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Computer simulation of a single kink in the [010] screw dislocation in anthracene crystals

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Abstract. The equilibrium configuration for the core of a single kink in the [010] screw dislocation in anthracene crystals has been calculated through computer simulations. The method was based on the assumption of a rigid-body molecule and intermolecular interactions were evaluated using the atom–atom potential method. It followed that a single kink of smooth type was realized in the screw dislocation. The formation energy of the kink was estimated as 0.5 eV. The Peierls stress for the side motion of the kink along the dislocation line, i.e. the Peierls stress of the second kind, was roughly estimated by means of applying an external shear stress. It was much smaller than one twentieth of the Peierls stress of the first kind of the [010] screw dislocation, $2.0 \times 10^{-1}\,\mu$, where μ is the shear modulus.

1. Introduction

The motion of dislocations in Peierls troughs goes through two processes at low temperature, i.e. nucleation of kink pairs in a straight dislocation and side motions of the kinks along the dislocation line. Knowledge on dislocation kinks—such as the shape and the formation energy—is indispensable in explaining how dislocations move at finite temperature. However, no investigation on dislocation kinks has yet been reported for organic materials.

In anthracene crystals, both (001)[010] slip systems and (001)[110] systems are dominantly operative [1, 2]. The slip deformation characteristics of anthracene crystals were divided into two temperature regions [3]; one is a high-temperature region above 180 K where the deformation is controlled through jogs produced on cutting forest dislocations, and the other is a low-temperature region below 180 K where the Peierls mechanism seems operative. However, neither the smooth-kink model [4, 5] nor the abrupt-kink model [6] could explain the strong temperature dependence of the yield stress at low temperature within the framework of continuum elasticity [3]. One problem of particular interest is that of what structure of the kink is realized in a crystal composed of disc-like molecules possessing a rigid body.

In our previous work, the molecular configurations around the [010](001) edge and [010] screw dislocations were investigated using computer simulations [7, 8], and Peierls stresses of those dislocations were evaluated by means of gradually increasing an external

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shear stress [8]. The Peierls stress of the screw dislocation, $2.0 \times 10^{-1}\,\mu$, was much larger than that of the edge dislocation, $1.0 \times 10^{-3}\,\mu$, where μ is the shear modulus. The former decreased rapidly as temperature increased [9]. In the present article we will report the structure, the formation energy and the Peierls stress for the side motion of a single kink in the [010] screw dislocation in anthracene crystals, because it is more important to investigate the screw dislocation possessing the higher Peierls stress.

2. Method

We begin by constructing the perfect crystal, which is stable under a given potential. The functional form used for the pairwise-additive atom–atom potentials is the Buckingham function

$$\phi_{ij} = -A_{ij}/r_{ij}^{\,6} + B_{ij}\exp(-C_{ij}r_{ij}) \tag{1}$$

where r_{ij} is the distance between non-bonded atoms and A_{ij}, B_{ij} and C_{ij} are empirical parameters. For the potential parameters we use the values presented by Williams in set IV [10], which are given in table 1. The cut-off radius of interaction between atoms is 8 Å. All parameters used in the present simulations, such as lattice and elastic constants, are estimated through use of this potential. The evaluated packing energy and lattice constants [11] agree well with experimental values [12] with errors within 2%.

Table 1. Potential parameters (Williams' set IV [10]).

Interaction	A_{ij} (kcal Å^6 mol^{-1})	B_{ij} (kcal mol^{-1})	C_{ij} (Å^{-1})
C···C	535	74 460	3.60
C···H	139	9411	3.67
H···H	36	4000	3.74

The model crystal used consists of two regions. One is a relaxable region where molecules are moved during the relaxation process so as to minimize the total potential energy. As the shape of the relaxable region, we take a cylindrical region with radius $r_{\rm rel}$ and length $l_{\rm rel}$. The screw dislocation runs along the cylinder and the centre of the kink is put at the centre of the cylindrical region. The other is a fixed region surrounding the relaxable region where molecules are fixed at the initial positions.

An initial configuration of molecules around a kink is constructed using the equilibrium configuration around the [010] screw dislocation [8]; the crystal containing the straight [010] screw dislocation is cut along the plane normal to the dislocation line, and the shift is by a_0, where a_0 is a unit lattice vector lying on the slip plane and perpendicular to the dislocation line. Hence, the initial shape of the kink is crank-like. Although the displacement field peculiar to the kink is not taken into account in the initial configuration, the influence of this on results is negligibly small for a model where the relaxable region is large enough. The dependence of the results on the radius $r_{\rm rel}$ is examined in the range from $6b$ to $12b$, and that on the length $l_{\rm rel}$ in the range from $4b$ to $20b$, where b is the magnitude of the Burgers vector, 5.91 Å.

To obtain an equilibrium configuration around the kink, we employ both the method of steepest descent and the Newton method combined with the line-search method in the relaxation process. The method of steepest descent is applied repeatedly until all matrices $(\partial^2 E^p/\partial x_i^p \partial x_j^p)$ become positive definite and remain so for more than ten steps, where E^p

and x_i^p denote the potential energy and the ith component of the coordinates of the pth molecule, respectively. The Newton method is then used to make convergence rapid.

3. Results

To examine the shape of the kink, the positions of the dislocation in the direction of the x_1 axis, x_p, are evaluated for each molecular plane normal to the x_2 axis using the following equation:

$$x_p(x_2) = \int_{-\infty}^{+\infty} x_1 \rho_2(x_1, x_2)\, dx_1 \left(\int_{-\infty}^{+\infty} \rho_2(x_1, x_2)\, dx_1 \right)^{-1} \tag{2}$$

where the x_1, x_2 and x_3 axes are parallel to the crystallographic axes a, b and c', respectively, and $\rho_2(x_1, x_2)$ indicates the Burgers vector density [13]. The Burgers vector density is defined as

$$\rho_k(x_1, x_2) = \frac{\partial}{\partial x_1} \left[u_k\left(x_1, x_2, +\tfrac{1}{2}c_0'\right) - u_k\left(x_1, x_2, -\tfrac{1}{2}c_0'\right) \right] \tag{3}$$

where $u_k(x_1, x_2, x_3)$ is the displacement field due to the dislocation lying on the $x_3 = 0$ plane with respect to the regular lattice and the c_0' is the x_3 component of the unit lattice vector c_0.

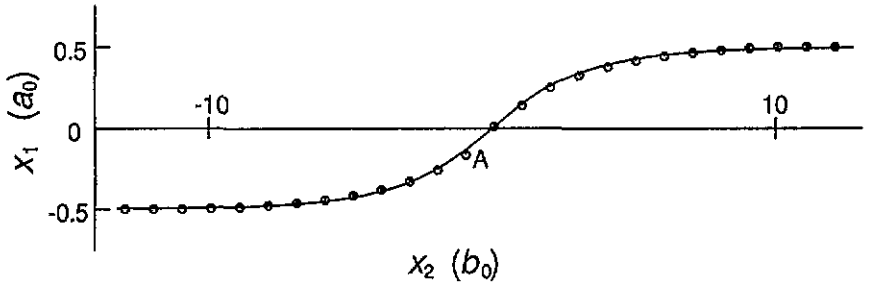

Figure 1. The shape of the kink after the relaxation ($r_{rel} = 6b$, $l_{rel} = 20b$). Circles show the positions of dislocation evaluated from equation (2) in each molecular plane normal to the x_2 axis. Units a_0 and b_0 are the lattice constants; $a_0 = 8.18$ Å and $b_0 = 5.91$ Å. Fitting curve (5) is also shown as a solid line.

The shape of the kink after the relaxation is shown with circles in figure 1. The values of x_1 for the circles correspond to x_p. It is obvious from the figure that the kink in the [010] screw dislocation is of smooth type. We defined the width of the extension of the kink, d_{kink}, as the difference between x_2 at $x_1 = -0.25$ and x_2 at $x_1 = 0.25$. Figure 2 shows the dependence of the width d_{kink} on the length of the relaxable region, l_{rel}. The width d_{kink} is still varying for the largest model with $l_{rel} = 20b$, but the difference between that extrapolated to an infinitely long model and that of the model with $l_{rel} = 20b$ is within 10%.

A dependence of the formation energy of the kink on the model size was also examined. Figure 3 shows the dependence of the formation energy E_{kink} on the length of the relaxable region, l_{rel}, for three relaxation radii r_{rel}. It is apparent that the formation energy E_{kink} depends linearly on the inverse of the length, l_{rel}^{-1}. The extrapolation of the energy to an infinitely long model gives 0.10, 2.9 and 3.7 eV for the models with $r_{rel} = 6b$, $8b$ and $12b$, respectively. Using these three values the dependence of the formation energy E_{kink} on the relaxation radius r_{rel} was also examined. This result is shown in figure 4. Although

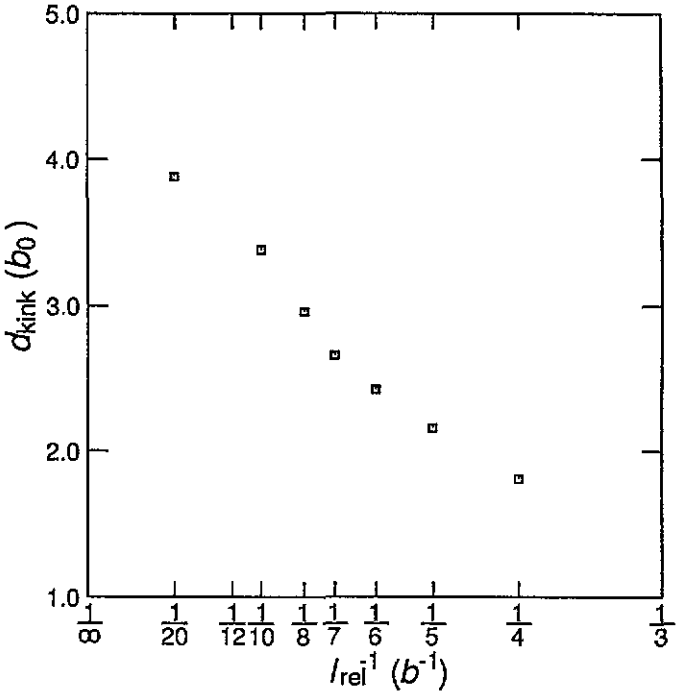

Figure 2. The dependence of the width of the extension of the kink, d_{kink}, on the length of the relaxable region, l_{rel} ($r_{rel} = 6b$).

even for the largest model the energy is still varying, the energy found by means of the extrapolation to $r_{rel} = \infty$ is about 0.5 eV.

Then we applied the shear stress σ_{23} to the kink in the same way as in our previous paper [8]. Under the stress $\sigma_{23} = 1.0 \times 10^{-2}\,\mu$, which is one twentieth of the Peierls stress of the [010] screw dislocation, the kink moves over more than $5b_0$, where b_0 is the lattice constant ($b_0 = b$). This suggests that the Peierls stress for the side motion of the kink, i.e. the Peierls stress of the second kind, is substantially lower than that stress.

4. Discussion

It was found that the kink in the screw dislocation had a smooth shape. This suggests that the height of the Peierls potential for the [010] screw dislocation is comparatively low. If the Peierls potential E_P is assumed to be quadratic as follows [4]:

$$E_P(x_1) = \begin{cases} \frac{1}{2}P\left(x_1 - \frac{1}{2}a_0\right)^2 & \left(\frac{1}{4}a_0 < x_1 < \frac{1}{2}a_0\right) \\ -\frac{1}{2}Px_1{}^2 + \frac{1}{16}Pa_0{}^2 & \left(-\frac{1}{4}a_0 < x_1 < \frac{1}{4}a_0\right) \\ \frac{1}{2}P\left(x_1 + \frac{1}{2}a_0\right)^2 & \left(-\frac{1}{2}a_0 < x_1 < -\frac{1}{4}a_0\right) \end{cases} \tag{4}$$

the functional form representing the shape of the kink can be derived as

$$x_1 = \begin{cases} -\frac{1}{4}a_0 \exp\left(\frac{\pi}{4}\right)\exp(-cx_2) + \frac{1}{2}a_0 & \left(\frac{1}{4}a_0 < x_1 < \frac{1}{2}a_0\right) \\ \frac{\sqrt{2}}{4}a_0 \sin(cx_2) & \left(-\frac{1}{4}a_0 < x_1 < \frac{1}{4}a_0\right) \\ \frac{1}{4}a_0 \exp\left(\frac{\pi}{4}\right)\exp(cx_2) - \frac{1}{2}a_0 & \left(-\frac{1}{2}a_0 < x_1 < -\frac{1}{4}a_0\right) \end{cases} \tag{5}$$

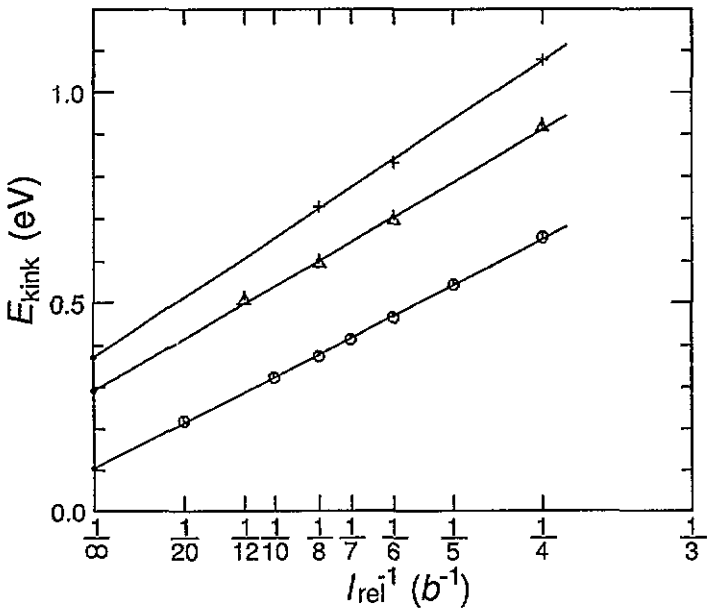

Figure 3. The dependence of the formation energy of the kink, E_{kink}, on the length of the relaxable region, l_{rel}. Crosses denote $r_{rel} = 12b$, triangles $r_{rel} = 8b$, and circles $r_{rel} = 6b$.

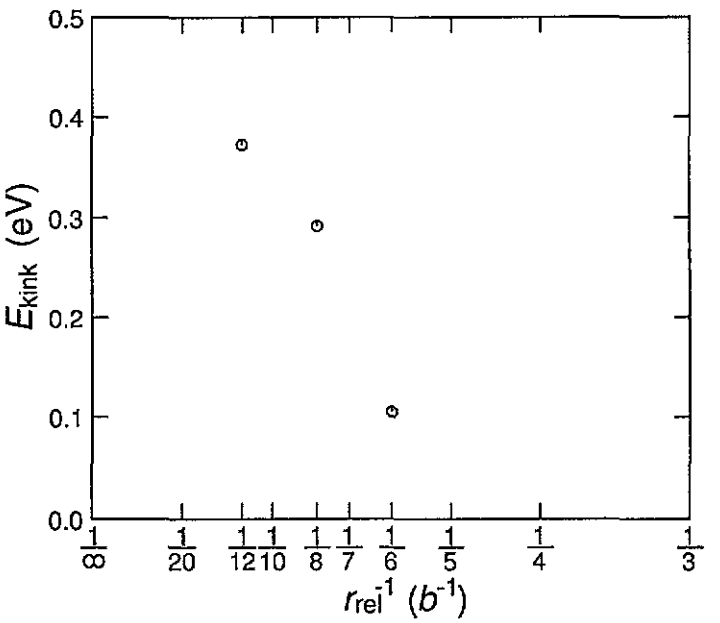

Figure 4. The dependence of the formation energy of the kink, E_{kink}, on the radius of the relaxable region, r_{rel}. Energies extrapolated to an infinitely long model ($l_{rel} = \infty$) are used.

where P and c are constants. The curve given by (5) could be fitted to the shape of the kink obtained through the simulation with the fitting parameter $c = 0.405\, b_0^{-1}$. The fitting curve is shown in figure 1. The fitting seems fairly satisfactory as a whole, although the circle A in figure 1 deviated somewhat from the curve. The constant c is represented as $c = (P/T)^{1/2}$,

where T is the line tension of the screw dislocation which is equal to the self-energy of the dislocation per unit length. Thus the value of P was estimated as 88.9 MPa using the self-energy of the dislocation evaluated by means of the pre-logarithmic energy factor [8]. This value of P is in good agreement with that estimated by changing the position of the straight screw dislocation around the minimum of the Peierls potential, 88.2 MPa [9]. Therefore it seems that the Peierls potential for the screw dislocation is approximately quadratic.

The Peierls stress of the [010] screw dislocation estimated under the assumption of the smooth-quadratic Peierls potential (4) is $1.2 \times 10^{-2}\,\mu$, which is smaller than the value, $2.0 \times 10^{-1}\,\mu$, obtained through the computer simulation [8]. This discrepancy would come from the breakdown of the assumption of the smooth Peierls potential; the Peierls potential should not be perfectly smooth, but somewhat ragged owing to the peculiar shape of the anthracene molecules. There probably exists a section which has a steep gradient in the Peierls potential, but does not deviate very much from the curve (4).

The formation energy of the single kink in the [010] screw dislocation was estimated from the present simulations as 0.5 eV. This value is about a half of the experimental activation energy for a kink pair nucleation, 0.95 eV [3]. Roughly speaking, the activation energy is comparable to the sum of the formation energy of the two single kinks, so the magnitude of the formation energy estimated in the present letter is regarded as reasonable.

The Peierls stress for the side motion of the kink was much lower than one twentieth of the Peierls stress of the screw dislocation. The motion of the screw dislocation at low temperature would be controlled by the formations of kink pairs, rather than by the propagation of kinks. It should be, thus, expected that the [010](001) slip systems will be controlled by the formations of kink pairs, i.e. by the Peierls mechanisms, at low temperature in anthracene crystals.

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