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The Properties of Shuffle Screw Dislocations in Semiconductors Silicon and Germanium

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Abstract: The dislocation widths, Peierls barriers and Peierls stresses for shuffle screw dislocations in diamond structure crystals, Si and Ge, have been calculated by the improved P-N theory. The widths are about 0.6b, where b is the Burgers vector. The Peierls barrier for shuffle screw dislocation in Si and Ge, is about 3.61~4.61meV/Å and 5.31~13.32meV/Å, respectively. The Peierls stress is about 0.28~0.33GPa and 0.31~0.53GPa, respectively. The calculated Peierls barriers and stresses are likely the results of shuffle screw dislocation with metastable core which is centered on the bond between two atoms.

Keywords: Dislocation width, Peierls barrier, Peierls stress, Shuffle screw dislocation.

1. INTRODUCTION

The mechanical properties of Si and Ge have been widely investigated due to their importance in the electronic industry. The plasticity of crystal materials is closely related to the dynamic properties of dislocations. The dislocations in diamond structure crystals Si and Ge can be present in the glide set or shuffle set configurations and the glide dislocation will dissociate into a pair of partial dislocations separated by an intrinsic stacking fault [1]. In experiments, Rabier and Demenet have showed that high external pressures on Si favor a pure shuffle dislocation popular over the partialized glide dislocation [2]. In order to make better use of semiconductors Si and Ge, studying the structure and motion of shuffle dislocation is important. Several attempts have been made to determine the Peierls stress of the shuffle 60^{o} dislocations. However, the screw dislocation has been less studied. *Ab initio* calculations carried out by Cai *et al*. predicted the Peierls stress at zero pressure for Si to be 3.3 ± 0.2GPa [3]. Density functional theory carried out by Pizzagalli *et al.* gives the result 4.1±0.3GPa [4].

Besides the numerical methods, the analytical P-N theory [1, 5, 6] is generally used for studying the structure and motion properties of dislocations. However, because of treating the crystal as an elastic continuum body, the classical P-N model becomes increasingly inaccurate for narrow dislocations [5, 7, 8]. Recently, professor Wang have obtained the improved P-N equation which has relaxed the continuum approximation successfully [9-11]. The research results have shown that the improved P-N theory can remarkably improve the agreement between theoretical prediction and the numerical result [12, 13].

In this paper, the core structure, Peierls barrier and Peierls stress for shuffle screw dislocations in Si and Ge have been studied by the improved P-N theory. An overview of this paper is as follows: Sec 1, Introduction; Sec 2, Dislocation equation, core structure, Peierls barrier and Peierls stress; Sec 3 is the result and discussion. The last section 4 is the conclusion.

2. DISLOCATION EQUATION, CORE STRUCTURE, PEIERLS BARRIER AND PEIERLS STRESS

Based on the lattice dynamics and the symmetry principle, the improved P-N equation for the straight dislocation that describes the balance of atoms on the border can be expressed as:

$$-\frac{\beta}{2}\frac{d^2u(x)}{dx^2}-\frac{K\sigma}{2\pi}\int_{-\infty}^{+\infty}\frac{dx'}{x'-x}\left(\frac{du}{dx}\right)|_{x=x'}=f(u), \tag{1}$$

where u is the displacement field, $f(u)$ is the restoring force, and they are defined along the Burgers vector. σ is the area of primitive cell in the misfit plane. The discrete parameter β and energy factor K can be represented as [1,14]:

$$\beta=\left(\frac{3c_{11}+5c_{12}}{24}\sin^2\theta+\frac{c_{11}-c_{12}}{16}\cos^2\theta\right)a_0^3,$$
$$K=\left(\frac{\sin^2\theta}{1-\nu}+\cos^2\theta\right)\mu \tag{2}$$

Where θ is the dislocation angel, μ and ν are the effective shear modulus and Poisson's ratio within {111} plane [1,5], c_{11} and c_{12} are the elastic constants, and a_0 is the lattice constant. The values for these constants are listed in Table **1**.

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Table 1. The effective shear modulus and Poisson's ratio μ and ν within {111} plane, elastic constants c_{11} and c_{12}, and the lattice constant a_0 for Si and Ge, where μ, c_{11} and c_{11} are in units of GPa, a_0 in unit of Å.

	μ	ν	c_{11}	c_{12}	a_0
Si	63.75	0.256	165.7	63.9	5.43
Ge	52.00	0.248	128.9	48.3	5.65

Table 2. The modification factors Δ_1 and Δ_2. SW and Baskes represent the γ-surface that has been calculated by Stillinger-Weber and MEAM-Baskes inter-atomic potential, respectively; LDA and GGA represent the γ-surface that has been calculated by Vienna *ab initio* simulation package (VASP) with the local density approximation and the generalized gradient approximation, respectively.

	Si		**Ge**	
	Δ_1	Δ_2	Δ_1	Δ_2
SW	-0.82	0.315	-0.40	0.26
Baskes	-0.10	-0.16	0.12	-0.38
LDA	-1.00	0.76	-1.10	0.84
GGA	-0.90	0.68	-1.20	0.90

The restoring force *f(u)* in Eq.(1) is given by the gradient of the γ-surface [15]

$$f = -\nabla\gamma(\mathrm{u})\sigma$$

The γ-surface of shuffle set for Si and Ge has been calculated by Kang and Cai [16], and it can be expressed as follows [17]:

$$\gamma_b(\mathrm{u}) = \frac{\mu b^2}{4\pi^2 d}(1+\cos\frac{2\pi u}{b})(1+\Delta_1\cos^2\frac{\pi u}{b} + \Delta_2\cos^4\frac{\pi u}{b}), \quad (3)$$

where *b* and *d* are the Burgers vector and the spacing between glide planes, respectively. Δ_1 and Δ_2 are the modification factors to the sinusoidal-force law. For fitting the γ-surface given in Ref. [16], Δ_1 and Δ_2 have been listed in Table **2**. The γ-surface and the fitted curve have been plotted in Fig. (**1**).

The dislocation Eq.(1) can be solved by truncating method proposed by professor Wang and the trial solution possesses the following form [14, 18]

$$u = \frac{b}{\pi}(\arctan q + \frac{cq}{1+q^2}), \quad (4)$$

with

$$q = kx, k = k_0(1-\mathrm{c}), \mathrm{k}_0 = \frac{2}{d}(\frac{\sin^2\theta}{1-\nu}+\cos^2\theta)^{-1}, \quad (5)$$

where the parameter *c* is a constant that can be determined by the dislocation equation.

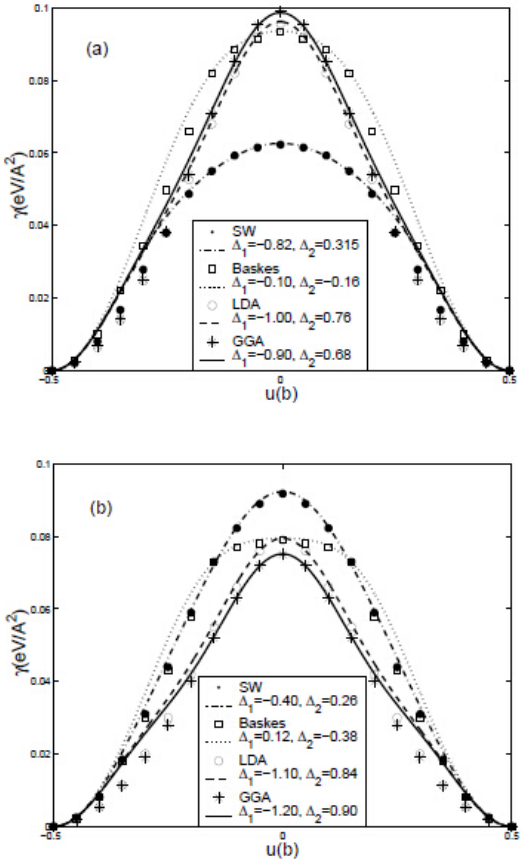

Fig. (1). The γ-surface along <110> direction of shuffle set for Si and Ge given by Kang *et al*. [16] and fitted by Eq. (3), where the Burgers vectors for Si and Ge are 3.84Å and 4.00Å, respectively.

Table 3. The core parameter *c* and half width ξ. c_0 and ξ_0 are given by the classical P-N model.

	Potential	c_0	c	$\xi_0(b)$	$\xi(b)$
	SW	0.85	0.88	0.99	1.21
Si	Baskes	0.62	0.76	0.46	0.66
	LDA	0.48	0.73	0.38	0.60
	GGA	0.46	0.72	0.37	0.58
	SW	0.39	0.69	0.35	0.54
Ge	Baskes	0.63	0.76	0.47	0.66
	LDA	0.50	0.74	0.38	0.62
	GGA	0.57	0.76	0.42	0.66

Substituting the solution Eq.(4) into dislocation equation and after complicated calculations, an algebraic equation about parameter *c* can be obtained as follows:

$$\frac{2\beta\mu}{K^2\sigma d}(1+2c)(1-c)^2-\frac{4c^2}{5}-\Delta_1(1+\frac{c}{5})-\frac{6\Delta_2}{5}=0. \quad (6)$$

It recovers the classical P-N model when the discrete parameter β equals to zero.

The core parameter *c* calculated from Eq.(6) and half width (the distance that *u* changes from 0 to *b*/4) are listed in Table **3**.

In the classical P-N theory, the Peierls barrier and stress are obtained by calculating misfit energy only. However, it has been shown that the contributions of strain energy and misfit energy are equally important [19]. The total energy which includes the contribution of misfit and strain energies should be evaluated to obtain the correct Peierls barrier and Peierls stress. For a dislocation with length *L*, the strain and misfit energies of dislocation per unit length are given by [14].

$$E_{str}(x_0)=\frac{1}{2}\sum_{l=-\infty}^{\infty}f_b(u_l)u_l\times\frac{\sigma}{a}, \quad (7)$$

$$E_{mis}(x_0)=\sum_{l=-\infty}^{\infty}\gamma_b(u_l)\times\frac{\sigma}{a}, \quad (8)$$

where $u_1=u(x_1-x_0)$ is the relative displacement for dislocation located at x_0, *a* is the length of the primitive vector (period in the direction of dislocation line). Just as shown in Fig. (**2**), sum is carried over the atoms located in the horizontal band in the misfit plane (the band width is *a*). According to Eq.(7) and Eq.(8), the total energy is:

$$E_{tot}=\sum_{l=-\infty}^{\infty}\frac{\mu b^2\sigma}{4\pi^2 ad}\{(1+\cos\frac{2\pi u_l}{b})(1+\Delta_1\cos^2\frac{\pi u_l}{b}+\Delta_2\cos^4\frac{\pi u_l}{b})+[(1+\Delta_1)\sin\frac{2\pi u_l}{b}+\frac{\Delta_1}{2}\sin\frac{4\pi u_l}{b}+3\Delta_2\sin\frac{2\pi u_l}{b}\cos^4\frac{\pi u_l}{b}]u_l\}. \quad (9)$$

Due to discreteness of lattice, a dislocation cannot move unless the applied stress exceeds the Peierls stress. The Peierls stress can be obtained from the maximum slope of the total energy:

$$\sigma_p=\max\left|\frac{1}{b}\frac{dE_{tot}(x)}{dx}\right|. \quad (10)$$

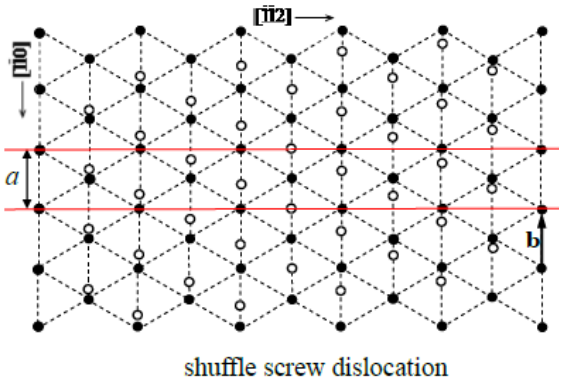

Fig. (2). Core structure of the shuffle screw dislocation. The black and white circles represent the atoms on the misfit planes that above and below the cut plane, respectively.

The calculated Peierls barriers and Peierls stresses are listed in Table **4**.

3. RESULT AND DISCUSSION

The width of dislocation is mainly related to the unstable stacking fault energy. The higher the unstable stacking fault energy, the narrower the dislocation is. The widths of shuffle screw dislocations in Si and Ge are about 0.6*b*. The Peierls barriers and Peierls stresses calculated from SW potential are much lower than those calculated from three other potentials. Besides, the results given by classical P-N theory calculated from Baskes potential are much lower than those calculated from LDA and GGA potentials. Thus, the results calculated from LDA and GGA potentials are thought to be more reliable. The Peierls barrier for shuffle screw dislocation in Si and Ge is 3.61~4.61meV/Å and 5.31~13.32meV/Å, respectively. Peierls stress is 0.28~0.33GPa and 0.31~0.53GPa, respectively. The calculated Peierls stress for Si is about one magnitude lower than the numerical results given in [3, 4]. The research on shuffle screw dislocation in Si shows that there exist two different core structures: core A is centered in the 6-member ring of atoms [20], core B is centered on the

Table 4. The Peierls barrier (meV/Å) and Peierls stress (meV/Å^3) for shuffle screw dislocation. $E_p(0)$ and $\sigma_p(0)$ are given by classical P-N model.

	Potential	$E_p(0)$	E_p	$\sigma_p(0)$	σ_p
	SW	2.19	1.45	0.54	0.36
Si	Baskes	13.85	6.52	4.13	1.65
	LDA	134.69	3.61	36.80	1.73
	GGA	137.72	4.61	37.35	2.07
	SW	128.55	9.16	30.13	2.09
Ge	Baskes	9.70	10.13	3.47	2.40
	LDA	99.86	5.31	29.57	1.93
	GGA	100.50	13.32	24.90	3.29

bond between two atoms [21]. Recent *ab initio* calculations show that core A is the ground state of a perfect screw dislocation, while core B is metastable, with an energy 0.38 eV/*b* higher than that of core A [3]. The Peierls barriers and Peierls stresses given in this paper are likely the results of metastable screw dislocations.

CONCLUSION

The core structures, Peierls barriers and Peierls stresses for shuffle screw dislocations in semiconductors Si and Ge, have been investigated. Our results indicate that the results calculated from LDA and GGA potentials are more reliable. The Peierls barrier for shuffle screw dislocation in Si and Ge, is about 3.61~4.61 meV/Å and 5.31~13.32 meV/Å, respectively. Peierls stress is 0.28~0.33 GPa and 0.31~0.53 GPa, respectively. The calculated Peierls barriers and Peierls stresses are likely the results of dislocations with metastable core which is centered on the bond between two atoms. Further studies will be carried out to better understand the mechanical properties of shuffle screw dislocation with different core structures.

CONFLICT OF INTEREST

The authors confirm that this article content has no conflict of interest.

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