Structure and Energy of Crystal Interfaces
II. A Simple Explicit Calculation

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Abstract

The variational method developed by Fletcher and Adamson is applied to calculate the energy of the interface between (100) faces of two cubic crystals for arbitrary relative twist displacements and for lattice parameter ratios between 0·6 and 2·0. A simplified interatomic potential is used for this calculation and this shows only a small number of cusped energy minima.

§ 1. Introduction

In the first paper of this series (Fletcher and Adamson 1966, to be referred to as I) a new method was developed for calculating the energy of an interface between two crystals of arbitrary crystal structure and relative orientation. Briefly, the method consists of bringing the two crystals into contact and then varying the positions of all the atoms near the interface until the total energy is a minimum. The method is designed to use realistic interatomic potentials and its main innovation consists in performing all manipulations in reciprocal space. This not only greatly reduces the number of variational parameters required in computation but also leads to an elegant theory from which many general features of the behaviour of interfacial energy can be deduced.

The development given in I was purely formal and it is the purpose of the present paper to present the results of a 'worked example' using a very simplified interatomic potential to demonstrate the scope of the method.

The potential used is not closely related to any real interatomic potential and was chosen in such a way as to reduce the computational effort involved. The computed results are therefore not directly applicable to any real materials, though broadly similar behaviour may be expected. What is demonstrated is the feasibility of such calculations using the present approach.

§ 2. The Interatomic Potential

Consider a crystal of material A whose atoms have nearest-neighbour distances a and a crystal of B with nearest-neighbour distances b. The theory set out in I is based upon the interaction potential $v_{AB}(r)$ between

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A and B atoms separated by a distance r. In practice such a potential might be a Lennard-Jones (12, 6) interaction in the case of rare-gas solids or a more complex oscillatory function (Ziman 1964, Harrison 1966) in the case of metals. These potentials present difficulties from the point of view of an exploratory calculation in that

(i) their extension in real space is great enough that second-neighbour interactions must be considered,

(ii) their extension in reciprocal space (due to the very sharply repulsive core) is rather large so that a considerable number of variational parameters should be used for an accurate solution.

Whilst both of these difficulties can be overcome within the theory of I at the expense of increased computer time, we have chosen rather to perform the calculation using a potential whose range in real space is short enough that only interactions with atoms lying in neighbouring planes parallel to the interface need be considered and whose repulsive core is not so hard as to give a very great extension in reciprocal space.

Fig. 1
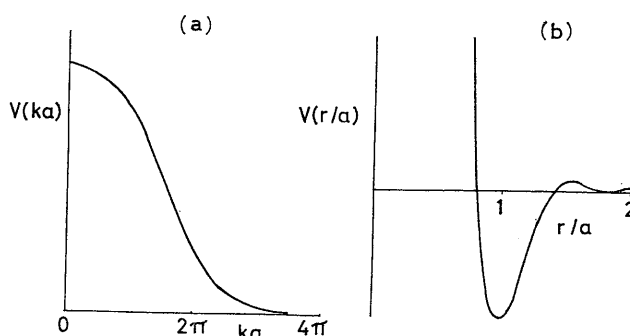
(*a*) The Fourier transform of the potential assumed for this calculation and given by eqn. (3), drawn for the case $b=a$. (*b*) This interatomic potential in real space.

To be explicit, the Fourier transform of the potential used in I is defined by:

$$v(\mathbf{k}) = \Omega^{-1} \int \exp\left(-i\,\mathbf{k}\cdot\mathbf{r}\right) v(r)\,d\mathbf{r}, \quad \ldots \ldots \quad (1)$$

which can be integrated over angle to give:

$$v(\mathbf{k}) = (4\pi/k\Omega) \int_0^\infty \sin\,(kr)\,v(r)\,r\,dr. \quad \ldots \ldots \quad (2)$$

The form chosen for this potential is given by the transformed function:

$$v(ka/2\pi) = \text{const} \times \left(\frac{a+b}{a}\right)^3 \{\exp\,[2\cdot5k\,(a+b)-4\cdot0]+1\}^{-1} \quad (3)$$

for $0 \leqslant k/2\pi < 3\cdot5/(a+b)$ and $v(ka/2\pi) = 0$ for larger k. This transform gives a potential $v(r)$ which has a minimum, of depth independent of b/a, at $r = \frac{1}{2}(a+b)$. The form of the potential and its representation in reciprocal space are shown in fig. 1. The constant in (3) is assigned the numerical value $5\cdot8$ to give a convenient scale for the interfacial energy.

§ 3. THE CRYSTAL PROBLEM

To define the problem we must specify the structures of the two crystals and their orientations relative to the plane of the interface. We have chosen to calculate the case of two simple cubic crystals with lattice parameters a and b respectively in contact on (100) faces and rotated through various angles about an axis normal to the interface. Again this represents an oversimplified situation not met in practice.

Fig. 2
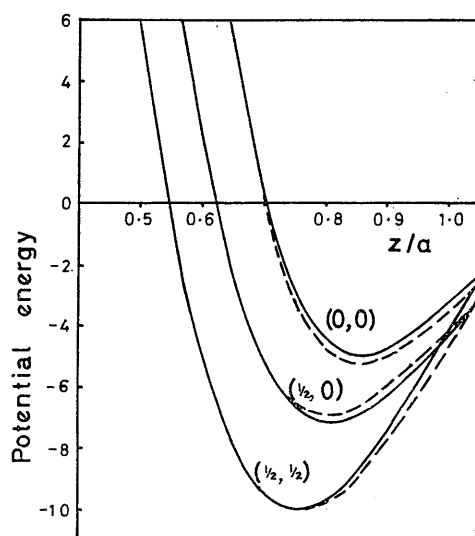
The potential, in units of $1/a^2$, experienced by an A atom at the point (x, y, z) just outside an xy surface of a crystal of B when $b = a$, for $2h = 3a$ (full lines) and $2h = 10a$ (broken lines). The curves show the potential profiles above three different (x, y) positions.

In I it was proposed that the calculation be simplified by supposing the potential just outside a crystal to repeat with a spatial period $2h$ normal to the interface instead of extending to infinity, thus reducing an integral over $\mathbf{k}$ components normal to the interface to a sum. This is clearly valid if h is much greater than the range of the potential but, to speed computation, h should be as small as possible.

Figure 2 shows potential profiles normal to the surface when $a = b$ for three different atomic positions and for $2h = 3a$ and $2h = 10a$, which latter

value approximates the result for $2h = \infty$. It is clear that, within the important region near the potential minima, $2h = 3a$ gives a good approximation to the true potential. This value is used in the calculation in the generalized form:

$$2h = 1 \cdot 5(a + b). \qquad \ldots \ldots \ldots \quad (4)$$

In the theory of I the elastic strain problem was simplified by defining three elastic moduli for each crystal, denoted by η_i and η_i' respectively. To further simplify the present calculation we assume $\eta_1 = \eta_2 = \eta_3 = \eta$ and $\eta_1' = \eta_2' = \eta_3' = \eta'$. If we assume that v_{AA} (r) and $v_{BB}(r)$ have the same general form as $v_{AB}(r)$ then we can write:

$$\eta = M/a^3 \, ; \quad \eta' = M/b^3, \qquad \ldots \ldots \ldots \quad (5)$$

where M is a constant. From the potential curves of fig. 2 we deduce that M is of the order of a few hundred in the energy units we are using so, for the present calculation, we assume $M = 500$.

§ 5. Numerical Results and Discussion

The computer programme minimized the total energy of the system, as given by eqns. (22), (19) and (21) of I, by successive minimization with respect to the distortion parameters, beginning with those of smallest K. The process converged rapidly and the programme, run on an Elliott 503 computer, took about 5 min per point, the number of variational parameters ranging from 3 to about 18. The computed results are summarized in figs. 3 and 4. The energy calculated is the total interaction energy of the two crystals, per unit area of interface, taking as zero the energy of the two separated crystals.

The computed results show a general similarity to those which have been derived using dislocation theory (Read and Shockley 1950) or a simplified interface model (Van der Merwe 1950). There is a sharply cusped energy minimum for exact matching $(b = a, \theta = 0)$ and subsidiary cusped minima for $b = \sqrt{2}a$ or $a/\sqrt{2}, \theta = 45°$. Crystal symmetry, however, is automatically included in the present calculation and there is exact 4-fold rotation symmetry.

It is interesting to note that, at any rate with this potential, the energy of a simple twist boundary $(b/a = 1 \cdot 0$ in fig. 3) is essentially independent of angle for twist angles between 30° and 45°. This is in agreement with the conclusions of Van der Merwe, whilst the dislocation model of Shockley and Read (extrapolated beyond its range of validity) predicts a maximum energy for a twist of rather less than 30°.

Finally, the energy has no appreciable cusped minima except those noted above. This is a true result for the potential considered and is due to the softness of the repulsive core. As shown in the general theory in I, such subsidiary minima have magnitudes determined by $v(k)$ for reasonably large k so that they will be more pronounced with a more realistic potential.

Fig. 3
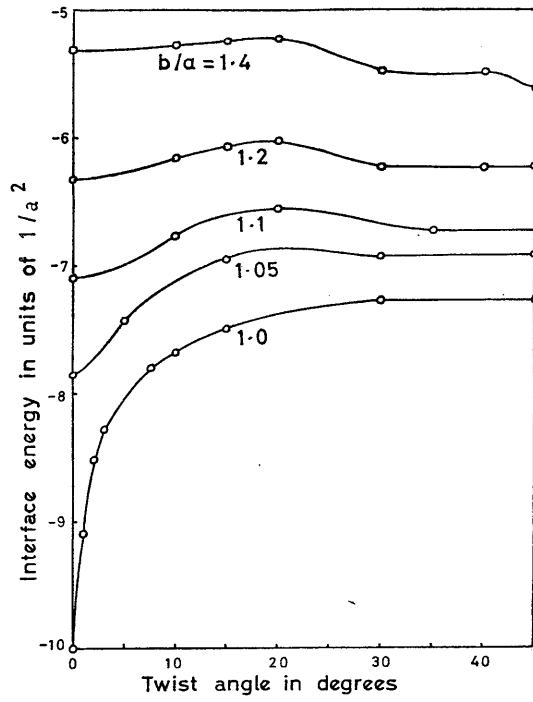
Energy, in units of $1/a^2$, of a twist boundary of angle θ between two crystals with lattice parameters a and b respectively.

Fig. 4
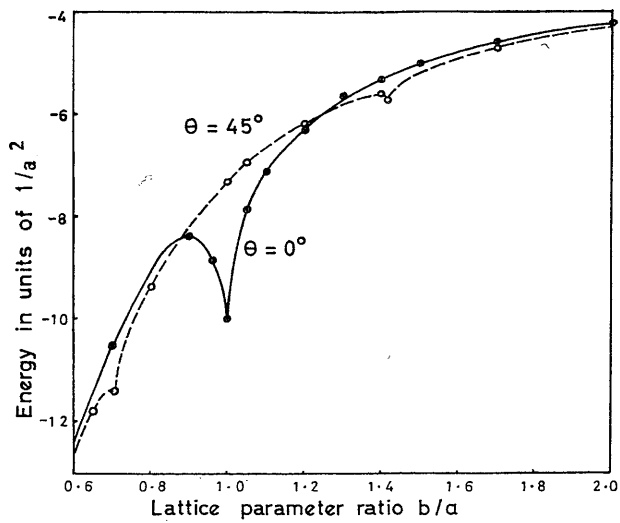
Energy, in units of $1/a^2$ of a boundary between two crystals with lattice parameters a and b for boundary twist angles of 0° and 45°.

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