Stacking-fault energies in simple metals: applications to BCC metals

John F Devlin

University of Michigan-Dearborn, 4901 Evergreen Road, Dearborn, Michigan 48128, USA

Abstract. We present a general method for calculating the stacking-fault energy in simple metals, and then we apply this to the {112} faults in body-centred cubic (BCC) metals. Our method contains no approximations for a given wavenumber characteristic (or equivalently the pair potential). Our results show that metastable faults do indeed exist in the simple BCC metals (Li, Na, K, Rb, Cs, Ca, Sr, Ba), but the currently available potentials do not yield sufficiently accurate stacking-fault energies because they do not predict BCC as the lowest energy phase.

1. Introduction

The stacking-fault energy problem has been extensively studied in the past. Most of these efforts have been directed towards the face-centred cubic (FCC) metals (see Simon 1979 for a review). The methods used have either been the direct space method or the reciprocal space method. In the direct space method the pair potential is summed over all pairs of ions that cross the stacking-fault plane. Because the known theoretical pair potentials (which are generated from pseudopotential theory) have a long-range oscillatory tail, convergence problems usually arise and hence cloud the reliability of the results. This convergence problem does not arise in the reciprocal space method because the Fourier transform of the pair potential, the wavenumber characteristic, is short-range. The only approximation made in the reciprocal space method is in the particular wavenumber characteristic used. Hence, this method is preferred for these long-range potentials. In the case of short-range potentials, which are empirically generated, the direct space method is preferable (see Vitek 1968 for examples of this method).

In an earlier paper (Devlin 1974), we presented the reciprocal space method for the stacking-fault energy of the simple FCC and hexagonal close-packed (HCP) metals. The particular method used there depended heavily on the special symmetry of the FCC and HCP stacking faults. In this paper, we present a more generalised expression for calculating the stacking-fault energy within the reciprocal space method. Our method is valid for any stacking fault in which the half-crystals on each side of the fault are translationally invariant. As such, this assumption of translational invariance of each half-crystal excludes us from considering relaxation effects in the vicinity of the boundary. In the case of FCC and HCP faults, our more general expression reduces to the usual result.

We have applied our new method to investigating the existence of {112} faults in body-centred cubic (BCC) metals. This is a rather stringent test of the method and of the potentials used because, unlike the FCC and HCP faults, the nearest-neighbour distances change across the BCC fault plane. Some controversy remains as to whether such faults even exist. The theoretical calculations have been split on this issue: Vitek (1968), Basinski *et al* (1970) and Rao (1975) do not find stable stacking faults on the {112} planes whereas Eichler and Pegel (1969) do. All four calculations used the direct space method and so are possibly suspect to convergence problems, depending on whether their potential is short- or long-range. When our reciprocal space method is applied to these {112} faults using long-range potentials, we do find metastable fault configurations in the vicinity of the hypothesised faults. However, for the metals concerned in this work the numerical results yielded stacking-fault energies which were negative for certain configurations, indicating that the BCC phase itself is unstable. Hence, none of the potentials currently available are reliable enough to show the BCC phase as being preferable over all other phases.

Specifically, we have calculated the twin and intrinsic stacking-fault energies of the metals Li, Na, K, Rb, Cs, Ca, Sr and Ba using the model pseudopotential of Appapillai and Williams (1973, to be referred to as AW) and in the case of Ca, Sr and Ba, we also used the d state pseudopotential of Moriarty (1972). Both of these potentials include the many-electron correlation effects known to be important in structural studies. The AW potential for Be, Mg and Al yielded good agreement between theory and experiment for the FCC and HCP faults. Hence, we feel that the AW potentials are the best pseudopotentials currently available for structural studies of the simple metals.

2. General method

In pseudopotential theory the structure-dependent part of the cohesive energy (per crystal ion) can be written as

$$E = \sum_{q}{}' |S(q)|^2 F(q) \tag{1}$$

where the prime indicates summing over all wavevectors, q, except $q = 0$. The function $F(q)$ is the Fourier transform of the pair potential between the ions. $S(q)$ is the static structure factor of the lattice

$$S(q) = \frac{1}{N} \sum_{R_i} \exp(-iq \cdot R_i) \tag{2}$$

where the R_i are the N ionic positions. To obtain the stacking-fault energy of just a single stacking fault, we have to take the difference in energy between two crystals: one faulted and one unfaulted. Then the stacking-fault energy (per crystal ion) is given by

$$E_{sf} = \sum_{q}{}' F(q)(|S_{faulted}(q)|^2 - |S_{unfaulted}(q)|^2). \tag{3}$$

In order to perform this delicate subtraction to obtain the stacking-fault energy *per fault ion*, we describe the crystal structure in the following manner. Each ion is

associated with a particular unit cell. The unit cells are chosen so that the lattice of unit cells is translationally invariant across the fault plane. The only difference in the unit cells across the fault plane is in their internal structure. This lattice of unit cells is frequently called the coincidence-site lattice (see Bollmann 1970 for a fuller discussion of these lattices). Then an ionic position is described with two labels:

$$R_{\mu\nu} = R_{\mu} + r_{\nu}$$

where the vector R_{μ} describes the particular unit-cell origin and the r_{ν} locates the individual ion within the unit cell. The set of $\{R_{\mu}\}$ forms the coincidence lattice. The set of $\{r_{\nu}\}$ would be different on each side of the fault plane. Then

$$S(q) = \frac{1}{N} \left(\sum_{\mu} \exp(-iq \cdot R_{\mu}) \right) \left(\sum_{\nu} \exp(-iq \cdot r_{\nu}) \right). \tag{4a}$$

Now, referring to figure 1, we consider our fault plane to be perpendicular to the z axis. Then every vector R_{μ} can be written as $R_{\mu} = R_{\mu\perp} + R_{\mu z}\hat{z}$, where the $R_{\mu\perp}$ is in the x–y plane. Similarly, we write $q = q_{\perp} + q_{z}\hat{z}$. Then the sum over all unit cells in a single x–y plane is easily performed:

$$\sum_{\substack{\mu \\ \text{(in one plane)}}} \exp(-iq_{\perp} \cdot R_{\mu\perp}) = N_{p}\delta_{q_{\perp}, G_{\perp}}$$

where the $G_{\perp}$ are the reciprocal lattice vectors of the x–y plane, N_{p} is the number of ions in one plane, and δ is the usual Krönecker delta function. Now we define partial-structure factors for the half-crystals

$$S_{1}(q_{z}) = \frac{1}{N_{z}} \sum_{\substack{\mu \\ \text{(left)}}} \exp(-iq_{z}R_{\mu z}) \tag{4b}$$

$$S_{2}(q_{z}) = \frac{1}{N_{z}} \sum_{\substack{\mu \\ \text{(right)}}} \exp(-iq_{z}R_{\mu z}) \tag{4c}$$

where the sum for S_{1} (S_{2}) is performed over all unit-cell origins along the z axis that are to the left (right) of the fault and N_{z} is the total number of unit-cell planes parallel to the fault plane. Finally, we define unit-cell structure factors
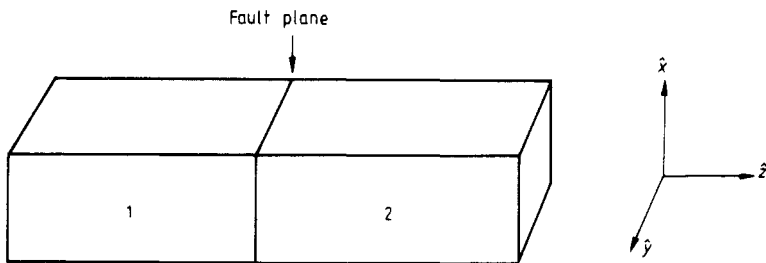
Figure 1. An idealisation of a faulted crystal. The crystal structure is assumed to be perfect on each side of the fault and the crystal is assumed perfectly long in the z direction which is normal to the fault plane.

$$f_1(q) = \frac{1}{N_c} \sum_{\substack{v \\ (\text{left})}} \exp(-iq \cdot r_v) \tag{5a}$$

$$f_2(q) = \frac{1}{N_c} \sum_{\substack{v \\ (\text{right})}} \exp(-iq \cdot r_v) \tag{5b}$$

where, again, the indices 1 and 2 refer to summations on the respective sides of the fault. Since $N = N_p N_z N_c$ the total structure factor for a faulted crystal is of the form

$$S_{\text{faulted}}(q) = \delta_{q_-,G_-}(S_1(q_z)f_1(q) + S_2(q_z)f_2(q)). \tag{6}$$

The structure factor for a perfect (unfaulted) crystal would then be

$$S_{\text{unfaulted}}(q) = \delta_{q_-,G_-}(S_1(q_z) + S_2(q_z))f_1(q) \tag{7a}$$

or

$$S_{\text{unfaulted}}(q) = \delta_{q_-,G_-}(S_1(q_z) + S_2(q_z))f_2(q) \tag{7b}$$

since the unfaulted crystal may be of either f_1 or f_2 structure, both of which, of course, have the same energy. For symmetry reasons we will find it convenient to use a combination of equations (7a) and (7b) for the squared magnitude of $S_{\text{unfaulted}}$:

$$|S_{\text{unfaulted}}(q)|^2 = \tfrac{1}{2}\delta_{q_-,G_-}|S_1(q_z) + S_2(q_z)|^2(|f_1(q)|^2 + |f_2(q)|^2). \tag{8}$$

Then the stacking-fault energy expression of equation (3) becomes

$$E_{sf} = \sum_q{}' \delta_{q_-,G_-} F(q)[S_1 S_2^*(f_1 f_2^* - \tfrac{1}{2}|f_1|^2 - \tfrac{1}{2}|f_2|^2) + S_1^* S_2(f_1^* f_2 - \tfrac{1}{2}|f_1|^2 - \tfrac{1}{2}|f_2|^2)] \tag{9}$$

where terms of the form $|S_i|^2|f_j|^2$ all drop out because each of the f_i correspond to the same structure and hence have the same crystal energy.

We assume the R_{nz} planes are spaced a distance d apart and, if we label them with integers n, we have

$$S_1(q_z) = \frac{1}{N_z} \sum_{n=(-N_z/2)+1}^{0} \exp(-iq_z nd) \tag{10a}$$

$$S_2(q_z) = \frac{1}{N_z} \sum_{n=1}^{N_z/2} \exp(-iq_z nd). \tag{10b}$$

In the spirit of Hodges (1967) we introduce convergence factors into each of the sums:

$$S_1(q_z) = \lim_{\varepsilon \to 0^-} \frac{1}{N_z} \sum_{n=(-N_z/2)+1}^{0} \exp[-i(q_z + i\varepsilon)nd] \tag{11a}$$

$$S_2(q_z) = \lim_{\varepsilon \to 0^+} \frac{1}{N_z} \sum_{n=1}^{N_z/2} \exp[-i(q_z - i\varepsilon)nd]. \tag{11b}$$

The small parameter ε is chosen so that for very large N_z, $\varepsilon d N_z \gg 1$. Then the sums are easily performed to yield

$$S_1 S_2^* = \left(\frac{-1}{4N_z^2} \right) \lim_{\varepsilon \to 0^-} \frac{1}{\sin^2(q_z + i\varepsilon)d/2} \tag{12}$$

so that the stacking-fault energy expression becomes

$$E_{\mathrm{sf}} = \lim_{\varepsilon \to 0^+} \frac{1}{4N_z^2} \sum_q' \delta_{q,G} \, F(q) \left(\frac{A(q)}{\sin^2(q_z + i\varepsilon)d/2} + \frac{A^*(q)}{\sin^2(q_z - i\varepsilon)d/2} \right) \tag{13}$$

where

$$A(q) = -(f_1(q)f_2^*(q) - \tfrac{1}{2}|f_1(q)|^2 - \tfrac{1}{2}|f_2(q)|^2). \tag{14}$$

In appendix 1 we show that this can be written as

$$\gamma_{\mathrm{sf}} = \frac{N_c}{4\pi^2} \sum_{G_-} \sum_{l=-\infty}^{+\infty} \left(\int_{-\infty}^{+\infty} \frac{F(l)\mathscr{F}^{\mathrm{E}}(l) - F(z)\mathscr{F}^{\mathrm{E}}(z)}{(z-l)^2} \, \mathrm{d}z + \pi \frac{\partial}{\partial z} (F(z)\mathscr{F}^0(z))|_{z=l} \right) \tag{15}$$

where γ_{sf} is the stacking-fault energy *per fault ion*, $F(z) = F(q(z))$, $q(z) = |q(z)|$, $q(z) = G_- + (2\pi z/d)\hat{z}$ and

$$\mathscr{F}^{\mathrm{E}}(z) = -[A(q(z)) + A^*(q(z))] \tag{16a}$$

$$\mathscr{F}^0(z) = -\mathrm{i}[A(q(z)) - A^*(q(z))]. \tag{16b}$$

As can be seen from equation (15) only the portions of $\mathscr{F}^{\mathrm{E}}$ that are even in z contribute to the integral sum, and only the portions of $\mathscr{F}^0$ that are odd in z contribute to the sum. Hence, these will be the only portions of the functions we will need to evaluate equation (15).

Equation (15) is the primary result of this paper. It was obtained by taking the limit $N_z \to \infty$, i.e. the crystal is infinitely long in the z direction with only one fault plane. The other limiting process $\varepsilon \to 0^+$ has also been taken care of exactly. Hence, equation (15) represents an exact result for the stacking-fault energy for a given wavenumber characteristic. The details of the particular stacking-fault structure are embodied in the two functions $\mathscr{F}^{\mathrm{E}}$ and $\mathscr{F}^0$. The results obtained previously for the stacking-fault energy of the FCC and HCP faults, using a different mathematical technique for obtaining equations (11a) and (11b), can also be cast into the form of equation (15) with a minor change in notation. In fact, equation (15) represents the general form for any stacking-fault energy problem in which the two half-crystals each have perfect crystal structure. So our method is then restricted to the unrelaxed stacking-fault structures.

In general, the wavenumber characteristic is separated into two components: the bandstructure contribution summarising the electron–ion effects and the electrostatic contribution summarising the bare ion–ion effects. We write

$$F(q) = F^{\mathrm{BS}}(q) + F^{\mathrm{ES}}(q).$$

The $F^{\mathrm{ES}}(q)$ is known exactly because it is the Coulomb repulsion between the positive ion cores of effective valence Z^*:

$$F^{\mathrm{ES}}(q) = 2\pi(Z^*e)^2/\Omega_0 q^2$$

where Ω_0 is the atomic volume. The contribution to the stacking-fault energy from F^{ES} can be evaluated separately. In appendix 2 we show that

$$\gamma_{sf}^{ES} = \frac{\pi d N_c}{4\Omega_0} (Z^*e)^2 \sum_{G} \frac{\mathcal{H}(G_\perp d/N_c)}{G_\perp \sinh^2(G_\perp d/2)} \tag{17}$$

where the $\mathcal{H}$ function is obtained from the $\mathcal{F}^E$ and $\mathcal{F}^0$ functions as follows:

$$\mathcal{H}(\xi) = \mathcal{F}^E(-i\xi) + i\mathcal{F}^0(-i\xi). \tag{18}$$

3. BCC {112} faults

In order to calculate the stacking-fault energy for a given fault configuration all we need to do is to find the functions $\mathcal{F}^E$ and $\mathcal{F}^0$ which contain the information about the ion positions on each side of the fault, and then evaluate equation (15).

For the {112} faults in BCC materials we chose the following basis vectors for the lattice of unit cells:

$$a = a_0(-\hat{i} + \hat{j}) \qquad b = a_0(-\tfrac{1}{2}\hat{i} - \tfrac{1}{2}\hat{j} + \tfrac{1}{2}\hat{k}) \qquad c = a_0(\hat{i} + \hat{j} + 2\hat{k})$$
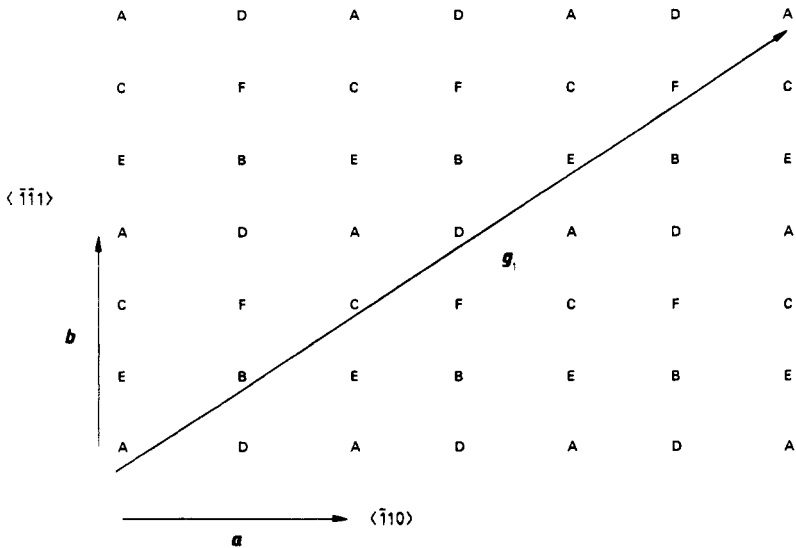
where a_0 is the usual BCC lattice constant. This cell contains six ions. The vectors $\hat{i}, \hat{j}$ and $\hat{k}$ are *not* the vectors $\hat{x}, \hat{y}$ and $\hat{z}$ of figure 1. The vector c does lie along $\hat{z}$, however. The reciprocal lattice vectors are

$$A = \frac{2\pi}{3a_0}(-\tfrac{3}{2}\hat{i} + \tfrac{3}{2}\hat{j}) \qquad B = \frac{2\pi}{3a_0}(-2\hat{i} - 2\hat{j} + 2\hat{k}) \qquad C = \frac{2\pi}{3a_0}(\tfrac{1}{2}\hat{i} + \tfrac{1}{2}\hat{j} + \hat{k})$$

and therefore, the basal plane reciprocal lattice vectors are

$$G_\perp = hA + kB$$

for all integers h and k.

Figure 2. The relative ion positions in the {112} plane. The layers are stacked in the sequence A, B, C, ... each $\tfrac{1}{6}$ the interplanar spacing d above the other.

Figure 2 shows the relative ionic positions in the {112} plane. The planes are stacked one upon the other in the sequences A plane, B plane, C plane, etc. It is convenient to choose the following ion positions for side 1 of the crystal:

$$
\begin{aligned}
&\text{A layer:} \quad r_1 = 0 \\
&\text{B layer:} \quad r_2 = \tfrac{1}{6}(g_1 + c) \\
&\text{C layer:} \quad r_3 = \tfrac{2}{6}(g_1 + c) \\
&\text{D layer:} \quad r_4 = \tfrac{3}{6}(g_1 + c) \\
&\text{E layer:} \quad r_5 = \tfrac{4}{6}(g_1 + c) \\
&\text{F layer:} \quad r_6 = \tfrac{5}{6}(g_1 + c)
\end{aligned}
\tag{19}
$$

where $g_1 = 3a + 2b$.

Stacking faults are created by disturbing the normal stacking sequence, ABCDEF. Table 1 presents some possible examples of faulted crystals on {112} planes. These are the faults that are commonly hypothesised for the simple BCC metals (Hirth and Lothe 1968). Note that the I_1 fault is geometrically equivalent to two twin faults on adjacent planes. The extrinsic fault is an example of a stacking fault which cannot be handled by the methods of this paper since there is not a single fault plane which divides the crystal into two perfect sequences.

3.1. Twin faults

If side 2 is to form a twin fault with respect to side 1, then one possible set of unit-cell ion positions for side 2 is

$$
\begin{aligned}
r_1 &= \tfrac{4}{6} g_1 \\
r_2 &= \tfrac{1}{6}(-g_1 + c) + \tfrac{4}{6} g_1 \\
r_3 &= \tfrac{2}{6}(-g_1 + c) + \tfrac{4}{6} g_1 \\
r_4 &= \tfrac{3}{6}(-g_1 + c) + \tfrac{4}{6} g_1 \\
r_5 &= \tfrac{4}{6}(-g_1 + c) + \tfrac{4}{6} g_1 \\
r_6 &= \tfrac{5}{6}(-g_1 + c) + \tfrac{4}{6} g_1.
\end{aligned}
\tag{20}
$$

Table 1. Possible stacking sequences of {112} planes in BCC materials. The asterisk indicates the fault plane.

Perfect crystal	A B C D E F A B C D E F
Twin fault	A B C D E F*E D C B A F
Intrinsic (I_1) fault	A B C D E F* E F A B C D
Intrinsic (I_2) fault	A B C D E F* C D E F A B
Extrinsic fault	A B C D E F* C D* A B C D

From equations (5), (19) and (20) we obtain the f functions

$$f_1 = \tfrac{1}{3}[\cos\tfrac{5}{2}(\zeta + \xi) + \cos\tfrac{3}{2}(\zeta + \xi) + \cos\tfrac{1}{2}(\zeta + \xi)]\exp[-\tfrac{5}{2}i(\zeta + \xi)]$$

$$f_2 = \tfrac{1}{3}[\cos\tfrac{5}{2}(-\zeta + \xi) + \cos\tfrac{3}{2}(-\zeta + \xi) + \cos\tfrac{1}{2}(-\zeta + \xi)]\exp[-\tfrac{5}{2}i(-\zeta + \xi) - 4i\zeta]$$

where

$$\zeta = \tfrac{1}{6}\boldsymbol{G}_{\perp}\cdot\boldsymbol{g}_1 \tag{21a}$$

$$\xi = \tfrac{1}{6}q_z\hat{z}\cdot\hat{c} = 2\pi x/6. \tag{21b}$$

Then the $\mathscr{F}^E$ and $\mathscr{F}^0$ functions are obtained from equations (14) and (16)

$$\mathscr{F}^E = \tfrac{2}{9}(\cos\zeta - 1)T_1^2 - \tfrac{2}{9}(\cos\zeta + 1)T_2^2 \tag{22a}$$

$$\mathscr{F}^0 = \tfrac{2}{9}(\sin\zeta)(T_1^2 - T_2^2) \tag{22b}$$

where

$$T_1 = \cos\tfrac{5}{2}\zeta\cos\tfrac{5}{2}\xi + \cos\tfrac{3}{2}\zeta\cos\tfrac{3}{2}\xi + \cos\tfrac{1}{2}\zeta\cos\tfrac{1}{2}\xi \tag{23a}$$

$$T_2 = \sin\tfrac{5}{2}\zeta\sin\tfrac{5}{2}\xi + \sin\tfrac{3}{2}\zeta\sin\tfrac{3}{2}\xi + \sin\tfrac{1}{2}\zeta\sin\tfrac{1}{2}\xi. \tag{23b}$$

We can simplify equation (22b) even further. Equation (15) says that only the parts of $\mathscr{F}^0$ that are odd in x, or equivalently odd in ξ, contribute since $F(x)$ is even in x. Therefore, the $\mathscr{F}^0$ of equation (22b) will contribute nothing since it is even in ξ. Hence, we need only use

$$\mathscr{F}^0(\xi) = 0 \tag{24}$$

for the twin fault.

The $\mathscr{H}$ function needed for the electrostatic contribution is obtained by the method of equation (18):

$$\mathscr{H}(\xi) = \mathscr{F}^E(-i\xi) + i\mathscr{F}^0(-i\xi)$$

$$= \tfrac{2}{9}(\cos\zeta - 1)Q_1^2 + \tfrac{2}{9}(\cos\zeta + 1)Q_2^2 \tag{25}$$

where

$$Q_1 = \cos\tfrac{5}{2}\zeta\cosh\tfrac{5}{2}\xi + \cos\tfrac{3}{2}\zeta\cosh\tfrac{3}{2}\xi + \cos\tfrac{1}{2}\zeta\cosh\tfrac{1}{2}\xi \tag{26a}$$

$$Q_2 = \sin\tfrac{5}{2}\zeta\sinh\tfrac{5}{2}\xi + \sin\tfrac{3}{2}\zeta\sinh\tfrac{3}{2}\xi + \sin\tfrac{1}{2}\zeta\sinh\tfrac{1}{2}\xi. \tag{26b}$$

3.2. Intrinsic faults

The intrinsic faults correspond to shifting side 2 with respect to side 1 in the direction of a basal plane vector. A general basal plane direction can be described by $\tfrac{1}{6}\alpha\boldsymbol{g}_1 + \tfrac{1}{2}\beta\boldsymbol{g}_2$ where α and β are arbitrary and $\boldsymbol{g}_2 = -\boldsymbol{a} + 4\boldsymbol{b}$ is orthogonal to $\boldsymbol{g}_1$. Then f_2 can easily be described in terms of f_1

$$f_2 = f_1\exp[-i(\alpha\zeta + \beta\rho)]$$

where

$$\rho = \tfrac{1}{2}\boldsymbol{g}_2\cdot\boldsymbol{G}_{\perp}. \tag{27}$$

From this we can obtain the required functions

$$\mathscr{F}^E = \tfrac{2}{9}[\cos(\alpha\zeta + \beta\rho) - 1](T_1^2 + T_2^2) \tag{28a}$$

$$\mathscr{F}^0 = \tfrac{4}{9}[\sin(\alpha\zeta + \beta\rho)]T_1 T_2. \tag{28b}$$

where the T_1 and T_2 terms are the same as those of equations (23a) and (23b). In obtaining equation (28) we again made use of the symmetry properties implied by equation (15); namely, that only the even parts of $\mathscr{F}^E$ contribute to the integral sum, and only the odd parts of $\mathscr{F}^0$ contribute.

The $\mathscr{H}$ function for the electrostatic contribution is

$$\mathscr{H} = \tfrac{2}{9}[\cos(\alpha\zeta + \beta\rho) - 1](Q_1^2 - Q_2^2) + \tfrac{4}{9}[\sin(\alpha\zeta + \beta\rho)]Q_1 Q_2 \tag{29}$$

where Q_1 and Q_2 are defined by equation (26). C W Krause (1977, private communication) has corroborated the functional form of equation (29) and also equation (25) using a variation on the method of Fumi and Tosi (1960) for evaluating these electrostatic summations.

By considering various possible values of α and β in equations (28) and (29) we can cover all possible shifts of one half-crystal with respect to the other. The I_1 fault listed in table 1 is described by $\alpha = 4$ and $\beta = 0$. while the I_2 fault is given by $\alpha = 2$, $\beta = 0$.

4. Numerical results

The integration of equation (15) was performed in the same manner as our previous work (Devlin 1974). For each of the metals we integrated out to a value of q where $F(q)$ was negligible. The tabular data for $F(q)$ was interpolated with a six-point Lagrange formula.

For the metals Li, Na, K, Rb, Cs, Ca, Sr and Ba we used the model potentials developed by AW. The potentials obtained by the AW method for the metals Al, Mg and Be were highly successful in our study of stacking faults in these FCC and HCP metals. Because the model potential theory is just as applicable to the metals Li, Na, K and Ca, we would expect the potentials so generated for these metals to also be valid to the same extent. For the higher atomic number metals, Rb, Sr, Cs and Ba, the model potentials are less reliable because of the localised d states which are neglected in model potential theory.

We have also used the Moriarty (1972) potentials for Ca, Sr and Ba. These potentials were obtained from a generalisation of the pseudopotential theory which incorporates the localised d states to some extent.

Table 2 summarises the results for the stacking-fault energies of the alkaline earth metals Ca, Sr and Ba. The Moriarty and AW potentials agree reasonably well for the metals Ca and Sr. There is a substantial discrepancy in the results of the two potentials in the case of the heaviest alkaline earth Ba. The AW Ba twin-fault energy is nearly twice that for the Moriarty twin fault because of the difference in signs for the γ_{BS} term. In all three metals $\gamma_{I_1} \simeq \gamma_{I_2} \simeq 2\gamma_{T}$. Because the I_1 fault is geometrically equivalent to two twin faults on adjacent planes and energetically $\gamma_{I_1} \simeq 2\gamma_{T}$, we are led to the conclusion that twin faults in these metals do not interact strongly with each other. This is consistent with the work done on the FCC stacking-fault interactions (Devlin 1975).

Table 2. Stacking-fault energies of Ca, Sr and Ba. The Moriarty (1972) and AW potentials were used. Here γ_{ES} is the electrostatic contribution, γ_{BS} is the bandstructure contribution, and γ_{total} is the sum of these. These stacking-fault energies are all reported in units of erg cm^{-2}.

	γ_{ES}	γ_{BS}	γ_{total}
Twin faults			
Ca (Moriarty)	114.3	− 30.1	84.2
Sr (Moriarty)	96.6	− 27.2	69.4
Ba (Moriarty)	101.5	− 45.1	56.4
Ca (AW)	100.1	− 28.6	71.5
Sr (AW)	79.4	− 12.2	67.2
Ba (AW)	79.6	+ 17.5	97.1
I_1 faults			
Ca (Moriarty)	230,5	− 61.3	169.2
Sr (Moriarty)	194.8	− 54.7	140.1
Ba (Moriarty)	204.8	− 79.7	125.1
Ca (AW)	201.8	− 63.3	138.5
Sr (AW)	160.1	− 32.6	127.5
Ba (AW)	160.5	+ 26.9	187.4
I_2 faults			
Ca (Moriarty)	228.7	− 61.3	167.4
Sr (Moriarty)	193.3	− 54.7	138.6
Ba (Moriarty)	203.1	− 79.7	123.4
Ca (AW)	200.2	− 63.4	136.8
Sr (AW)	158.8	− 32.6	126.2
Ba (AW)	159.2	+ 27.0	186.2

Table 3. Stacking-fault energies of the alkali metals. The AW potential was used in each case. Here γ_{ES} is the electrostatic contribution, γ_{BS} is the bandstructure contribution, and γ_{total} is the sum of these. All results are reported in units of erg cm^{-2}.

	γ_{ES}	γ_{BS}	γ_{total}
Twin faults			
Li	46.9	31.6	78.5
Na	27.4	− 1.7	25.7
K	15.7	− 0.3	15.4
Rb	13.0	− 0.9	12.1
Cs	11.0	− 0.6	10.4
I_1 faults			
Li	94.7	47.3	142.0
Na	55.2	− 4.1	51.1
K	31.6	− 1.3	30.3
Rb	26.3	− 2.4	23.9
Cs	22.3	− 1.8	20.5
I_2 faults			
Li	93.9	47.3	141.2
Na	54.8	− 4.2	50.6
K	31.3	− 1.3	30.0
Rb	26.1	− 2.4	23.7
Cs	22.1	− 1.8	20.3

Table 3 summarises the results for the stacking-fault energies of the alkali metals. Again, we see that $\gamma_{I_1} \simeq \gamma_{I_2} \simeq 2\,\gamma_T$ indicating weakly interacting twin faults. Note that for the alkalis the electrostatic term is the main contributor to the stacking-fault energy except in the case of Li.

The results reported for the intrinsic faults I_1 and I_2 in tables 2 and 3 are the results of the ideal intrinsic faults as listed in table 1. We have also considered arbitrary shifts of one half-crystal with respect to another. A general shift (see §3.2) is described by $\delta = \frac{1}{6}\alpha g_1 + \frac{1}{2}\beta g_2$ where the α and β are arbitrary. Each pair of α, β produces a stacking-fault energy $\gamma(\alpha, \beta)$. A plot of $\gamma(\alpha, \beta)$ in three space yields a two-dimensional surface called the gamma surface. An investigation of the gamma surface yields the possible (meta)stable stacking faults. In figures 3 and 4 we have plotted $\gamma(\alpha, \beta)$ for certain directions in the (α, β) space. These plots are for Na with the AW potential. The plots suggest minima in the γ values. The minima in figure 3 are in fact true minimas, not saddle points. These minimas are located close to the ideal stacking faults of table 1. The I_1 fault is ideal when $\alpha = 4$, $\beta = 0$. We find the minima nearest this to be at $\alpha \simeq 4.15$, $\beta \simeq 0.0$. The value of γ at the minima is 14.9 erg cm^{-2} while the ideal structure for I_1 yields a value of 51.1 erg cm^{-2}. Hence, γ is sensitive to small displacements about the minima. The ideal I_2 fault corresponds to $\alpha = 2$, $\beta = 0$. The minima nearest this occurs at $\alpha \simeq 2.00$, $\beta \simeq 0.15$. The value of γ at the minima is -42.6 while the ideal structure has $\gamma_{I_1} = 50.6$. A negative fault energy at the I_2 minima indicates that the BCC phase is unstable with respect to this type of deformation. Thus, the AW potential does not predict the ideal BCC structure as the most stable phase for Na. A separate structural energy calculation for Na for the perfect crystal structures shows that the HCP structure (with an ideal axial ratio) is preferred over the FCC and BCC structures. In such a case then it is not too surprising that the BCC structure with one defect has less energy than the perfect BCC structure.

A negative γ value also occurs near the point $\alpha = 5.85$, $\beta = 0$ (see figure 3). In fact, the slope of the $\gamma(\alpha, 0)$ versus α curve is positive in the region $\alpha = 6$ (or equivalently
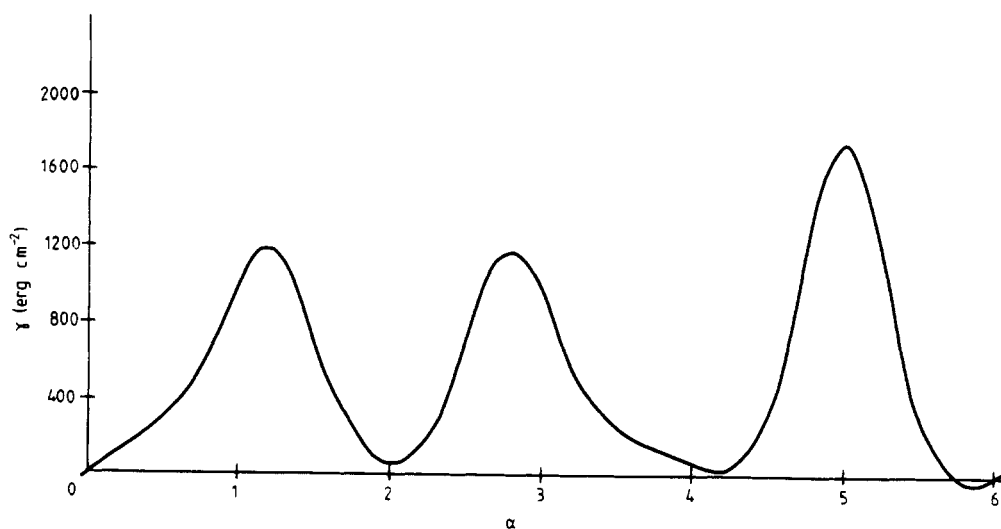

Figure 3. Plot of the $\gamma(\alpha, \beta)$ surface along the $\beta = 0$ direction. For sodium with the AW potential.
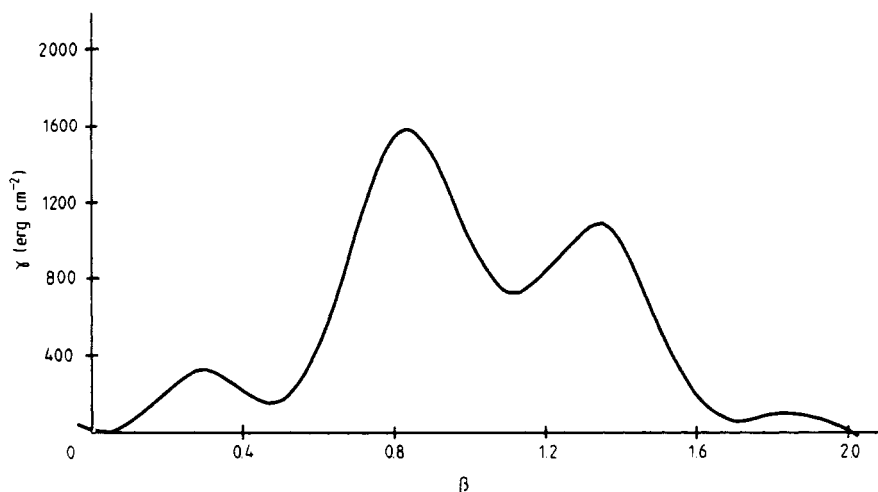
Figure 4. Plot of the $\gamma(\alpha, \beta)$ surface along the $\alpha = 0$ direction. For sodium with the AW potential.

$\alpha = 0$). So again, the BCC phase is unstable with respect to certain distortions when the AW potential is used. This negative value of γ for small positive displacements along g_1 was noted for all of the eight metals reported here even when two different potentials were available. Coinciding with this is the fact that our separate structural calculations show that neither the AW nor Moriarty potentials predict BCC as the preferred phase with the sole exception of Li. In the case of Li, the BCC phase is slightly preferred over the FCC and HCP phase, but this particular preference does not in any way prove that the BCC phase has the absolute lowest energy of *all* possible crystal structures. Such a search for the absolute lowest energy structure would be computationally unfeasible. Our conclusion then is that negative fault energies are indicative of potentials that cannot correctly predict the known crystal structures. Such predictions are extremely difficult to make since the energy difference between the phases is one part in 10^5 of the total structure-dependent energy and would indeed be a severe test of any model or pseudopotential.

Notwithstanding negative fault energies, the ability of these potentials to predict metastable faults seems assured. The minima in $\gamma(\alpha, \beta)$ that we have found for these BCC faults are well-defined and in the expected regions. The actual values of γ, however, are suspect. Ba is a good example of this effect. Both the AW and Moriarty potential predict that the I_1 fault minima would occur approximately at the $\alpha = 4.15$, $\beta = 0$ point; however, the Moriarty potential yields $\gamma = -5.5$ erg cm^{-2} at that point, while the AW potential yields $\gamma = 100.1$ erg cm^{-2}.

5. Summary and conclusions

We have developed a general procedure for calculating the stacking-fault energy of unrelaxed stacking faults, i.e. faults which are perfect crystal structures up to the fault plane. The only approximations that enter into this procedure enter through the wavenumber characteristic.

Our procedure was used to study the {112} stacking faults in BCC structures. The AW potentials were used to study the BCC phases of Li, Na, K, Rb, Cs, Ca, Ba and Sr, while the Moriarty potentials were used for Ca, Ba and Sr. In each of the metals (and for each of the potentials) we noted stable stacking-fault configurations in the vicinity of the predicted structures. The actual values of the stacking-fault energies cannot be compared directly with experiment for two reasons. First, two of these metals (Ca and Sr) do not even exist in the BCC phase. Second, with the exception of Li, neither potential predicts BCC to be the most stable crystal phase, and therefore, some of the stacking-fault energies turn out to be negative. Hence, the model and pseudopotentials are inadequate for these metals when doing structural studies on the BCC phase.

The possible role played by relaxing the ions in the region of the fault to produce realistic configurations is still open to question. Our fault energies for the unrelaxed faults would clearly be upper bounds on the relaxed fault energy since any relaxation would be to minimise the energy.

Since we already have negative energies for some of the BCC faults, any relaxation effects that we might introduce would not be very effective in adding to our knowledge of the true structure and energy of the BCC faults.

Acknowledgment

Appendix 1

Here we derive equation (15) from equation (13).

Writing $q_z = 2\pi z/d$, $\sigma = \varepsilon d/2\pi$, and converting the sum over q_z to an integral over z we have

$$E_{sf} = \lim_{\sigma \to 0^-} \frac{1}{4N_z} \sum_G \int_{-\infty}^{+\infty} dz\, F(G_\perp, q_z(z)) \left(\frac{A(G_\perp, q_z(z))}{\sin^2(\pi z + i\pi\sigma)} + \frac{A^*(G_\perp, q_z(z))}{\sin^2(\pi z - i\pi\sigma)} \right) \quad \text{(A.1)}$$

Hereafter, we will only show explicitly the z dependence of $F(G_\perp, q_z(z))$ and $A(G_\perp, q_z(z))$. Now using the identity

$$\frac{1}{\sin^2 \pi(z + i\sigma)} = \frac{1}{\pi^2} \sum_{l=-\infty}^{+\infty} \frac{1}{(z - l + i\sigma)^2} \quad \text{(A.2)}$$

and setting $\Phi(z) = F(z) A(z)$ we have

$$E_{sf} = \lim_{\sigma \to 0} \frac{1}{4\pi^2 N_z} \sum_G \sum_{l=-\infty}^{+\infty} \int_{-\infty}^{+\infty} dz \left(\frac{\Phi(z)}{(z - l + i\sigma)} + \text{cc} \right)$$

where cc is the complex conjugate. Now we add and subtract the same terms to the equation

$$E_{sf} = \lim_{\sigma \to 0^-} \frac{1}{4\pi^2 N_z} \sum_G \sum_{l=-\infty}^{+\infty} \int_{-\infty}^{+\infty} dz \left(\frac{\Phi(z) - \Phi(l)}{(z - l + i\sigma)^2} + \text{cc} \right)$$
$$+ \lim_{\sigma \to 0^-} \frac{1}{4\pi^2 N_z} \sum_G \sum_{l=-\infty}^{+\infty} \int_{-\infty}^{+\infty} dz \left(\frac{\Phi(l)}{(z - l + i\sigma)^2} + \text{cc} \right). \quad \text{(A.3)}$$

For the $(z - l + i\sigma)^{-2}$ term we use the following identity in the first part of E_{sf}

$$\lim_{\sigma \to 0^+} \frac{1}{(z - l + i\sigma)^2} = P \frac{1}{(z - l)^2} + i\pi\delta'(z - l) \tag{A.4}$$

where P represents the principal part integral and δ' represents the derivative of the Dirac delta function. Then equation (A.3) becomes

$$E_{sf} = \frac{1}{4\pi^2 N_z} \sum_{G_\perp} \sum_{l = -\infty}^{+\infty} \left(P \int_{-\infty}^{+\infty} \frac{(\Phi(z) - \Phi(l)) + cc}{(z - l)^2} \, dz \right.$$

$$\left. + \int_{-\infty}^{+\infty} [(\Phi(z) - \Phi(l)) i\pi\delta'(z - l) + cc] \, dz \right) + E_{sf}^{(2)} \tag{A.5}$$

where

$$E_{sf}^{(2)} = \lim_{\sigma \to 0^+} \frac{1}{4\pi^2 N_z} \sum_{G_\perp} \sum_{l = -\infty}^{+\infty} \int_{-\infty}^{+\infty} dz \left(\frac{\Phi(l)}{(z - l + i\sigma)^2} + cc \right).$$

Now we note that

$$\Phi(z) + \Phi^*(z) = F(z)(A(z) + A^*(z)) = -F(z)\mathscr{F}^E(z)$$

$$\Phi(z) - \Phi^*(z) = F(z)(A(z) - A^*(z)) = iF(z)\mathscr{F}^0(z)$$

where the $\mathscr{F}^1$ and $\mathscr{F}^0$ functions are as defined in equations (16a) and (16b), respectively. Then equation (A.5) becomes

$$E_{sf} = \frac{1}{4\pi^2 N_z} \sum_{G_\perp} \sum_{l = -\infty}^{+\infty} \left(P \int_{-\infty}^{+\infty} \frac{F(l)\mathscr{F}^E(l) - F(z)\mathscr{F}^E(z)}{(z - l)^2} \, dz \right.$$

$$\left. - \int_{-\infty}^{+\infty} \pi(F(z)\mathscr{F}^0(z) - F(l)\mathscr{F}^0(l))\delta'(z - l) \, dz \right) + E_{sf}^{(2)}.$$

By the usual properties of the Dirac delta function, this can be written as

$$E_{sf} = \frac{1}{4\pi^2 N_z} \sum_{G_\perp} \sum_{l = -\infty}^{+\infty} \left(P \int_{-\infty}^{+\infty} \frac{F(l)\mathscr{F}^E(l) - F(z)\mathscr{F}^E(z)}{(z - l)^2} \, dz \right.$$

$$\left. + \pi \frac{\partial}{\partial z} F(z)\mathscr{F}^0(z)|_{z = l} \right) + E_{sf}^{(2)}.$$

The principal value notation on the integral above is unnecessary at this point since the integral is analytic at $z = l$. To get γ_{sf}, the stacking-fault energy per fault ion, we multiply by $N_c N_z$

$$\gamma_{sf} = \frac{N_c}{4\pi^2} \sum_{G_\perp} \sum_{l = -\infty}^{+\infty} \left(\int_{-\infty}^{+\infty} \frac{F(l)\mathscr{F}^E(l) - F(z)\mathscr{F}^E(z)}{(z - l)^2} \, dz \right.$$

$$\left. + \pi \frac{\partial}{\partial z} F(z)\mathscr{F}^0(z)|_{z = l} \right) + N_c N_z E_{sf}^{(2)}. \tag{A.6}$$

Equation (A.6) is the same as equation (15) except for the term $E_{sf}^{(2)}$. We shall show

that $E_{sf}^{(2)}$ is zero. The integration over z in the definition of $E_{sf}^{(2)}$ can be performed as follows

$$E_{sf}^{(2)} = \lim_{\sigma \to 0^+} \frac{1}{4\pi^2 N_z} \sum_{G_\perp} \sum_{l=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \int_{-1/2}^{+1/2} dz \left(\frac{\Phi(l)}{(z + n - l + i\sigma)^2} + cc \right).$$

However

$$\sum_{n=-\infty}^{+\infty} \frac{1}{(z + n - l + i\sigma)^2} = \frac{\pi^2}{\sin^2 \pi(z - l + i\sigma)} = \frac{\pi^2}{\sin^2 \pi(z + i\sigma)}$$

so

$$E_{sf}^{(2)} = \lim_{\sigma \to 0^+} \frac{1}{4N_z} \sum_{G_\perp} \sum_{l=-\infty}^{+\infty} \int_{-1/2}^{+1/2} dz \left(\frac{\Phi(l)}{\sin^2 \pi(z + i\sigma)} + cc \right).$$

By choosing a contour in the upper half of the complex plane, it is possible to show that

$$\lim_{\sigma \to 0^+} \int_{-1/2}^{+1/2} dz \frac{1}{\sin^2 \pi(z + i\sigma)} = 0.$$

Hence, $E_{sf}^{(2)} = 0$ and therefore equation (A.6) leads to equation (15).

Appendix 2

Here we derive equation (17) from equation (15) for the case of the electrostatic wavenumber characteristic

$$F^{ES}(q) = \frac{2\pi(Z^*e)^2}{\Omega_0 q^2} = \frac{2\pi(Z^*e)^2}{\Omega_0[G_\perp^2 + (2\pi z/d)^2]}. \tag{A.7}$$

We begin by defining

$$\mathscr{F}(z) = \mathscr{F}^E(z) + i\mathscr{F}^O(z) \tag{A.8}$$

and, with the use of equation (A.4), equation (15) can be written as

$$\gamma_{sf}^{ES} = \lim_{\sigma \to 0^+} \frac{N_c}{8\pi^2} \sum_{G_\perp} \sum_{l=-\infty}^{+\infty} \left(\int_{-\infty}^{+\infty} dz \frac{F^{ES}(l)\mathscr{F}(l) - F^{ES}(z)\mathscr{F}(z)}{[z - (l + i\sigma)]^2} + cc \right).$$

Now the $\mathscr{F}(z)$ function, since it is obtained from the f_1 and f_2 functions of equation (5), can, in general, be expressed as a sum of exponentials

$$\mathscr{F}(z) = \sum_j a_j \exp(ib_j z)$$

where a_j and b_j are constants.

We separate $\mathscr{F}(z)$ into two parts, one with positive (or zero) b_j and one with negative b_j:

$$\mathscr{F}^+(z) \equiv \sum_{\substack{j \\ b_j \geqslant 0}} a_j \exp(ib_j z)$$

$$\mathscr{F}^-(z) \equiv \sum_{\substack{j \\ b_j < 0}} a_j \exp(ib_j z).$$

Now we define

$$g^+(z) = \frac{1}{[z - (l + i\sigma)]^2} \left(\frac{\mathscr{F}^+(z)}{G_\perp^2 + (2\pi z/d)^2} - \frac{\mathscr{F}^+(l)}{G_\perp^2 + (2\pi l/d)^2} \right)$$

$$g^-(z) = \frac{1}{[z - (l + i\sigma)]^2} \left(\frac{\mathscr{F}^-(z)}{G_\perp^2 + (2\pi z/d)^2} - \frac{\mathscr{F}^-(l)}{G_\perp^2 + (2\pi l/d)^2} \right).$$

Hence

$$\gamma_{sf}^{ES} = \lim_{\sigma \to 0^+} \frac{-N_c}{8\pi^2} \frac{2\pi(Z^*e)^2}{\Omega_0} \sum_{G_-} \sum_{l = -\infty}^{+\infty} \int_{-\infty}^{+\infty} [(g^+(z) + g^-(z)) + \mathrm{cc}] \, \mathrm{d}z. \tag{A.9}$$

The integrals in equation (A.9) can be performed by contour integration. The function $g^+(z)$ is bounded in the upper half plane, while $g^-(z)$ is bounded in the lower half plane. The functions have poles at $z = l + i\sigma$ (second order) and $z = \pm (2\pi i/d)G_\perp$ (first order). The integral for $g^-(z)$ is easily obtained

$$\int_{-\infty}^{+\infty} g^-(z) \, \mathrm{d}z = \frac{d}{2G_\perp} \frac{\mathscr{F}^-(-iG_\perp d/2\pi)}{(l + i\sigma + iG_\perp d/2\pi)^2} \tag{A.10}$$

and for $g^+(z)$

$$\int_{-\infty}^{+\infty} g^+(z) \, \mathrm{d}z = \frac{d}{2G_\perp} \frac{\mathscr{F}^+(iG_\perp d/2\pi)}{(l + i\sigma - iG_\perp d/2\pi)^2} + 2\pi i \frac{\partial}{\partial z} \left(\frac{\mathscr{F}^+(z)}{G_\perp^2 + (2\pi z/d)^2} \right)_{z = l + i\sigma} \tag{A.11}$$

Then equation (A.9) becomes

$$\gamma_{sf}^{ES} = \lim_{\sigma \to 0^+} \frac{-N_c}{8\pi^2} \frac{2\pi(Z^*e)^2}{\Omega_0} \sum_{G_-} \sum_{l = -\infty}^{+\infty} \left\{ \left[\frac{d}{2\pi} \frac{\mathscr{F}^-(-iG_\perp d/2\pi)}{(l + i\sigma + iG_\perp d/2\pi)^2} \right. \right.$$

$$\left. \left. + \frac{d}{2\pi} \frac{\mathscr{F}^+(iG_\perp d/2\pi)}{(l + i\sigma - iG_\perp d/2\pi)^2} + 2\pi i \frac{\partial}{\partial z} \left(\frac{\mathscr{F}^+(z)}{G_\perp^2 + (2\pi z/d)^2} \right)_{z = l + i\sigma} \right] + \mathrm{cc} \right\}$$

which with the use of equation (A.2) yields

$$\gamma_{sf}^{ES} = \frac{N_c}{8\pi} \frac{2\pi(Z^*e)^2}{\Omega_0} \sum_{G_-} \left\{ \left[\frac{\pi^2 d}{2G_\perp} \left(\frac{\mathscr{F}^+(iG_\perp d/2\pi) + \mathscr{F}^-(-iG_\perp d/2\pi)}{\sinh^2(G_\perp d/2)} \right) \right. \right.$$

$$\left. \left. + 2\pi i \sum_{l = -\infty}^{+\infty} \frac{\partial}{\partial z} \left(\frac{\mathscr{F}^+(z)}{G_\perp^2 + (2\pi z/d)^2} \right)_{z = l} \right] + \mathrm{cc} \right\}. \tag{A.12}$$

Now we define

$$h(z) = [\exp(2\pi i z) - 1]^{-1} \frac{\partial}{\partial z}\left(\frac{\mathscr{F}^+(z)}{G_\perp^2 + (2\pi z/d)^2}\right).$$

This function is bounded everywhere at infinity so that

$$\oint h(z)\,dz = 0$$

where the contour encloses the whole complex plane. Then the sum of the residues of this function is zero. This leads to the following identity

$$2\pi i \sum_{l=-\infty}^{+\infty} \frac{\partial}{\partial z}\left(\frac{\mathscr{F}^+(z)}{G_-^2 + (2\pi z/d)^2}\right)_{z=l} = \frac{d\pi^2}{2G_+}\frac{\mathscr{F}^+(iG_\perp d/2\pi) - \mathscr{F}^+(-iG_\perp d/2\pi)}{\sinh^2(G_\perp d/2)}.$$

Then equation (A.12) becomes

$$\gamma_{sf}^{ES} = \frac{N_c}{8\pi^2}\frac{2\pi(Z^*e)^2}{\Omega_0}\sum_G\left\{\left[\frac{d\pi^2}{2G_+}\left(\frac{\mathscr{F}^+(iG_\perp d/2\pi) + \mathscr{F}^-(-iG_\perp d/2\pi)}{\sinh^2(G_\perp d/2)}\right)\right.\right.$$
$$\left.\left. - \frac{d\pi^2}{2G_-}\left(\frac{\mathscr{F}^+(iG_\perp d/2\pi) - \mathscr{F}^+(-iG_\perp d/2\pi)}{\sinh^2(G_\perp d/2)}\right)\right] + cc\right\}.$$

Since $\mathscr{F}^{-*}(\alpha) = \mathscr{F}^-(-\alpha)$, $\mathscr{F}^{+*}(\alpha) = \mathscr{F}^+(-\alpha)$, we have our final result

$$\gamma_{sf}^{ES} = \frac{\pi d N_c(Z^*e)^2}{4\Omega_0}\sum_G \frac{\mathscr{F}^+(-iG_\perp d/2\pi) + \mathscr{F}^-(-iG_\perp d/2\pi)}{G_\perp \sinh^2(G_\perp d/2)}.$$

In terms of the ξ variable, $\xi = 2\pi z/N_c$, we have

$$\gamma_{sf}^{ES} = \frac{\pi d N_c(Z^*e)^2}{4\Omega_0}\sum_G \frac{\mathscr{F}^E(-iG_\perp d/N_c) + i\mathscr{F}^0(-iG_\perp d/N_c)}{\sinh^2(G_\perp d/2)}$$

where we have reverted back to the $\mathscr{F}^E$ and $\mathscr{F}^0$ functions. Hence, the definition in equation (18) leads to equation (17).

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