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LETTER TO THE EDITOR

An improved method of calculating the lattice friction stress using an atomistic model

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Abstract. We present an efficient and accurate method of calculating the lattice friction barrier to dislocation motion. This method makes use of an atomistic model of the dislocation core structure. Results of calculations for the lattice friction barrier and the Peierls stress of $\frac{1}{2}a\langle 110\rangle$ edge dislocations in the ionic crystals MgO and KCl are presented and compared with experiment.

An important parameter for understanding the mechanical behaviour of materials is the lattice friction barrier to dislocation motion in a stressed crystal. To date, the more accurate calculations of this barrier have been made using atomistic models of the dislocation's core structure (Basinski *et al* 1972, Puls and Norgett 1976). In such atomistic models, the initial zero-stress equilibrium core configuration of the dislocation is obtained by allowing the atoms to interact via a specified potential. The core region is surrounded by an elasto-atomic boundary region throughout which the equilibrium positions of the atoms are specified by linear elasticity theory.

In most of the previous calculations, the boundary atoms were held rigidly in place while the core configuration was calculated using a suitable energy and force minimization technique. Using such a rigid boundary model, two approaches for obtaining the lattice friction stress have been tried. The first (e.g. Granzer *et al* 1968, Puls and Norgett 1976) involves moving the dislocation to successive crystallographically non-equivalent positions in the crystal and, without any further relaxation, calculating the resulting increase in energy, $E_p(x_c)$, as a function of the dislocation position, x_c. The lattice friction stress, $\sigma_p(x_c)$, is then given by

$$\sigma_p(x_c) = \frac{1}{b}\frac{dE_p(x_c)}{dx_c}, \qquad (1)$$

where b is the Burgers vector. The maximum value of the above stress is commonly referred to as the Peierls stress. It is clear that this approach does not take account of possible changes in the dislocation core structure when a shear stress is applied to the crystal. Hence, the second method (e.g. Basinski *et al* 1972) involves applying an external shear stress to the crystal by superimposing a homogeneous shear displacement (corresponding to the stress according to linear elasticity theory) on the equilibrium core and boundary atoms and subsequently minimizing this configuration. The Peierls stress, consequently, is the minimum stress required to move the dislocation (after minimization) a distance of at least $1-2b$ before it is stopped by the rigid boundary. This method is, however, time consuming and inaccurate. The inaccuracy derives from the fact that even for a rather large core region, the force on the dislocation due to the rigid boundary is significant and comparable to the Peierls stress.

More recently, an attempt was made by Hoagland (1973) to calculate the Peierls stress in the above manner using a flexible-boundary model. However, his calculation has two main shortcomings. Firstly, the Green function calculated by Hirth and Lothe (1973) using the anisotropic linear elasticity theory and used by Hoagland for rearranging the boundary atoms is inaccurate when the point, $\boldsymbol{x}$, at which the displacement is determined is close to the source force position, $\boldsymbol{x}'$. In fact, this Green function diverges when $\boldsymbol{x}$ and $\boldsymbol{x}'$ coincide. Secondly, the quenched dynamical method (Gehlen *et al* 1968) used to minimize the energy of the core region seems unsuitable for a Peierls stress calculation. According to Hoagland (1973), the reason for this is as follows. Using the minimization in the usual manner, with the kinetic energy quench turned on, the dislocation moves too slowly and takes too much computer time for the dislocation to reach equilibrium even when the applied stress is lower than the Peierls stress. However, used without the kinetic energy quench, the excessive kinetic energy acquired by the atoms causes the dislocation to overshoot the Peierls barrier even for the case when the applied stress is lower than the Peierls stress. Thus, Hoagland was unable to determine an accurate value of the Peierls stress. Nevertheless, his method provided him with a lower bound to the Peierls stress, while an upper bound value could be estimated from the minimum value of the external stress that caused ready movement of the dislocation.

We have recently used a modified version of the above flexible-boundary model to calculated the configuration and energy of $\frac{1}{2}a\langle 110\rangle$ edge dislocations in MgO (Puls and Woo 1976). The main modifications of our model involve: (i) using a 'lattice' Green function for very close separations between the source force and the atom to be displaced, and (ii) using a conjugate gradient optimization technique (Sinclair and Fletcher 1974) rather than the quenched dynamical method for the minimization of the core energy. To obtain the zero-stress core configuration, the optimization technique is used to obtain the 'equilibrium' core atom positions while the boundary atoms are held rigidly in place. Then, to take account of the new core configuration, the boundary plus the core atoms are adjusted using the Green function (Puls and Woo 1975). If, at the first attempt, this step does not result in complete equilibrium throughout the crystal (as is usually the case), the process is repeated. A rather accurate and efficient determination of the dislocation configuration has been obtained this way.

It is the purpose of this letter to report that the above procedure for the zero-stress core configuration can be used for an accurate and efficient evaluation of the entire lattice friction barrier of a straight dislocation. We have made use of this scheme to obtain the entire lattice friction barrier of a straight $\frac{1}{2}a\langle 110\rangle$ edge dislocation in MgO and KCl using only two runs (each run with a different value of the applied stress). A brief description of the calculation is given in the following. A more detailed account of this method and more results will be given at a later date.

We start with a zero-stress equilibrium dislocation configuration with its centre (see Hoagland 1973 for a definition) at x_{c0}. We apply a shear stress, $\sigma_{ex} > \sigma_p$. During the rigid-boundary relaxation, the dislocation will move. It is opposed by the lattice friction force, $F_p(x_c)$, and a rigid boundary force, F_{rb}, which represents the mismatch between core and boundary configurations. If we denote $x_c - x_{c0}$ by Δx_c, then F_{rb} will be an increasing function of Δx_c. The dislocation will move on until F_{ex} is balanced out by

F_p and F_{rb}. Equilibrium is thus achieved when

$$F_p(x_c) + F_{rb}(x_c, \Delta x_c) - F_{ex} = 0. \quad (2)$$

Note that $F_p(x_c)$ and F_{ex} are related to the lattice friction stress and the external stress, respectively, via $F_p(x_c) = b\sigma_p(x_c)$ and $F_{ex} = b\sigma_{ex}$. At this point, the boundary and the core configuration are relaxed using the Green function method. This yields a new value for x_{c0}. In this configuration, F_{rb} vanishes (practically). The above process is then repeated until the dislocation has moved through a distance of at least $1b$. Note that x_{c0} and x_c always represent the positions of the dislocation at the start and finish, respectively, of the rigid-boundary relaxation. The results of this procedure yield the upper three curves Δx_c versus x_c shown in figure 1. Each point on the curves represents one iteration.

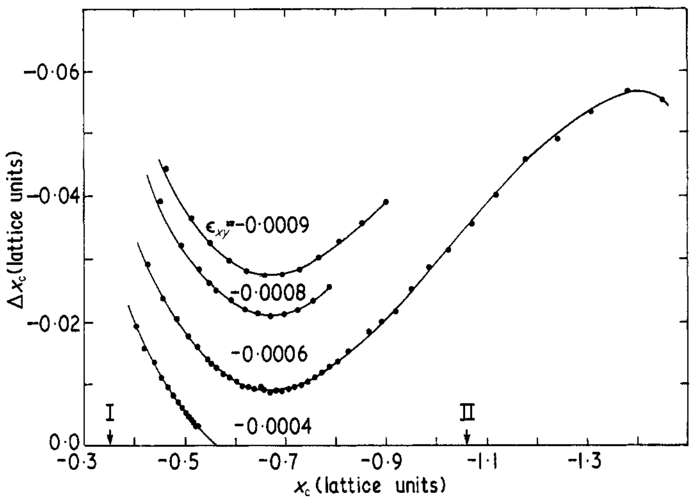

Figure 1. Plots of Δx_c versus x_c for different applied shear strains. Lattice unit distances are measured in units of $\frac{1}{2}a$ where a is the lattice parameter. The locations of the dislocation's centre, x_c, for the two symmetry configurations I and II are indicated by the arrows. These positions are a distance $\frac{1}{2}b$ apart.

To solve for $F_p(x_c)$ in equation (2) we must have a value for $F_{rb}(x_c, \Delta x_c)$. One can see that, with respect to the boundaries parallel to the slip plane, the force F_{rb} is derived from a shear stress, while with respect to the boundaries perpendicular to the slip plane, it is derived from a compressive or tensile stress. Each of these stresses, and therefore the total force on the dislocation due to the boundary, is a function of the relative displacement between the boundary atoms and those core atoms close to the boundary. These displacements are proportional to, but much smaller than, Δx_c. Hence, if Δx_c is also small, linear theory applies and $F_{rb} = K(x_c)\Delta x_c$, where $K(x_c)$ is a force constant depending only slightly on x_c. Thus equation (2) becomes

$$F_p(x_c) = F_{ex} - K(x_c)\Delta x_c. \quad (3)$$

Application of a different external stress yields a similar equation to equation (3), i.e.

$$F_p(x_c) = F'_{ex} - K(x_c)\Delta x'_c. \tag{4}$$

Using equations (3) and (4), we can solve for $K(x_c)$ and $F_p(x_c)$. Having obtained $F_p(x_c)$ and hence $\sigma_p(x_c)$, the Peierls energy barrier, $E_p(x_c)$, can be obtained by integrating equation (1), i.e.

$$E_p(x_c) = b\int_0^{x_c} \sigma_p(x_c)\,dx. \tag{5}$$

As shown in figure 1, a plot of Δx_c versus x_c for MgO has the general shape expected for the lattice friction barrier. Note that a minimum in Δx_c implies a maximum for $\sigma_p(x_c)$. The different plots are essentially parallel; $K(x_c, \Delta x_c)$, as expected, is only slightly dependent on x_c and independent of σ_{ex}. The x_c dependence of $K(x_c, \Delta x_c)$ is apparently due to a combined effect of the proximity of the rigid boundary and deviation from the linear assumption. The corresponding lattice friction stress has been calculated from

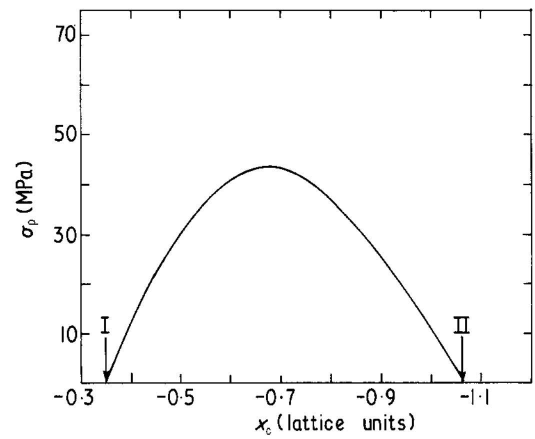

Figure 2. Plot of lattice friction stress, σ_p, versus x_c for MgO calculated from the curves of figure 1. The maximum value of this stress is the Peierls stress .The arrows refer to the two dislocations symmetry positions I and II.

equations (3) and (4) using the points given in figure 1, and plotted in figure 2. The following points can be made about figure 2:

(i) The values of the lattice friction stress at the two symmetry positions I and II are correctly calculated to be zero.

(ii) From figure 1 (lowest curve) application of a shear strain of $-0{\cdot}0004$ (σ_{ex} = 38 MPa) results in a stable relaxed dislocation of configuration corresponding to the dislocation's centre having climbed part way up the Peierls hill to $x_c = -0{\cdot}565$. In figure 2, the lattice friction stress at this point calculated using the above equations is exactly 38 MPa. This demonstrates the validity of our assumptions.

(iii) The lattice friction stress always pushes the dislocation from symmetry position

II to symmetry position I. This is consistent with the fact that for MgO (using Model 1 potential—Puls and Norgett 1976) symmetry II is an unstable configuration.

Similar consistency is observed for KCl (Hoagland 1973) and MgO using the Model 2 potential (Puls and Norgett 1976). The Peierls stresses obtained are compared with the experimental results and other calculated results in table 1. It can be seen that the present results agree very satisfactorily with experiment. Note that the experimental results quoted for MgO using two different methods are not consistent. However, it appears that Singh and Coble's (1974) results are more reliable (Puls and Norgett 1976).

Table 1. Results of the Peierls stress calculations for $\frac{1}{2}a\langle 110\rangle$ edge dislocations in MgO and KCl using different models and methods of calculation. Comparison with experimental values. Values are in units of MPa.

	Theoretical			Experimental		
Material	Result	Method	Reference	Result	Method	Reference
MgO	46	Flex-II, Model 1	Present calculation	60	Flow stress	Singh and Coble (1974)
	68·5	Flex-II, Model 2	Present calculation	5	Bordoni peak	Chang (1961)
				1·9		Ikushima and Suzuki (1963)
	162–383	Rigid Boundary, Model 1	Puls and Norgett (1975)			
KCl	15·2	Flex-II	Present calculation	4·2–14·7	Bordoni peak	Ikushima and Suzuki (1963)
	12·7–32·4	Flex-II	Hoagland (1973)			

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