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Metastablity of the undissociated state of dissociated dislocations

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Abstract

Undissociated, metastable dislocations have been observed in various crystals in addition to stable dissociated dislocations by high-resolution transmission electron microscopy. The origin of the metastablity of the undissociated state has been discussed specifically for the dissociation into Shockley partial dislocations in fcc or hcp lattice. It is shown that the metastability is due either to a high Peierls–Nabarro stress larger than a few percent of the shear modulus of the partial dislocations and/or to the increase of the total core energy by an increase of the dangling bonds. The metastablity of undissociated dislocations in zincblende III–V compounds is concluded to be due to a contribution of the latter effect.

Keywords: Dislocation dissociation; Shockley partial dislocation; Metastability; Peierls–Nabarro stress; Dangling bond

1. Introduction

It is well established that dislocations in crystals are dissociated into partial dislocations bounding a stacking fault between them when there exists a stable stacking fault in the crystal. The separation between the partials or the dissociation width w is determined so as to minimize the total energy or by the balance between the repulsive force of the partials and the surface tension of the stacking fault. Electron microscopy observation of dislocations has shown, however, that in many occasions undissociated dislocations are also present in addition to the dissociated dislocations. Long constricted segments have been observed in Si by weak-beam technique [1]. Both dissociated and undissociated core structures have been observed by high-resolution electron microscopy for III–V compounds of GaAs [2,3], InP [4] and GaN [5], for II–VI compounds of CdS, CdSe [6] and ZnO [7]. These observations indicate that undissociated state can be metastable for the stable dissociated dislocation. In this paper, we discuss the origin of the metastability of the undissociated state.

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2. Strain energy consideration

The energy of a perfect dislocation can be represented by the sum of the elastic energy outside the core radius r_c where the elastic strain can be described by the linear elasticity theory, and the core energy inside the radius r_c. The value of r_c is (2–3)b, where b is the strength of the Burgers vector of the dislocation. Assuming elastic isotropy, the elastic energy is expressed as:

$$E_{el} = \frac{KGb^2}{4\pi} \ln \frac{R}{r_c}, \quad (1)$$

where R is the outer-cutoff radius which is of the order of the average dislocation spacing in the crystal, G the shear modulus of the crystal and the factor K depends on the dislocation character: $K = 1$ for screw dislocation and $K = (1-\nu)^{-1}$ (ν: Poisson's ratio) for edge dislocation. The core energy depends on the type of the crystal and cannot be expressed in a universal way; so that the core energy contribution is usually incorporated in the total energy by using an effective cutoff parameter r_0 ($<r_c$) and thus the total energy E_u (subscript u stands for undissociated dislocation) is written as:

$$E_u = \frac{KGb^2}{4\pi} \ln \frac{R}{r_0}. \quad (2)$$

In metallic crystals r_0 is about $b/3$ [8–11]. In real situations, the outer-cutoff radius is variable and so we may regard R/r_0 in Eq. (2) a variable parameter. For a typical dislocation density of $10^6\ \mathrm{cm}^{-2}$, $R/r_0 \approx 10^5$.

The total energy of a dissociated dislocation is the sum of the self-energies of the two partial dislocations, the interaction energy between the partial dislocations and the energy of the stacking fault between the partials. Let b_1 and b_2 be the strength of the partial Burgers vector, θ_1 and θ_2 be the angle between the dislocation line and the Burgers vector of partial 1 and partial 2, respectively, and Γ be the stacking fault energy per unit area and x the distance between the partial 1 and partial 2. Then, the total energy of the dissociated dislocation E_d (subscript d stands for dissociated dislocation) is given as:

$$E_\mathrm{d}(x) = \frac{K_1 G {b_1}^2}{4\pi} \ln\frac{R}{r'_0} + \frac{K_2 G {b_2}^2}{4\pi} \ln\frac{R}{r'_0} + \frac{\beta G b_1 b_2}{2\pi} \ln\frac{R}{x} + \Gamma x \quad \text{with}$$

$$K_{1,2} = \frac{1-\nu\cos^2\theta_{1,2}}{1-\nu}$$

$$\beta = \cos\theta_1\cos\theta_2 + \frac{1}{1-\nu}\sin\theta_1\sin\theta_2. \tag{3}$$

The equilibrium width w of the dissociated dislocation is determined by the condition $\mathrm{d}E_\mathrm{d}(x)/\mathrm{d}x = 0$, which gives

$$w = \frac{\beta G b_1 b_2}{2\pi\Gamma}. \tag{4}$$

We should note that the interaction energy term in Eq. (3) is valid only for x larger than the core radius r'_c for partials, where the linear elasticity theory can apply.

Now, we consider the energy change in the dissociation process of an undissociated dislocation into partial dislocations. In the following, we treat the most popular dissociation scheme of Heidenreich–Shockley extended dislocation in fcc and hcp lattices, i.e., the dissociation into Shockley partial dislocations, which is represented by the following equation for the case of fcc crystals.

$$\frac{1}{2}[1\,1\,0] = \frac{1}{6}[2\,1\,1] + \text{stacking fault} + \frac{1}{6}[1\,2\,\bar{1}] \tag{5}$$

In the numerical evaluation of the energy, we assume that Poisson's ratio is 1/3 and the effective inner-cutoff radius r_0 or r'_0 is one-third of the corresponding Burgers vector. We should note that the ambiguity of taking the inner-cutoff radius is equivalent to the ambiguity on the outer-cutoff radius because these two values appear in the energy equation as their ratio.

Fig. 1 shows the energy of an edge dislocation for unit length as a function of the separation distance of the Shockley partials for three equilibrium dissociation widths of $w = 5b$, $10b$ and $20b$, and for $R = 10^4b$. We note that the energy versus distance curves for $R = 10^3b$ and 10^5b are the same as that for $R = 10^4b$ but shifted by $0.275\,Gb^2$ downwards or upwards, respectively. Fig. 2 shows the results for a mixed dislocation where the dislocation line and the Burgers vector make 60°, and Fig. 3 the results for a screw dislocation again for $w = 5b$, $10b$ and $20b$. In these figures, we have assumed that the interaction term in Eq. (3) is valid approximately for $x \geq 2b$. In the case of 60°dislocation and screw dislocation, the change

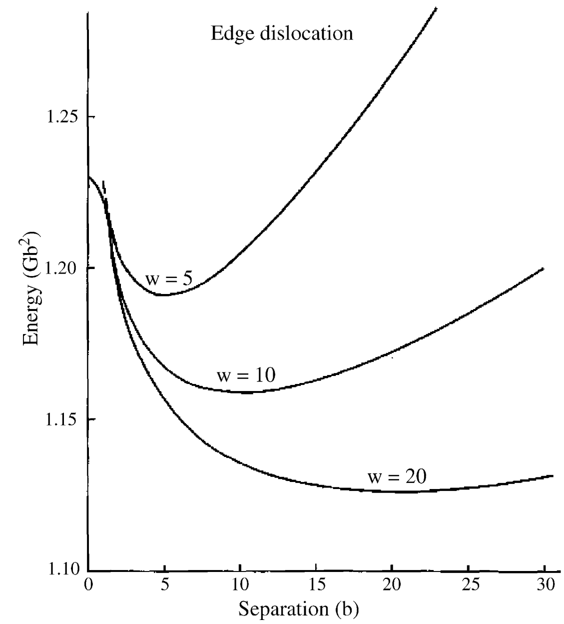

Fig. 1. Change of the strain energy of an edge dislocation with dissociation into Shockley partial dislocations for three different stacking fault energies giving equilibrium dissociation widths of $w = 5b$, $10b$ and $20b$.

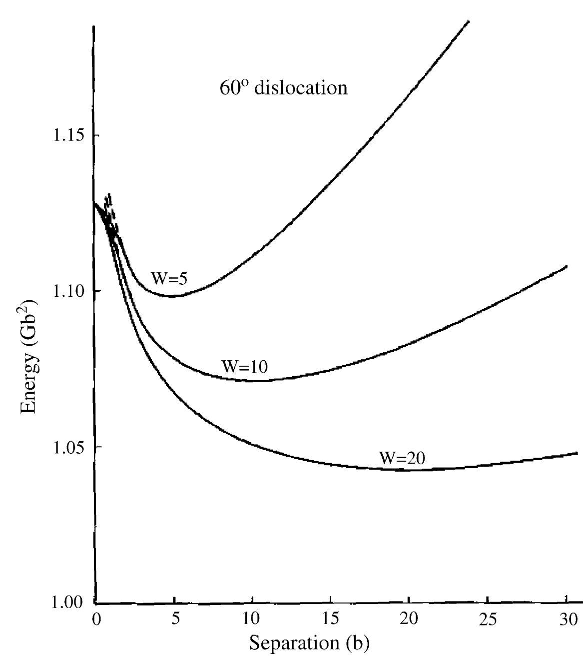

Fig. 2. Change of the strain energy of a 60°-dislocation with dissociation into Shockley partial dislocations for three different stacking fault energies giving equilibrium dissociation widths of $w = 5b$, $10b$ and $20b$.