LETTER TO THE EDITOR

Coincidence site lattice twist boundary energies for metals with long-ranged potentials

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Abstract. We have calculated the coincidence site lattice Σ twist boundary energies for copper and aluminium. The boundaries were on (100) planes and we considered Σ values of 5, 13, 17, 25, 29 and 37. The method employed was a wavenumber space summation which includes all effects due to the long-ranged potentials. The trend was for the twist boundary energy, γ, to be proportional to Σ independent of the metal and the potential used.

There have been numerous efforts to determine the grain boundary energy and structure of Σ twist boundaries in metals (see, e.g., Weins *et al* 1971, Chaudhari and Charbau 1972, Lodge and Fletcher 1975, Guyot and Simon 1976, Bristowe and Crocker 1978, Bristowe and Sass 1980). All of these previous determinations were based either on short-ranged potentials (including only up to the third nearest neighbours) or they assumed an elastic continuum outside the vicinity of the boundary plane. Yet it is well known (Harrison 1966) that potentials derived from first principles (pseudopotentials or model potentials) have long-ranged oscillatory tails. In this letter we point out how these long-ranged potentials may be included into a grain boundary energy calculation. The appropriate mathematical procedure for dealing with this type of potential is to perform the necessary summations in reciprocal space (wavenumber space) where the Fourier transform of the potential, the wavenumber characteristic $F(q)$, is relatively short-ranged.

The essence of this letter is to point out that an expression recently developed for the reciprocal space summation for the energy of a general stacking fault (Devlin 1981) can also be used for unrelaxed coincidence site lattice (CSL) grain boundaries. From that paper the requisite expression is

$$\gamma = \frac{N_c}{4\pi^2 N_f} \sum_{G_\perp} \sum_{l=-\infty}^{+\infty} \left(\int_{-\infty}^{+\infty} \frac{\mathscr{F}^E(l) F(q(l)) - \mathscr{F}^E(z) F(q(z))}{(z-l)^2} \, \mathrm{d}z \right.$$
$$\left. + \pi \frac{\mathrm{d}}{\mathrm{d}z} \left[\mathscr{F}^0(z) F(q(z)) \right]_{z=l} \right). \tag{1}$$

In developing this expression it was assumed that the faulted crystal could be described by an orthogonal CSL extending throughout an infinite bicrystal. Here N_c is the number of ions per CSL unit cell, N_f is the number of ions in a boundary

layer CSL unit cell that lie on the boundary plane, the $G_\perp$ are the reciprocal lattice vectors of the CSL boundary plane, and $q(z) = (G_\perp + (2\pi z/d)^2)^{1/2}$ with d being the CSL cell dimension normal to the boundary plane. The functions $\mathscr{F}^E$ and $\mathscr{F}^0$ contain the specific information concerning the unit cell structures on each side of the boundary layer of the bicrystal. Equation (1) is the lowest order structure-dependent term for the grain boundary energy in pseudopotential theory. It includes *no* approximations other than the choice of potential (or equivalently, wavenumber characteristic) for a given atomic volume (which is taken to be constant everywhere in the bicrystal). The difficulty in applying equation (1) to a general boundary lies in determining the $\mathscr{F}^E$ and $\mathscr{F}^0$ functions as they can be quite complicated even for CSL boundaries.

We have succeeded in applying equation (1) to CSL Σ twist boundaries on (100) planes in FCC metals. The extension to other planes and other phases is evidently also possible. For the FCC structures $N_c = 2\Sigma$. In the case of (100) boundary planes, $N_f = \Sigma$, $d = a_0$ (the lattice constant), and the basal plane reciprocal lattice vectors are of the form

$$G_\perp = \frac{2\pi}{a_0(\frac{1}{2}\Sigma)^{1/2}} (h\hat{x} + k\hat{y}) \tag{2}$$

where h and k are integers. We have taken the boundary normal to lie along the $\hat{z}$ axis. In order to determine the $\mathscr{F}^E$ and $\mathscr{F}^0$ functions we assumed the following unrelaxed ionic positions using the direct basis vectors (a, b, c),

$$r_n^A = \frac{n-1}{\Sigma} (a + mb) \qquad \text{for } n = 1, \Sigma$$

$$r_{n+\Sigma}^A = r_n^A + \frac{1}{2\Sigma} (a + mb) + \tfrac{1}{2}c \qquad \text{for } n = 1, \Sigma \tag{3}$$

for the A side of the bicrystal, and the ionic positions on the B side are of the same form except a is replaced by $-a$. Here the integer m depends on the particular geometry of the CSL unit cell. The value of m can be shown to be determined by the smallest integer solution of

$$m = [2\Sigma(i^2 + j^2) - 1]^{1/2} \tag{4}$$

where i and j are also integers. The Σ values studied are listed in table 1 along with the appropriate values of m. Figure 1 shows an example of the ionic positions when $\Sigma = 5$, in which case $m = 3$.

Using the ionic positions of equation (3) the methods of Devlin (1981) lead to $\mathscr{F}^0 = 0$ for all $G_\perp$ vectors and the only values of h and k for which $\mathscr{F}^E$ is non-zero

Table 1. Geometrical parameters for the Σ twist boundaries. θ is the rotation angle between the half crystals and m is the integer parameter of equation (3).

Σ	θ (deg)	m
5	36.78	3
13	22.62	5
17	61.93	13
25	16.26	7
29	43.60	17
37	71.08	31

(a)   (b)
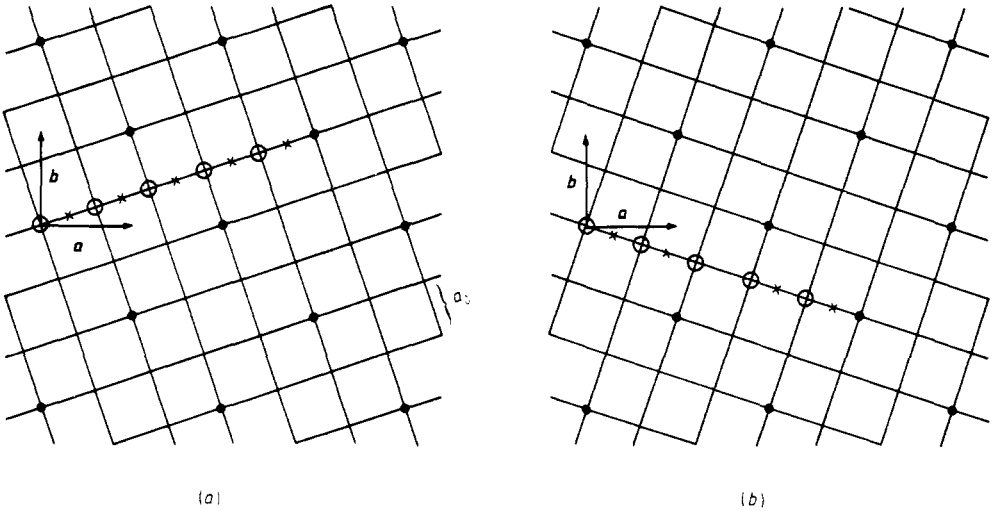
Figure 1. Ionic positions for the respective halves of the $\Sigma = 5$ bicrystal. The open circles represent in plane ions, crosses represent ions displaced half a plane above. The full circles represent some of the coincidence sites.

are those for which $mk + h = 0$ (modulo Σ) when $mk - h \neq 0$ (modulo Σ) or those values for which $mk - h = 0$ (modulo Σ) when $mk + h \neq 0$ (modulo Σ). Specifically, if $mk \pm h = j\Sigma$ while $mk \mp h \neq 0$ (modulo Σ) then

$$\mathscr{F}^{E}(z) = \begin{cases} -\sin^2 \dfrac{\pi z}{2} & \text{if } j \text{ is an odd integer} \\[3mm] -\cos^2 \dfrac{\pi z}{2} & \text{if } j \text{ is an even integer.} \end{cases} \tag{5}$$

These functions lead to relatively simple integrations in equation (1). Furthermore, the restrictions on h and k for non-zero values of $\mathscr{F}^{E}$ yield a rather restricted sum for the reciprocal lattice vector sum. Hence, for these boundaries equation (1) is an inexpensive calculation for each value of Σ and the effect of Σ on the grain boundary energy, γ, is thereby easily determined.

We have performed our numerical calculations using the aluminium potential of Appapillai and Williams (1973) and the copper potential of Moriarty (1972). Both of these long-ranged potentials were found to be useful in stacking fault studies (Devlin 1974). The integral sums were carried out to about $q = 8 k_F$ where k_F is the Fermi wavevector. This would normally correspond to 296 basal plane reciprocal lattice vectors in the case of $\Sigma = 17$ but the restrictions on contributing vectors reduced the sum to one over only thirty vectors. This reduction was typical of the other Σ values, too. Our results for γ are presented in table 2. In that table γ^{ES} refers to the contribution due to $F^{ES}(q)$, the electrostatic interaction wavenumber characteristic representing the interaction between the bare ion cores, while γ^{BS} refers to the contribution coming from $F^{BS}(q)$, the band structure contribution to the wavenumber characteristic which summarises the electron–ion effect. The total $F(q) = F^{ES}(q) + F^{BS}(q)$.

In general our values for γ are quite large compared to experimental values (of approximately 600 ergs cm^{-2}). Our results, because of our choice of ionic positions

Table 2. Twist boundary energies for aluminium and copper. The aluminium results were obtained using the wavenumber characteristic of Moriarty (1972) while the copper results were obtained with the wavenumber characteristic of Appapillai and Williams (1973). All results are in ergs cm^{-2}.

	γ^{ES}	γ^{BS}	γ_{total}
Aluminium			
Σ_5	-15414	20750	5337
Σ_{13}	-40076	54066	13990
Σ_{17}	-52407	70702	18295
Σ_{25}	-77070	103974	26904
Σ_{29}	-89401	120610	31209
Σ_{37}	-114063	153881	39818
Copper			
Σ_5	-922	3982	3060
Σ_{13}	-2402	10376	7974
Σ_{17}	-3141	13569	10428
Σ_{25}	-4619	19954	15334
Σ_{29}	-5358	23147	17789
Σ_{37}	-6836	29532	22696

in equation (3), are only for unrelaxed twist boundaries, so a direct comparison is not appropriate. Undoubtedly, the inclusion of relaxations in the ionic positions in the region of the boundary would reduce our γ values.

The trend in our $\gamma(\Sigma)$ values for both metals is that (except for $\Sigma = 5$), $\gamma(\Sigma_i) = (\Sigma_i/\Sigma_j)\gamma(\Sigma_j)$, where Σ_i and Σ_j are different Σ values. In other words $\gamma(\Sigma)$ is proportional to the Σ value. This is along the lines of the expected trend (Bollmann 1970) and is the reason low Σ CSL boundaries are hypothesised to be common in metals because of this lower energy. This trend does not seem to be just a function of the FCC structure, as we have also performed similar calculations on the simple cubic phase and achieved the same result. It is doubtful though that this would be the correct physical trend for large Σ values. Our results are clearly limited to small values of Σ (say $\Sigma \leqslant 100$) where relaxation effects would not completely dominate the total grain boundary energy.

In summary then we have shown that the wavenumber space formulation can be used to include the important long-ranged potentials into a grain boundary energy calculation. In particular this formulation leads to a computationally quick result for the twist boundaries in FCC structures, which are physically reasonable at least for small Σ values. The extension to large Σ values would necessitate including relaxation effects into this formulation. We are presently extending the formulation to include these important effects.

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