35, 36]:

$$\Phi(\eta) = \frac{1}{2!} \sum_{ijkl} C_{ijkl} \eta_{ij} \eta_{kl} + \frac{1}{3!} \sum_{ijklmn} C_{ijklmn} \eta_{ij} \eta_{kl} \eta_{mn} + \dots, \quad (1)$$

where η is the Lagrangian strain tensor, and it can be defined as [37]

$$\eta_{ij} = \frac{1}{2} \sum_k (J_{ki} J_{kj} - \delta_{ij}), \quad (2)$$

where δ_{ij} is a unit matrix; the deformation tensor $J_{ij} = (\partial x'_i / \partial x_j)$ constructs the connection of initial configuration x_j and strained configuration x'_i at the equilibrium state.

The α th – order ($\alpha \geq 2$) elastic constants were defined by Brugger as [38]

$$C_{ijklmn\dots} = C_{IJK\dots} = \frac{\partial^\alpha \Phi}{\partial \eta_{ij} \partial \eta_{kl} \partial \eta_{mn} \dots} \Big|_{\eta=0}, \quad (3)$$

where I, J , and K are Voigt subscripts, and the Lagrangian strain tensor η links this notation by

$$\eta = (\eta_1, \eta_2, \eta_3, \eta_4, \eta_5, \eta_6). \quad (4)$$

Because of the cubic symmetry, there are three independent SOECs (C_{11} , C_{12} , and C_{44}) and six TOECs (C_{111} , C_{112} , C_{123} , C_{144} , C_{155} , and C_{456}). Introducing six Lagrangian strain tensors in terms of a single parameter ζ to calculate the SOECs and TOECs, the strain energy per unit mass can be written as a polynomial of the strain parameter ζ [41],

$$\Phi(\eta) = A_2 \zeta^2 + A_3 \zeta^3 + O(\zeta^4), \quad (5)$$

where the coefficients A_2 and A_3 are comprised by the SOECs and TOECs of the crystal. The applied strains η_α with $\alpha = A$ to F and the corresponding coefficients A_2 and A_3 are listed in Table 1 [42].

To obtain accurate TOECs, ζ is changed from -0.064 to 0.064 with the step of 0.008 . For covalent bonding materials, the maximal amplitude 0.064 of the deformations is enough to obtain the accurate TOECs. The elastic constants can be obtained from the least-square polynomial fitted from the strain-energy relation given by the first-principles total-energy calculations.

We perform first-principles total-energy calculations based on the density functional theory (DFT), using the *ab-initio* simulation package (VASP 4.6) [43–45]. In order to compare the performance of two different density functionals in the first-principles prediction of the lattice constant and SOECs, the local density approximation (LDA) and the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional for generalized gradient approximation (GGA) are, respectively, used. A plane-wave basis set is employed within the framework of the projector augmented wave (PAW) method [46, 47]. In the calculation, the wave functions are expanded as a plane wave basis with the cut-off energy of 550 eV. For the first Brillouin zone integrals, reciprocal space is represented by the Monkhorst-Pack special k -point scheme [48] with $21 \times 21 \times 21$ grid meshes. The convergence of energy and force are set to 1.0×10^{-6} eV and 1.0×10^{-4} (eV/Å), respectively. The equilibrium theoretical crystal structures are determined by minimizing the Hellmann–Feynman force on the atoms and stress on the unit cell.

The lattice constant and SOECs obtained with the LDA and GGA are presented in Table 2. The results show that the GGA overestimates, while the LDA underestimates the lattice constants, which is in agreement with [19] and [49]. And, it is obvious that the predictions of LDA are in better agreement with the experiment results, regardless of the lattice constant or the SOECs. Consequently, the calculation of the TOECs and the GSFE in the present paper is based on the LDA functional.

TABLE 1: The applied strains η_α and the corresponding coefficients A_2 and A_3 in equation (5) as combinations of SOECs and TOECs for crystals with cubic symmetry.

Strain type	A_2	A_3
$\eta_A = (\zeta, 0, 0, 0, 0, 0)$	$(1/2)C_{11}$	$(1/6)C_{111}$
$\eta_B = (\zeta, \zeta, 0, 0, 0, 0)$	$C_{11} + C_{12}$	$(1/3)C_{111} + C_{112}$
$\eta_C = (\zeta, \zeta, \zeta, 0, 0, 0)$	$(3/2)C_{11} + 3C_{12}$	$(1/2)C_{111} + 3C_{112} + C_{123}$
$\eta_D = (\zeta, 0, 0, \zeta, 0, 0)$	$(1/2)C_{11} + (1/2)C_{44}$	$(1/6)C_{111} + (1/2)C_{144}$
$\eta_E = (\zeta, 0, 0, 0, \zeta, 0)$	$(1/2)C_{11} + (1/2)C_{44}$	$(1/6)C_{111} + (1/2)C_{155}$
$\eta_F = (0, 0, 0, \zeta, \zeta, \zeta)$	$(3/2)C_{44}$	C_{456}

TABLE 2: Comparison of the calculated equilibrium lattice constants, SOECs, and TOECs with the experimental data and previous calculations. All data are in unit of GPa except of the lattice constant in Å.

	This work	Previous study	Experiment
a_0	5.763 ^a , 5.626 ^b	5.671 (GGA) ^h , 5.604 (LDA) ^h , 5.75 (GGA) ⁱ	5.653 ^j , 5.65325 ^l
C_{11}	100 ^a , 117 ^b	126 ^g , 118 ^h , 100 ⁱ , 133 ^k	119.0 ^c , 118.8 ^d
C_{12}	47 ^a , 57 ^b	55 ^g , 54 ^h , 49 ⁱ , 57 ^k	53.8 ^c , 53.7 ^d
C_{44}	50 ^a , 58 ^b	61 ^g , 61 ^h , 52 ⁱ , 62 ^k	59.5 ^c , 59.4 ^d
C_{111}	-691	-615 ^f , -600 ^g , -561 ⁱ	-675 ^c , -622 ^d , -620 ^e
C_{112}	-407	-386 ^f , -401 ^g , -337 ⁱ	-402 ^c , -387 ^d , -392 ^e
C_{123}	-67	-81 ^f , -94 ^g , -83 ⁱ	-4 ^c , -57 ^d , -62 ^e
C_{144}	3	11 ^f , 10 ^g , -14 ⁱ	-70 ^c , 2 ^d , 8 ^e
C_{155}	-280	-282 ^f , -305 ^g , -244 ⁱ	-320 ^c , -269 ^d , -274 ^e
C_{456}	-24	-46 ^f , -43 ^g , -22 ⁱ	-69 ^c , -39 ^d , -43 ^e

^aThis work of GGA. ^bThis work of LDA. ^cRef [13] ($T = 298$ K). ^dRef [14] ($T = 298$ K). ^eRef [15] ($T = 298$ K). ^fRef [16]. ^gRef [17]. ^hRef [18]. ⁱRef [19]. ^jRef [49]. ^kRef [50]. ^lRef [51].

2.2. Results and Discussion. The strain energies from first-principles calculations and the fitted polynomials are shown in Figure 1. It is found that, for GaAs with the Lagrangian strain up to 6.4%, considering the terms up to third order in energy expansion is sufficient to obtain good consistency with the first-principles results. In addition, the strain energies with positive strains are always smaller than ones with negative strains; therefore, the values of TOECs are typically negative. In order to examine in which range of strains the third-order effects affect the properties of GaAs, the curves of the nonlinear elasticity comparison with the linear elasticity and the DFT results of a particular deformation η_C are shown in Figure 2. One can see that when the applied deformations are larger than approximately 1.5%, the linear elasticity is not sufficient and the third-order effects must be considered. The calculated results for lattice constant and elastic constants are presented in Table 2. The results are all agreeing well with the previous results and experimental data except for C_{144} . The TOEC C_{144} given by the present paper is a positive value, and the estimated value of 3 GPa agrees well with the experimental result of 2 GPa given in [14]. The results given by the present paper can provide a reference for understanding the elasticity of GaAs.

3. GSFE and Mechanical Properties of 30° Partial Dislocations

3.1. First-Principles Calculations of GSFE. The first-principles total-energy calculations were used to calculate the GSFE, and the process of optimization is the same as the calculation of elastic constants. While for the Brillouin zone, the calculations of GSFE employ $21 \times 21 \times 1$ grid meshes. Because

of the zinc-blende structure, there are two different slip planes (see Figure 3). The widely and closely spaced $\{111\}$ planes, respectively, correspond to the shuffle set and glide set. For discussing the properties of 30° partial in GaAs, the GSFE along $(1/2)\langle 112 \rangle$ on glide set has been calculated with a slab calculation. In order to simulate the process of stacking fault, we employ a slab consisting of 12 atomic layers in the $\langle 111 \rangle$ direction. The vacuum space of 15 Å normal to $\{111\}$ plane between the periodically repeated slab is chosen to avoid the interactions between two slabs. To obtain the reasonable results, we performed that the fluctuations of calculated results' vacuum gap of 15 Å and 18 Å are less than 0.1%. The GSFE was generated by a set of rigid shifts of the upper slab along $(1/2)\langle 112 \rangle$ with respect to the lower slab. For the relaxed GSFE, all atoms of the system are allowed to move only in the $\langle 111 \rangle$ by minimization of the Hellmann–Feynman forces on each atom. The calculated GSFE is shown in Figure 4. The unstable stacking fault energy with relaxation is about two-thirds of that without relaxation.

3.2. Mechanical Properties of 30° Partial Dislocation. The mechanical properties of 30° partial in GaAs have been studied theoretically based on the improved P - N model [28]. As done generally, the restoring force is given by the gradient of the GSFE as suggested by Christian and Vitek [34]; the dislocation equation given by the improved P - N model is

$$-\frac{\beta}{2\sigma} \frac{d^2 u}{dx^2} - \frac{K}{2\pi} \int_{-\infty}^{+\infty} \frac{dx'}{x' - x} \left(\frac{du}{dx} \right) \Big|_{x=x'} = -\nabla \gamma(u). \quad (6)$$

FIGURE 1: The strain-energy relations for GaAs. The discrete points denote the values of DFT calculations; solid curves represent the results obtained from third-order polynomial fitting.

FIGURE 2: Energy as a function of Lagrangian strain parameter ξ for particular deformation η_C . Empty points denote the results of DFT calculations; dashed and solid curves indicate the results obtained from linear and nonlinear elasticity theory, respectively.

FIGURE 3: The two slip planes (glide set and shuffle set) for GaAs.

FIGURE 4: GSFE curves along $(1/2)\langle 112 \rangle$ of the glide set for GaAs. The lines denote the fitted curves from Fourier series (equation (9)), and the discrete points denote the results given by first-principles calculations.

The second-order derivative term proportional to β represents the correction from the discrete effect caused by the interaction among the atoms on the misfit plane. σ is the area of the primitive cell in the misfit plane, and u is the displacement field. The energy factor K is [53]

$$K = \mu \left(\frac{\sin^2 \theta}{1 - \nu} + \cos^2 \theta \right), \quad (7)$$

where θ is the dislocation angle and μ and ν are the effective shear modulus and Poisson's ratio in $\{111\}$ surface [53]. The discrete parameter β for zinc-blende structure crystals has been investigated based on a simple dynamics model [54]. For glide partials, the parameter β is

$$\beta = \frac{(c_{11} - c_{12})a_0^3}{16} \sin^2 \theta. \quad (8)$$

$\gamma(u)$ can be obtained by fitting the calculated GSFE data with

$$\gamma(u) = \gamma \cos^2 \frac{\pi u}{b} \left(1 + \Delta_1 \cos^2 \frac{\pi u}{b} + \Delta_2 \cos^4 \frac{\pi u}{b} \right), \quad (9)$$

where b is the Burgers vector; the fitting curves are shown in Figure 4, and the fitting parameters γ , Δ_1 , and Δ_2 are listed in Table 3.

TABLE 3: The fitting parameters of GSFE, half width ξ , and Peierls stress σ_p of 30° partial in GaAs. ξ_0 and σ_p^0 are the results without considering the discrete effect ($\beta = 0$). The half width and Peierls stress are, respectively, in units of Burgers vector b and GPa.

	γ	Δ_1	Δ_2	ξ_0	ξ	σ_p^0	σ_p
Relaxed	0.14	-0.71	0.27	0.16	0.22	8.11	4.29
Nonrelaxed	0.14	-0.34	0.15	—	0.17	—	9.79

The core structure can be determined by solving dislocation equation (6) with the truncating method proposed by Wang, and the Peierls stress can be obtained from the maximum slope of the dislocation energy [54, 55]. The calculated half width ξ and Peierls stress σ_p of 30° partial in GaAs are listed in Table 3.

It is found that the core structure calculated from the relaxed GSFE is wider, and the Peierls stress is smaller. Because of bond flip appearing for large distortion, the results obtained from the relaxed GSFE is more reliable. The narrow core is reasonable for dislocations in covalent materials. Furthermore, it can be seen that the dislocations will be widened by the discrete effect, and consequently, the Peierls stress will be decreased. The discrete effect is especially important for the narrow dislocations in covalent crystals since it is related to the interaction among the atoms on the misfit plane. The estimated 4 GPa is in good agreement with the experimental results of 2~3 GPa [20, 21]. Furthermore, the Peierls stress of 30° partial in GaAs given by the classical P - N model is 23 GPa [22], about larger by one order of magnitude than that given by improved P - N theory. In addition to negligence of the discrete effect, another possible reason for the difference is that the law of sinusoidal force is applied in [22], while the dimensionless parameters Δ_1 and Δ_2 have been introduced for modifying the sinusoidal force in the present paper.

4. Summary and Discussion

In this paper, the SOECs, TOECs, and GSFEs for semiconductor GaAs are investigated using the first-principles total-energy calculations. The predictions of SOECs and TOECs are obtained from the coefficients of the fitted polynomials of the energy-strain functions. It is found that the nonlinear elastic effects must be considered when the applied deformations are larger than approximately 1.5%. And, with the Lagrangian strains up to 6.4%, the terms included up to the third order in energy expansion functions are sufficient to obtain good agreement with our calculated results. The elastic constants given in this work agree well with the previous results and experimental data except C_{144} . Regarding the disagreement in the magnitude and sign of the TOEC C_{144} , the result given by the present paper is a positive value, and the magnitude of 3 GPa agrees well with the experiment result of 2 GPa given in [14]. Our result can provide a reference for understanding the elasticity of GaAs.

The GSFE has been calculated, respectively, without and with structural relaxation. The unstable stacking fault energy

with relaxation is about two-thirds of that without relaxation. Based on the improved P - N theory, the dislocation width and Peierls stress of 30° partial in GaAs have been calculated. The dislocation is very narrow, and it is reasonable for covalent materials. Because of bond flip appearing for large distortion, the results obtained from the relaxed GSFE are more reliable. The estimated Peierls stress in this work is about 4 GPa; it is in good agreement with the experimental results of 2~3 GPa [20, 21]. Furthermore, according to the Peierls stresses given by the classical P - N model and improved P - N model, it is found that the discrete effect is very important and must be considered when investigating the narrow dislocations in covalent crystals.

Data Availability

The data used to support the findings of the study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

The work was supported by the National Natural Science Foundation of China (Grant no. 11104120).

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