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On the Properties of Shuffle Dislocation in BC_5: Core Structure and Peierls Barrier and Stress†

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The dislocation widths for shuffle 60º and screw dislocations in diamond like BC_5 have been calculated by the improved Peierls-Nabarro theory in which the discrete effect has been taken into account. For the dislocations with same angles, the width of dislocation located between B-C layers is about 1.2 times wider than that located between C-C layers. For the dislocations located between same layers, the width of 60º dislocation is about 1.4 times wider than that of the screw dislocation. Peierls barriers and stresses have been evaluated with considering the contribution from both misfit and strain energies. The Peierls barriers for shuffle 60º and screw dislocations in BC_5 are, respectively about 0.059 and 0.167 eV/Å, Peierls stresses are, respectively about 5 and 15 GPa. The results calculated in this paper are useful for data analysis of experiments.

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

INTRODUCTION

The applications of diamond are limited due to its reaction with ferrous metals and nonresistant to oxidation[1]. Doping a small amount of boron can improve the oxidation resistance[2], reduce the energy band gap[3] and increase the superconducting transition temperature[4-9] of the original diamond crystals. Solozhenko *et al.*[10] have synthesized diamondlike BC_5 with the ultimate boron solubility in diamond. They reported that the BC_5 has extreme Vickers hardness (71 GPa) which depends strongly on plastic deformation. However, the available information about the plastic deformation of BC_5 is very sparse[11]. As is well known, the plastic deformation of materials is closely related to the dislocations. Study the dislocations in BC_5 is therefore necessary.

Besides the numerical method, the analytical Peierls-Nabarro (P-N) theory[12-14] is the best for investigating basic properties of dislocations. However, the classical P-N model becomes increasingly inaccuracy for narrow dislocations[13,15,16] due to it has treated the crystal as an elastic continuum body and the discrete effect is missed in the continuum approximation. The discrete effect will remarkably modify the core structure where the displacement field varies rapidly[17]. Recently, Wang[17-19] has successfully relaxed the continuum approximation and obtained the improved P-N equation based on the lattice dynamics. The discrete effect is represented by a term proportional to the second-order derivative of displacement. It is found that the agreement between theoretical prediction given by improved P-N theory and the numerical results can be remarkably improved[20-28]. In this paper, the core structures of shuffle dislocations in BC_5 have been studied by the improved P-N equation and the Peierls barriers and stresses have been evaluated with considering the contribution from strain energy.

Dislocation equation and γ-surface: According to the two-dimensional dislocation equation for straight dislocations[19] and the method given in Ref. 13 and Ref. 20, the dislocation equation for an arbitrary mixed dislocation takes the following form

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

where u and $f_b(u)$ are defined along Burgers vector, σ is the area of primitive cell of the misfit plane (which is a two-dimensional triangular lattice for BC_5). The coefficients β and K are, respectively

$$\beta=\beta_e\sin^2\varphi+\beta_s\cos^2\varphi, K=K_e\sin^2\varphi+K_s\cos^2\varphi \qquad (2)$$

where φ is the dislocation angle, K_e and K_s are, respectively the energy factors for edge and screw dislocations[12], β_e and β_s

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are the discrete parameters for edge and screw dislocations[21]. The energy factors can be expressed in terms of effective shear modulus and Poisson's ratio within the {111} plane[13]

$$K_e = \frac{\mu_e}{(1-\nu_e)},\ K_s = \mu_e \quad (3)$$

with the values μ_e = 363 GPa, ν_e = 0.162 for BC_5[1,12]. The discrete parameters and for dislocations in diamondlike crystals have been derived from a simple dynamics model[21]. For shuffle dislocations, β_e and β_s are, respectively

$$\beta_e = \frac{(3c_{11}+5c_{12})a^3}{24}, \qquad \beta_s = \frac{(c_{11}-c_{12})a^3}{16}$$

where c_{11} and c_{12} are the elastic constants. For BC_5, c_{11} = 865 GPa and c_{12} = 177 GPa[1]. a = 3.606 Å is the lattice constant.

The restoring force $f_b(u)$ in dislocation eqn. 1 can be obtained from the gradient of the γ-surface as suggested by Christian and Vitek[29]

$$f = -\nabla\gamma(u)$$

The γ-surface of shuffle set for BC_5 has been calculated by Lazara and Podloucky[30]. The calculated unstable stacking fault energies of γ-surface that slip between widely spaced B-C layers and C-C layers are, respectively about 6.2 and 8.2 J/m^2. It is noted that the γ-surface along <110> direction of shuffle set can be approximately expressed as

$$\gamma_b(u) = \gamma_0\left(1+\cos\frac{2\pi u}{b}\right)\left(1+\Delta_1\cos^2\frac{\pi u}{b}+\Delta_2\cos^4\frac{\pi u}{b}\right) \quad (4)$$

where b is the Burgers vector, Δ_1 and Δ_2 describe the modification to the sinusoidal-force law. In Table-1, the fitting parameter γ_0 and modification factors Δ_1 and Δ_2 are listed for fitting γ-surface given in Ref. 30.

TABLE-1
FITTING PARAMETERS γ_0, Δ_1 AND Δ_2, B-C AND C-C RESPECTIVELY REPRESENT SLIP BETWEEN WIDELY SPACED B-C LAYERS AND WIDELY SPACED C-C LAYERS, γ_0 IS IN UNIT OF J/m^2

	γ_0	Δ_1	Δ_2
B-C	3.007	0.033	0.000
C-C	2.728	1.049	-0.544

The profiles of the γ-surface and the restoring force are plotted in Fig. 1. The γ-surface can be satisfactorily fitted by eqn. 4.

The dislocation eqn. 1 can be solved by truncating method proposed by Wang[31] and the solution is

$$u = \frac{\pi}{b}\left(\arctan p + \frac{cp}{1+p^2}\right) \quad (5)$$

$$\text{with } p = kx,\ k = k_0(1-c),\ k_0 = \frac{2}{d}\left(\frac{\sin^2\varphi}{1-\nu_e}+\cos^2\varphi\right)^{-1} \quad (6)$$

where d is the spacing between glide planes. After complicated calculations, the algebraic equation about core parameter c can be obtained

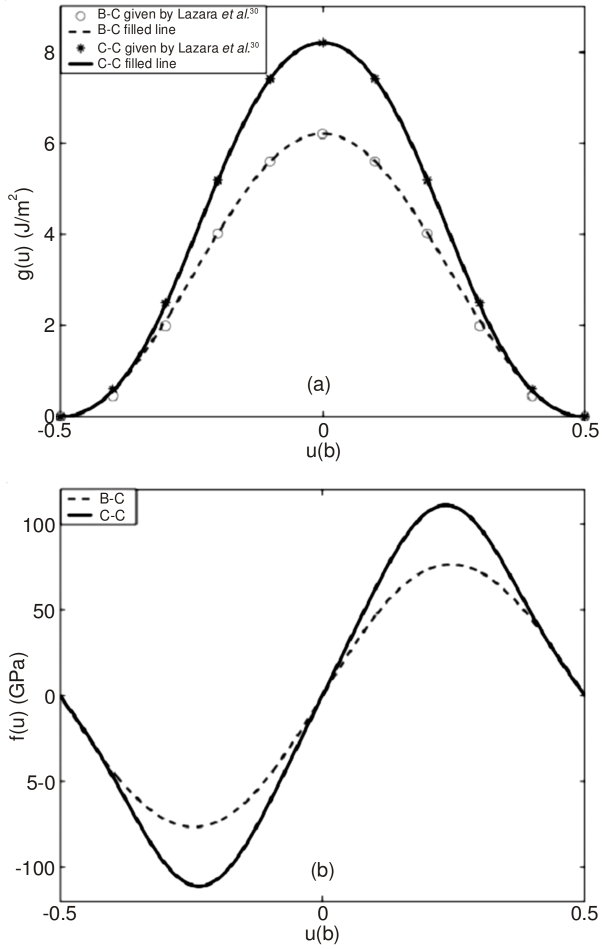

Fig. 1. (a) γ-Surface along <110> direction of shuffle set for BC_5 given by Lazara and Podloucky[30] and fitted by eqn. 4, where B-C and C-C, respectively represent the slip between widely spaced B-C layers and widely spaced C-C layers; (b) The corresponding restoring force

$$\frac{\beta\mu_e^2 b^2}{K^2\pi^2\gamma_0\sigma d^2}(1+2c)(1-c)^2 + \frac{\mu_e b^2}{6\pi^2\gamma_0 d}(1-c)(2+3c)$$

$$-\frac{2}{15}(10+5c-3c^2) - 2\Delta_1\left(1+\frac{c}{5}\right) - \frac{12\Delta_2}{5} = 0 \quad (7)$$

If parameter β equals to zero, eqn. 7 recovers the classical P-N model with generalized stacking fault restoring force. For convenience, we have listed the elementary constants in Table-2.

TABLE-2
ELEMENTARY CONSTANTS BURGERS VECTOR b, SPACING d, DISCRETE PARAMETER β AND ENERGY FACTOR K FOR 60° AND SCREW DISLOCATIONS

Dislocation	b (Å)	d (Å)	β (eV)	K (eV/Å^3)
60°	2.55	1.56	35.02	2.60
Screw	2.55	1.56	12.60	2.27

Dislocation width and Peierls barrier and stress: The core parameter c calculated from eqn. 7 and half width ξ, defined as the distance over which μ changes from 0 to b/4 are listed in Table-3.

Obviously, after considering the correction from discrete effect, the width of dislocation becomes wider. For γ-surface slip between widely spaced C-C layers (γ_0 = 2.728 J/m^2), the

TABLE-3
CALCULATED CORE PARAMETER C AND HALF WIDTH ξ FOR SHUFFLE 60° AND SCREW DISLOCATIONS IN BC_5, c_0 AND ξ_0 ARE THE RESULTS GIVEN BY CLASSICAL P-N MODEL WITH THE SAME γ-SURFACE. THE WIDTH IS GIVEN IN UNIT OF BURGERS VECTOR b. B-C (C-C) REPRESENTS THE DISLOCATION IS LOCATED BETWEEN B-C (C-C) LAYERS

Dislocation	Layers	c_0	c	ξ_0	ξ
60°	B-C	0.41	0.77	0.40	0.78
60°	C-C	–	0.71	–	0.65
Screw	B-C	0.41	0.71	0.35	0.56
Screw	C-C	–	0.60	–	0.44

unstable stacking fault energy is so high that the parameter c_0 has no real root. For the dislocations located between same layers (B-C layers or C-C layers), the width of 60° dislocation is about 1.4 times wider than that of screw dislocation. Besides, the dislocation located between widely spaced B-C layers is about 1.2 times wider than that located between the widely spaced C-C layers, it is mainly resulted from that the unstable stacking fault energy of the γ-surface slip between B-C layers is lower (Fig. 1). Therefore, it is reasonable to expected that the Peierls barrier and stress of the dislocation located between B-C layers are lower than that located between C-C layers.

In the classical P-N theory, the Peierls barrier and stress are obtained by calculating the misfit energy only. However, it has been shown that the contribution from strain energy is as important as that from the misfit energy[21,32]. Therefore, the total energy including contribution from both misfit and strain energies should be evaluated to obtain correct result. For a dislocation, the misfit and strain energies per unit length are given by[21]

$$E_{mis}(x) = \sum_{l=-\infty}^{\infty}\frac{\sigma}{a_0}\times\gamma_b(u_l), E_{str}(x) = \frac{1}{2}\sum_{l=-\infty}^{\infty}\frac{\sigma}{a_0}\times f_b(u_l)u_l \quad (8)$$

where $u_l = u(x_l - x_0)$ is the relative displacement for dislocation located at x_0, $a_0 = a/\sqrt{2}$ is the length of the primitive vector (period in direction of dislocation line), sum is carried over the atoms in the horizontal band with width a_0 in a misfit plane (Fig. 2).

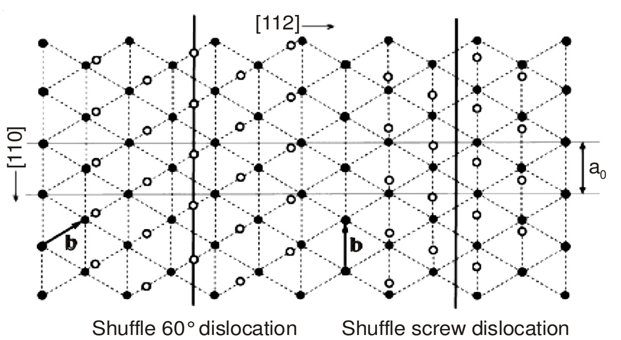

Fig. 2. Core structure of shuffle 60° and screw dislocations. The solid and empty circles, respectively represent the atoms on the misfit planes that below and above the cut plane. For simplicity, the distortion is shown by the relative displacements of atoms on the upper misfit plane

Substituting eqn. 4 and resulted force into above equations and according to $E_{tot} = E_{mis} + E_{str}$, we can obtain the total energy per unit length

$$E_{dis} = \sum_{l=-\infty}^{\infty}\frac{\sigma}{a_0}\gamma_0\left[\left(1+\cos\frac{2\pi u_l}{b}\right)\left(1+\Delta_1\cos^2\frac{\pi u_l}{b} + \Delta_2\cos^4\frac{\pi u_l}{b}\right) + \frac{\pi}{b}\sin\frac{2\pi u_l}{b}\left(1+\Delta_1+\Delta_1\cos\frac{2\pi u_l}{b} + 3\Delta_2\cos^4\frac{\pi u_l}{b}u_l\right)\right] \quad (9)$$

For a narrow dislocation, the series in the summation converges rapidly apart from an additional constant which has no contribution to the Peierls barrier and stress[15].

As a function of dislocation position, the misfit, strain and total energies have been calculated and plotted in Fig. 3 and the calculated Peierls barriers have been listed in Table-4. The results clearly tell us that the discrete effect lowered the Peierls barrier greatly. When a dislocation moves, both strain and misfit energies change periodically. They possess the same order amplitudes, but opposite phases. Therefore, the discrete effect and the contribution from strain energy can not be neglected.

The Peierls stress is the minimum stress to move a dislocation, it can be obtained from the maximum slope of the dislocation energy[12]

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

The calculated Peierls stresses have been listed in Table-4.

Similarly to Peierls barrier, the discrete effect lowered the Peierls stress greatly. For the dislocations located between same layers, the Peierls barrier and stress of the screw dislocation are higher than those of 60° dislocation. Besides, the Peierls barrier and stress of the dislocation located between B-C layers are much lower than that located between C-C layers. The Peierls barriers for 60° and screw dislocations located between B-C layers are respectively about 0.012 and 0.046 eV/Å, for dislocations located between C-C layers, the Peierls barriers are respectively about 0.059 and 0.167 eV/Å. The Peierls stresses for 60° and screw dislocations located between B-C layers are respectively about 0.006 V/Å^3 (~ 1 GPa) and 0.026 eV/Å^3 (~ 4 GPa), for dislocations located between C-C layers, the Peierls stresses are respectively about 0.033 eV/Å^3 (~ 5 GPa) and 0.096 eV/Å^3 (~ 15 GPa). However, the structure of BC_5 is found to be chemically disordered by Jiang *et al.*[33] through performing first-principle density-functional calculations. It means that the islocation gliding in a {111} shuffle plane will cut B-C but also C-C bonds, and therefore, the Peierls stresses for moving the dislocations will be the larger ones: the Peierls stresses for shuffle and screw dislocations in diamondlike BC_5 should be respectively 5 and 15 GPa. The critical shear stresses for {111} <110> and {111} <112> slip system of BC_5 given by Wang *et al.*[11] are respectively 28.7 and 27.0 GPa. These values for Si calculated by *ab initio* approaches are 9.6 GPa for the {111}<110> slip system[34] and 8.1 GPa for the {111} <112> slip system[35]. Although the value 9.6 GPa for {111} <110> is higher than that of 5 GPa computed for the Peierls stress of shuffle 60° dislocation in BC_5, the difference is rather low. Consequently, the plasticity

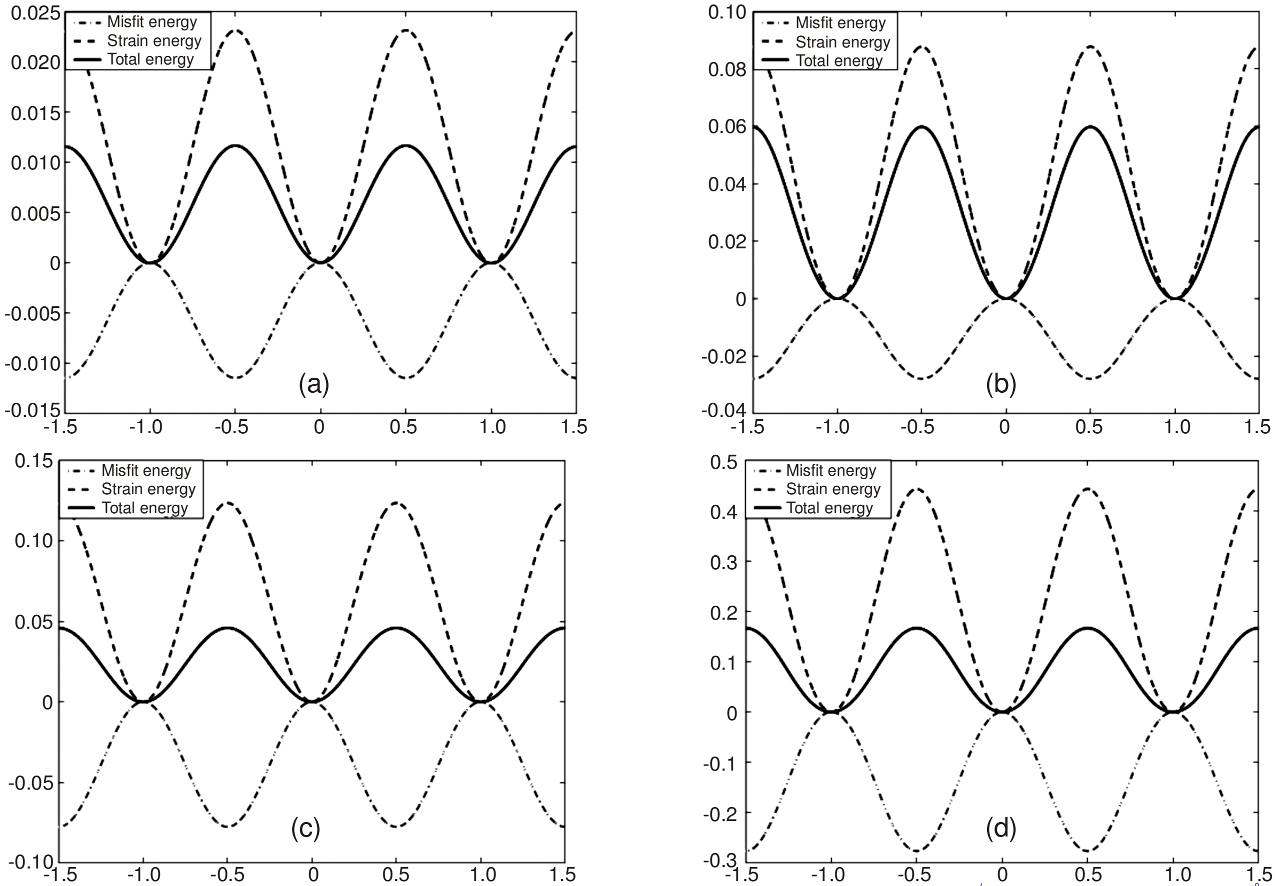

Fig. 3. Misfit, strain and total energies as a function of dislocation position, where x axis is in unit of the period $\sqrt{3}a_0/2$ and y axis in unit of eV/Å. The ground energy is taken to be zero-point. (a) 60º dislocation located between B-C layers; (b) dislocation located between C-C layers; (c) screw dislocation located between B-C layers; (d) screw dislocation located between C-C layers

TABLE-4
PEIERLS BARRIER IN UNIT OF eV/Å AND PEIERLS STRESS IN UNIT OF eV/Å^3 FOR SHUFFLE 60º AND SCREW DISLOCATIONS IN BC5. E_p and σ_p ARE OBTAINED FROM THE TOTAL ENERGY, $E_p^m(0)$, $\sigma_p^m(0)$ and E_p^m, σ_p^m ARE OBTAINED FROM THE MISFIT ENERGY ONLY, $E_p^m(0)$ and $\sigma_p^m(0)$ HAVE NOT CONSIDERED THE CORRECTION FROM DISCRETE EFFECT

Dislocation	Layers	$E_p^m(0)$	E_p^m	E_p	$\sigma_p^m(0)$	σ_p^m	σ_p
60º	B-C	0.267	0.011	0.012	0.150	0.006	0.006
60º	C-C	–	0.028	0.059	–	0.016	0.033
Screw	B-C	0.348	0.077	0.046	0.197	0.043	0.026
Screw	C-C	–	0.276	0.167	–	0.155	0.096

of BC_5 must be very poor and the crystal is expected to be brittle.

Conclusion

The dislocation width, Peierls barrier and stress of shuffle 60º and screw dislocations in diamondlike crystal BC_5 have been calculated. In calculation, the discrete effect and contribution from elastic strain energy which have been ignored in classical P-N theory have been taken into account. It is found that for the dislocations with same angles, the width of dislocation located between B-C layers is wider (about 1.2 times) than that located between C-C layers. For the dislocations located between same layers, the width of 60º dislocation is wider (about 1.4 times) than that of screw dislocation. The differences between calculated Peierls barriers (stresses) for different shuffle dislocations in BC_5 are very large. Considering the chemically disordered structure of BC_5, the Peierls barriers for shuffle 60º and screw dislocations are, respectively 0.059 and 0.167 eV/Å, the Peierls stresses are, respectively 5 and 15 GPa. The results calculated by us are correspond to the critical shear stress 9.6 GPa for the {111} <110> slip system of Si, therefore, the plasticity of BC_5 must be very poor. The results calculated by us are useful for data analysis of experiments.

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