A THERMODYNAMIC MODEL FOR THE STACKING-FAULT ENERGY

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Abstract—A general thermodynamic model for calculating the energy of stacking faults is presented and applied to f.c.c. Fe–Cr–Ni alloys. A distinction is made between ideal stacking faults and real stacking faults which are associated with an ideal stacking-fault energy (SFE) and an effective SFE, respectively. The ideal SFE is characterized by a chemical energy volume term and an interphase surface energy term, whereas the effective SFE is defined by an additional strain energy volume term. The chemical and strain energy terms are evaluated from theoretical considerations. The interphase surface energy is calculated based on a comparison with experimental values obtained from Transmission Electron Microscopy (TEM) measurements. The results of this analysis show a good agreement between the calculated and experimental values. The model enables the determination of the ideal and effective stacking fault energies as a function of the Cr and Ni contents. The SFE dependence on the Cr vs Ni contents has the shape of a hyperbola.

1. INTRODUCTION

A basic understanding of the deformation characteristics and mechanical behavior of materials, requires the knowledge of the stacking-fault energy (SFE). This aspect is relevant because various mechanical properties such as strength, toughness and fracture are severely affected by the SFE due to its direct influence on the slip mode, deformation twinning and martensitic transformations. Thus, in alloy design, it is important to understand how the SFE is affected by composition.

Thermodynamic calculations of SFEs have been treated by several authors [1–12]. Most of the treatments consider the fault as either exhibiting a volume energy [2–8] or a surface energy [9, 10]. A few authors have expanded this concept and considered the fault as comprising both volume energy and surface energy contributions [1, 11, 12]. However, these approaches either associate non-intrinsic measurements with intrinsic properties, or, they do not uniformly consider the volume free energies of both matrix and faulted phases, and the effect imposed by the presence of partial dislocations. The latter aspect is particularly important, since in the case where a terminated stacking-fault phase (SFP) has a distorted lattice with respect to the matrix, elastic strains will contribute to the energy of the defect. This has been discussed in another paper [13], where a distinction was made between an ideal SFE $\gamma^i$ (intrinsic material property corresponding to an infinite stacking fault) and an effective SFE $\gamma^e$ (non-intrinsic material property which includes a strain energy term in addition to the ideal SFE).

This paper attempts to predict both the ideal and effective SFE, based on a simple general thermodynamic model where two systems in equilibrium are compared. In principle, the procedure proposed herein is a general one and can be applied to any crystal structure. However, due to the simplicity of the f.c.c. lattice, this system is chosen to outline the concepts of the model. In particular, the model is applied to Fe–Cr–Ni alloys where information on some of the data necessary to verify the model is available in the literature. One of the features of the model is that it can predict the effect of Cr and Ni contents on the SFE.

2. THE INTERFACE AND STACKING-FAULT PHASE CONCEPTS

An infinite [Fig. 1(a)] or terminated stacking fault [Fig. 1(b)] can be formed by a shear displacement of the top half crystal on the glide plane of the matrix phase whereby the shear vector is not a lattice vector. This displacement disrupts the crystal stacking and produces an interface separating the matrix [Figs 1(a) and (b)]. This interface exhibits a different chemical bonding than that present in the bulk and thus can be treated as a specific case of a Gibbs interface.
can be expressed as Fig. 1(a). Thus, the change in Gibbs free energy approach and assuming an ideal stacking fault same. In both cases, however, the difference in Gibbs free energy per unit volume of SFP, \( G^\text{SFP} \) is the Gibbs free energy per unit volume of matrix, and \( \sigma \) is the interfacial energy per unit area of interphase boundary. Thus, the following equations can be written:

\[
\Delta G_{\text{surf}} = A\gamma^\infty \tag{1}
\]

where \( A \) is the interfacial area and \( \gamma^\infty \) the interfacial energy per unit area of the interface.

On the other hand, based on the volume approach [Fig. 2(a)], the presence of the SFP results in a free energy change which can be expressed by

\[
\Delta G_{\text{vol}} = V^\text{SFP}(G^\text{SFP} - G^M) + 2A\sigma \tag{2}
\]

where \( V^\text{SFP} \) is the volume of the SFP, \( G^\text{SFP} \) is the Gibbs free energy per unit volume of SFP, \( G^M \) is the Gibbs free energy per unit volume of matrix, and \( \sigma \) is the interfacial energy per unit area of interphase boundary.

Thus, the following equations can be written:

\[
\Delta G_{\text{surf}} \equiv \Delta G_{\text{vol}} \tag{3a}
\]

\[
\frac{\partial \Delta G_{\text{surf}}}{\partial A} = \frac{\partial \Delta G_{\text{vol}}}{\partial A} \tag{3b}
\]

\[
\gamma^\infty = 2s(G^\text{SFP} - G^M) + 2\sigma \tag{3c}
\]

where \( s \) is the interplanar spacing between the close-packed planes parallel to the fault plane. Equation (3c) represents a force per unit length, i.e. an energy per unit area. This will be called the ideal stacking-fault energy (SFE, \( \gamma^\infty \)).

Now consider the situation where the fault is bounded by two partial dislocations [Figs 2(b) and 2(b)]. Hence, the self energies of the dislocations and their interaction energy must be included in the energetics of the system. In this fashion, equation (1) can be rewritten in the form

\[
\Delta G_{\text{surf}}^* = A\gamma^* + W_1 + W_2 + W_{12} \tag{4}
\]

where \( \gamma^* \) is the interfacial energy per unit area of interface (not necessarily equal to \( \gamma^\infty \)). \( W_1 \) is the self energy of partial dislocation 1, \( W_2 \) the self energy of partial dislocation 2, and \( W_{12} \) the interaction energy between two parallel partial dislocations.

In the case of the stacking fault being a volume defect, a difference in the interplanar spacing between the matrix and the SFP will produce an elastic strain field, which should also be taken into account. Thus, equation (2) is modified to give

\[
\Delta G_{\text{vol}}^* = V^\text{SFP}(\Delta G^\text{SFP} - \Delta G_\text{M}) + 2A\sigma + W_1 + W_2 + W_{12} \tag{5}
\]

where \( \Delta G_\text{M} \) is the strain energy per unit volume of stacking fault. Following the same reasoning as in equations (3a)–(c)

\[
\gamma^* = 2s(\Delta G^\text{SFP} - \Delta G_\text{M}) + 2\sigma = \gamma^\infty + 2s\Delta G_\text{S} \tag{6}
\]

which will be called the effective stacking fault energy \( \gamma^* \) [13]. The strain energy term \( \Delta G_\text{S} \) is shape dependent [14], thus, \( \gamma^* \) is not an intrinsic material property, i.e. is very specific to the configuration of

3. THERMODYNAMIC MODEL

As discussed before, the stacking fault can either be treated as an interface or as a second phase. In both cases, however, the difference in Gibbs free energy of the systems in equilibrium, must be the same.

Start by calculating \( \Delta G \) according to the surface approach and assuming an ideal stacking fault [Fig. 1(a)]. Thus, the change in Gibbs free energy can be expressed as

\[
\Delta G = \Delta G^\infty + \Delta G^M + \Delta G_\text{S} \tag{7}
\]

where \( \Delta G^\infty \) is the change in Gibbs free energy per unit area of the interface, \( \Delta G^M \) is the change in Gibbs free energy per unit volume of matrix and \( \Delta G_\text{S} \) is the strain energy per unit volume of stacking fault.

Another possible approach is to consider an infinite stacking fault as a separate phase with a different stacking where two interphase boundaries exist parallel to the faulted planes [Fig. 2(a)]. The nature of these interfaces is due to differences in layer spacing between layers in the matrix and SFP structures. In the more realistic case of terminated stacking faults, additional interphase boundaries exist perpendicular to the faulted planes which can be represented by partial dislocations [Fig. 2(b)]. As a result, if lattice distortions are present, coherency strains and consequently a strain energy term will emerge.

Fig. 1. The classical model approach for the stacking fault, assumes the fault to be an interface separating two rigidly displaced crystals: (a) infinite stacking fault represented by stacking operators; (b) terminated stacking fault formed after dislocation dissociation. The stacking operators describe the relationship between a pair of layers. For the f.c.c. crystal structure, B layer above A, C above B or A above C is denoted by \( \Delta \), whereas C above A, B above C or A above B is denoted by \( \Delta \).

Fig. 2. An alternative model approach for the stacking fault considers the stacking fault as two layers of material which exhibit a different stacking sequence: (a) infinite stacking fault; (b) terminated stacking fault which includes the presence of two partial dislocations which are bounding the fault. 
the dislocations, presence of nearby defects, and sample dimensions.

In the particular case of two parallel partial dislocations, \( \Delta G_s \) has been estimated [13] and can be written as

\[
\Delta G_s = \pi De^2 \frac{2}{2} = \frac{\mu e^2}{4(1-v)}
\]

(7)

where \( D = \mu/2\pi(1-v) \), \( \mu \) is the shear modulus, \( v \) is Poisson’s ratio and \( e \) is the strain normal to the fault plane. Hence, equation (6) can be rewritten to give

\[
\gamma^* = \gamma^\infty + \frac{\mu e^2}{2(1-v)}.
\]

(8)

4. APPLICATION OF THE MODEL

4.1. Calculation of the iso-SFE lines

In order to verify the model, an attempt will be made to predict the ideal and effective stacking fault energies of f.c.c. Fe–Cr–Ni alloys. This system is chosen because of the great practical interest of these alloys and also due to the available literature on some of the important parameters required for the calculations. When available, the predicted results will be compared with TEM stacking-fault energy measurements.

Start by computing equation (3c), noting that for f.c.c. crystals, the structure of the SFP is hexagonal closed packed (h.c.p.). The determination of \( \Delta G_t \) is based on the work of Kaufman [15] and Breedes and Kaufman [16], according to the following expression:

\[
\Delta G_{FeCrNi}^{f.e.c.-h.c.p.} = X_{Fe} \Delta G_{Fe}^{f.e.c.-h.c.p.} + X_{Cr} \Delta G_{Cr}^{f.e.c.-h.c.p.}
\]

(9)

\[
+ X_{Ni} \Delta G_{Ni}^{f.e.c.-h.c.p.}
\]

\[
+ X_{Fe}X_{Cr} \Delta E_{FeCr}^{f.e.c.-h.c.p.}
\]

(10)

\[
+ X_{Fe}X_{Ni} \Delta E_{FeNi}^{f.e.c.-h.c.p.}
\]

\[
+ X_{Cr}X_{Ni} \Delta E_{CrNi}^{f.e.c.-h.c.p.}
\]

\[
+ X_{Fe} \gamma^\infty
\]

where \( X_{Fe} \), \( X_{Cr} \), and \( X_{Ni} \) are the mole fractions of elements Fe, Cr, and Ni, respectively; \( \Delta G_{Fe}^{f.e.c.-h.c.p., FeCrNi} \), \( \Delta G_{Cr}^{f.e.c.-h.c.p., FeCrNi} \), \( \Delta G_{Ni}^{f.e.c.-h.c.p., FeCrNi} \), and \( \Delta G_{FeCrNi}^{f.e.c.-h.c.p., FeCrNi} \) are the change in Gibbs free energy for the f.c.c./h.c.p. transformation due to the elements Fe, Cr, and Ni, respectively; \( E_{FeCr} \), \( E_{FeNi} \), and \( E_{CrNi} \) are the excess free energy coefficients for the systems FeCr, FeNi, and CrNi, respectively, and \( E_{FeCrNi} \) is the ternary excess free energy coefficient. These thermodynamic values were taken from Miodownik [12] and transformed into the units of energy per volume (Appendix A).

The ternary excess free energy coefficient was neglected in the absence of any data. The strain normal to the fault plane was assumed to be independent of composition and approximately 2% [17]. The lattice parameter \( a = 3.5893 \) Å was determined by X-ray analysis on a 310 stainless steel.

Now, the remaining calculation is that of the interfacial energy term. As a first approximation, one might be tempted to estimate it after subtracting the calculated volume \( \Delta G_t \) contribution from experimentally measured SFEs. However, as discussed before, it is not correct to compare the ideal SFE with experimental measurements unless \( \gamma^\infty = \gamma^* \), which is not true for Fe–Cr–Ni alloys [13]. Therefore, the best alternative is to compute the effective SFE, and from there, determine the value of the interfacial energy term, from comparison with experimental values.

Consider two alloys. A stainless steel type 316, where \( \mu = 7.5 \times 10^9 \text{N/m}^2 \) [18], \( v = 0.294 \) [18], and \( \gamma^* = 23 \text{mJ/m}^2 \) [19], and a stainless steel type 310 where \( \mu = 7.31 \times 10^9 \text{N/m}^2 \) [18], \( v = 0.305 \) [18], and \( \gamma^* = 35 \text{mJ/m}^2 \) [19]. The strain normal to the fault plane \( e = 0.02 \) [17] is assumed to be the same for both alloys. After substituting these values in equation (8), together with the calculated values for \( \Delta G_t \), an average value of \( 2e = 14 \text{mJ/m}^2 \) is obtained, which is a reasonable value for this type of coherent interfaces. Thus, as a first approximation, assuming \( \sigma \) to be independent of composition (cf. Section 5), the ideal SFE \( \gamma^\infty \) can be calculated based on equation (3c), for any Fe–Cr–Ni composition.

4.2. Effect of composition on the ideal SFE

An examination of equation (9) shows that \( \Delta G_t \) can be represented by an equation of second order, and consequently by rearranging equation (3c), the SFE \( \gamma^\infty \) can be expressed as

\[
\gamma^\infty = C_1 X_{Cr}^2 + C_2 X_{Cr} X_{Ni} + C_3 X_{Ni}^2
\]

(10)

\[
+ C_4 X_{Cr} + C_5 X_{Ni} + C_6
\]

where \( C_1 = 322.24 \text{mJ/m}^2 \), \( C_2 = -301.61 \text{mJ/m}^2 \), \( C_3 = -108.27 \text{mJ/m}^2 \), \( C_4 = -50.58 \text{mJ/m}^2 \), \( C_5 = 194.37 \text{mJ/m}^2 \), and \( C_6 = 1.62 \text{mJ/m}^2 \). The associated matrix of this equation can be written as

\[
A = \begin{bmatrix}
322.24 & -108.27 \\
-150.82 & -108.27
\end{bmatrix}
\]

(11)

which has eigenvalues \( \lambda_1 = 369.81 \text{mJ/m}^2 \) and \( \lambda_2 = -155.84 \text{mJ/m}^2 \). Since the eigenvalues have different signs, the conic expressed by equation (10) is a hyperbola or degenerate hyperbola. Equation (10) can be simplified by a suitable rotation and translation of the axes (Appendix B) and reduces to

\[
\frac{X_{Ni}^2}{p^2} - \frac{X_{Cr}^2}{q^2} = 1
\]

(12)

where \( p^2 = (40.36 - \gamma^\infty)/(-\lambda_2) \) and
A partial representation of this hyperbola is depicted in Fig. 3, which shows a plot of equation (10) for different values of SFE. It is interesting to note that the same SFE can be obtained based on drastically different chemical compositions. In particular, for a constant Ni content, there are two different Cr contents which give the same SFE. The element nickel seems to cause an increase of the SFE for a fixed chromium composition, whereas for a fixed content of Ni, the SFE goes through a minimum.

4.3. Effect of composition on the effective SFE

Qualitatively, the effective SFE $\gamma^*$ dependence on the components fraction is equivalent to the ideal SFE $\gamma^\infty$, since $\gamma^*$ differs from $\gamma^\infty$ simply by a constant [equation (8)]. However, quantitatively, due to the existence of the strain energy term, for the same composition, the effective SFE has a significantly larger value (Fig. 4) [13]. Note that this difference possibly depends on the composition, but in this work, an average value has been assumed for the strain energy term based on the stainless steels 316 and 310.

Figure 5 shows a plot of the effective SFE as a function of the molar fractions of Cr and Ni, where experimental average values [19] have been also included for comparison. All experimental values have been obtained by measurements on straight parallel dislocations and thus, the shape dependence of the effective SFE can be neglected.

5. DISCUSSION

5.1. Physical validity of equations (3c) and (8)

The first aspect of importance is that both $\gamma^\infty$ and $\gamma^*$ hold the right units of energy per unit area. In the cases where for a temperature increase, the stability of the f.c.c. phase is increased (e.g. Fe and Co alloys [15, 20]), $\Delta G_F$ is increased and consequently the model predicts an increase of the ideal and effective SFEs, which is consistent with experimental evidence [11, 21–23]. For the temperature where $\Delta G_F=0$, a barrier still exists for the dislocation dissociation. In the case of the ideal SFE, this is due to the contribution of the interfacial energy, whereas for the effective SFE, an additional barrier exists caused by the strain energy. This suggests, as discussed by Olsen and Cohen [1], that the formation of the fault will not occur spontaneously unless $\gamma^\infty$ and $\gamma^*$ have a negative value, which is possible for some systems at low temperatures. It is also evident from equation (8), that in
the case where the strain normal to the fault plane is zero, the ideal and effective SFE are identical. In this case, measurements of the SFE will be independent of the geometry of the fault.

5.2. Assumptions on the application of the model

In the above treatment several assumptions have been made, which will now be discussed. The idea of considering the stacking fault to be equivalent to an interface or to a second phase is a reasonable one, since the gradient of energy across the faulted planes as a result of the shear displacement can be approximated either as being the energy of a sharp interface between two identical crystals or the energy of a new phase with corresponding interphase energies.

The assumption of \( \Delta G_S \) being composition independent is made owing to a lack of enough experimental evidence [17]. Although some strain energy difference as a function of the components fraction is expected due to the composition dependence of the elastic constants, the variation is in principle small [17], and a very sensitive technique is required to establish accurately the absolute magnitudes.

The value of \( \sigma \) has been treated as an average value obtained from experimentally measured values of two alloys and then assumed to be independent on the composition. This is a rough approximation, although the role of the composition is mainly to alter the quantity \( \Delta G^{f.c.c. \rightarrow h.c.p.} \), and to a much lesser degree the interfacial energy \( \sigma \), since the interface remains coherent.

5.3. The hyperbola-like shape SFE dependence on composition

Another issue which is worthwhile discussing, concerns the result obtained by equation (12). The terms \( p^2 \) and \( q^2 \) approach zero for \( \gamma = 40.36 \text{ mJ/m}^2 \). This means that the hyperbola is transformed to a degenerate hyperbola. Further increase of the SFE \( \gamma = \) would revert the axes. These considerations are important since they impose on the model a limit for its application. This natural limitation is not fully understood, although it is suggested that it might be a consequence of the absence of the ternary excess free energy coefficient for high Ni and Cr contents [equation (9)], or the fact that the regular solution model, on which equation (9) is based, becomes inappropriate for highly concentrated alloys. On the other hand, for SFE values below 40.36 \text{ mJ/m}^2, the model seems to agree with the experimentally measured values (Fig. 5), except for one of the measurements (marked with a * in Fig. 5). The origin of this discrepant value is unknown, although it is argued that for such a composition, the effective SFE should be expected to be larger, on the basis of the other results obtained by Bampton et al. [19]. In fact, the trend shown in their paper [23], reported an increase of the SFE for a constant Ni content and an increase in the Cr content, for Cr amounts above 16 wt% which corresponds to a molar fraction \( \chi_{Cr} \) of approximately 0.17.

Finally, it should be emphasized that the results of this model can only be compared with measurements obtained from straight parallel dissociated dislocations. For comparison with other dislocation configurations, the strain energy term would need to be considered differently.

6. CONCLUSIONS

A thermodynamic model for calculating the SFE, based on a volume approach for the stacking fault is proposed. The fault energy can be described in terms of volume energy, surface energy and strain energy contributions. The model is applied to f.c.c. Fe–Cr–Ni alloys, for which most of the necessary data is available in the literature. The model offers the possibility of predicting the SFE dependence on the composition and agrees well with experimental results. The following conclusions can be drawn:

1. A real stacking fault is well represented by a volume defect bounded by partial dislocations. However, calculated and experimental values can only be compared on the basis of identical dislocation configurations, except when the strain normal to the fault plane is negligible.

2. In f.c.c. Fe–Cr–Ni alloys, the SFE dependence on the Cr and Ni contents can be represented by hyperbolas. The SFE increases with increasing Ni content whereas for an increase of the amount of Cr, the SFE goes through a minimum.

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REFERENCES


**APPENDIX A**

Transformation from energy/mole to energy/volume

In Fe–Cr–Ni alloys, the f.c.c. → h.c.p. phase transformation can be approximated as exhibiting a 2% contraction along the h.c.p. c-axis [23]. Since the (0001) plane of the h.c.p. phase is parallel to the (111) plane of the f.c.c. phase the volume of the h.c.p. phase can be determined.

The volume of the h.c.p. phase transform-


dation can be approximated as exhibiting a 2% contraction


tion can be written as

Thus the original equation (10) becomes


\[
\begin{align*}
\gamma = \hat{\lambda}_1 X'_{Cr} + \hat{\lambda}_2 X'_{Ni} - 106.70 X_{Cr} + 170.14 X_{Ni} + 1.62.
\end{align*}
\]

The polynomial given by equation (10) may be further simplified by translating the $X'_{Cr}$ and the $X'_{Ni}$ axes, in the form


\[
\begin{align*}
X_{Cr} = X'_{Cr} + \alpha \\
X_{Ni} = X'_{Ni} + \beta
\end{align*}
\]

Thus, taking $a = 3.893 \text{ Å}$, the volume of the h.c.p. unit cell can be written as


\[
\begin{align*}
V_{h.c.p} = \left( \frac{a \sqrt{3}}{2} \right)^2 \frac{2a}{\sqrt{3}} (1 - 0.02) = 2.621 \times 10^{-20} \text{ m}^3.
\end{align*}
\]

Since in the h.c.p. unit cell there are two atoms, the volume occupied by 1 mol of atoms can be found and consequently the number of moles per unit volume. On this basis, the following expression can be obtained for the relation between energy/mole and energy/volume:

\[
\frac{\text{energy (J)}}{\text{volume (m}^3\text{)}} = \frac{\text{energy (J)}}{\text{mole}} \times 126935. \quad (A4)
\]

**APPENDIX B**

Linear transformation of the quadratic equation

Following the calculation of the eigenvalues, determination of the orthonormal eigenvectors, gives the orthogonal matrix $P$ which transforms the conic to the principal axes

\[
P = \begin{pmatrix}
0.95367 & 0.30085 \\
-0.30085 & 0.95367
\end{pmatrix} \quad (B1)
\]

and the change of variables is given by

\[
X_{Cr} = 0.9537 X'_{Cr} + 0.3008 X'_{Ni} \quad (B2a)
\]

\[
X_{Ni} = -0.3008 X'_{Cr} + 0.9537 X'_{Ni} \quad (B2b)
\]

where $X'_{Cr}$ and $X'_{Ni}$ are the new coordinated axes rotated −17.5 deg from the original axes.

Thus the original equation (10) becomes

\[
\gamma' = \hat{\lambda}_1 X'_{Cr} + \hat{\lambda}_2 X'_{Ni} - 106.70 X'_{Cr} + 170.14 X'_{Ni} + 1.62.
\]

The expression for the stacking-fault energy

\[
\begin{align*}
\frac{X_{Cr}}{P^2} - \frac{X_{Ni}}{q^2} = 1
\end{align*}
\]

where $P^2 = (40.36 - \gamma' \hat{\lambda}_1 - \hat{\lambda}_2)$ and $q^2 = (40.36 - \gamma' \hat{\lambda}_1 - \hat{\lambda}_2)$. 

\[
\gamma' = \hat{\lambda}_1 X_{Cr} + \hat{\lambda}_2 X_{Ni} - 106.70 X_{Cr} + 170.14 X_{Ni} + 1.62.
\]