Dislocation energies and mobilities in B2-ordered Fe–Al alloys

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Anisotropic elasticity theory was used to calculate the energies and mobilities of dislocations belonging to the slip systems $\{1\,1\,0\}\langle 1\,1\,1\rangle$ and $\{1\,1\,0\}\langle 1\,0\,0\rangle$ in B2-ordered Fe–Al alloys. Based only on the energy values, it was not possible to predict the experimentally observed room-temperature slip system $\{1\,1\,0\}\langle 1\,1\,1\rangle$. However, when the mobility parameter, as modified by the consideration of atomic radii ratio R_{Fe}/R_{Al} was taken into account, the operative slip system could be predicted correctly.

1. Introduction

In a number of studies [1–4], anisotropic elasticity theory has been used to calculate the energies and mobilities of dislocations of possible slip systems in the B2 compounds (ordered b c c crystal structure). The calculated values have been used to predict the preferred slip systems. The dislocations with minimum energy of formation, i.e., minimum elastic energy are thought to be most abundantly available to initiate slip; however, if the energy difference between dislocations belonging to different slip system is small (say, < 20%), then the slip system having dislocations of highest mobility dominates the slip process. It has been shown [4] that other factors involving the relative values of ordering energies and the separation width of superlattice dislocations may also play a role in predicting the slip systems.

The formulations to calculate elastic energies are straight forward, however, the mobility parameter, M, originally formulated by Eshelby [5], is actually a ratio of the stress needed to move dislocations in a given slip plane to the stress needed to rigidly slip the entire plane of atoms over the adjacent plane. It would be preferable to calculate directly the numerator of this ratio, which is a measure of lattice friction stress. However, such a calculation is complex and may involve considerations of the assumed interatomic potential and core structure of screw dislocations. As a first approximation, the magnitude of stress needed for rigid translation of two adjacent atomic planes can be assumed to be proportional to the maximum vertical displacement, d_v, of the atomic planes during translation. The vertical displacement, in turn, depends upon ratio of the atomic radii of the component elements as well as upon the slip direction and can be calculated based upon simple geometric considerations. To a first approximation, M times d_v is a measure of lattice friction stress and thus provides a better indicator of dislocation mobility than the value of M alone.

The B2 Fe–Al alloys cover a wide composition range, Fe–35 to ~ 52 at % Al. The slip systems in these alloys have been determined experimentally in a number of studies [6–11]. However, no detailed theoretical calculations of dislocation energies and mobilities have been published. This paper presents results of the theoretical calculations to predict slip systems in Fe–35 at % Al, Fe–40 at % Al, and Fe–50 at % Al alloys. The calculations indicate that the predictions are in accord with the experimentally observed slip systems when the values of atomic radii ratio and resulting vertical displacements, d_v, are taken into account.

2. Basic equations

The theoretical background and the equations required for calculating the energy and mobility of dislocations have been discussed in detail in a previous publication [4]; and, in the present case, the same calculation procedure has been followed.

As is the case of NiAl and some other B2-ordered compounds, FeAl is anisotropic in its single-crystal elastic behaviour. The degree of anisotropy is characterized by the Zener factor,

$$A = 2C_{44}/C_{11}-C_{12} \qquad (1)$$

where C_{44} and C_{12} are the primary elastic constants. If $A = 1$ the material is isotropic; and if A deviates from unity, the elastic properties are anisotropic. For FeAl, $A = 2.94$ which means that FeAl is highly anisotropic. In isotropic materials, the dislocation energies are proportional to μb^2, where μ is the shear modulus independent of crystallographic orientation and b is the magnitude of Burger's vector. However, in anisotropic materials, energies are proportional to Kb^2, where the parameter K (called the energy factor) is strongly orientation dependent. Computation of K involves complex fourth-order tensor transformations; for the slip systems involving low-indices planes, expressions for K as a function of elastic constants have been derived by Foreman [12].

For the present B2 alloys calculations are made

for the two slip systems $\langle 1\,1\,1\rangle\{1\,1\,0\}$ and $\langle 0\,1\,0\rangle$ $\{1\,0\,1\}$. The other slip systems $\langle 1\,1\,0\rangle\{1\,1\,0\}$ and $\langle 1\,0\,0\rangle\{0\,1\,0\}$ are excluded from consideration because, as shown in a previous publication [4], during the glide process itself like atoms are brought into nearest-neighbour contact, a situation not favoured energetically. For $\langle 1\,1\,1\rangle$ slip, the Burger's vector which will not disrupt the atomic order is $a\langle 1\,1\,1\rangle$, however, the dislocation can lower its energy by splitting into a pair of dislocations:

$$a\langle 1\,1\,1\rangle \rightarrow 1/2\,a\langle 1\,1\,1\rangle + 1/2\,a\langle 1\,1\,1\rangle$$

$$+ \text{ antiphase boundary (APB)}$$

The present calculations are, therefore, made for both the unit $a\langle 1\,1\,1\rangle$ dislocation and superlattice $a/2\langle 1\,1\,1\rangle$ dislocations; for the latter, the interaction energy of the paired dislocations of like Burger's vectors and APB energy need to be computed.

Equations needed to make the calculations are given below.

2.1. Elastic energy of a dislocation

$$E = \frac{Kb^2}{4\pi}\ln\,(R/r_0) \qquad (2)$$

where K is the appropriate energy factor for an edge or a screw orientation, R the outer cut-off radius of a dislocation (assumed to be 2.5×10^{-4} cm, a typical distance between dislocations), r_0 the inner cut-off radius (assumed to be on the order of 0.1 nm) and b the magnitude of Burger's vector (in the case of superlattice dislocations, $b = 1/2\,a\langle 1\,1\,1\rangle$).

2.2. Elastic energy of a superlattice dislocation

$$E_{sl} = 2E + E_1 + \gamma\omega \qquad (3)$$

where E = self-energy of the component dislocation, Equation 2, E_1 the interaction energy of the component dislocations which form the superlattice dislocation, γ the antiphase boundary (APB) energy and ω the separation width between the component dislocation $= Kb^2/2\pi\gamma$. The interaction energy is given by

$$E_1 = \frac{Kb^2}{2\pi}\ln\,(R/w) \qquad (4)$$

The antiphase boundary is given by

$$\gamma = 0.707\,(kT_c/a_0^2) \qquad (5)$$

where R is the Boltzmann constant, T_c the order–disorder temperature, a_0 the lattice parameter and s the factor taking into account the degree of substoichiometry.

2.3. Mobility parameter [5]

$$M = 4\pi\frac{\delta}{b}\exp\,(-2\pi\delta/b) \qquad (6)$$

$$\delta/b = \frac{1}{2}\frac{Kd}{Cb} \qquad (7)$$

where δ is the width of the dislocation core, d the inter-

planar spacing of the slip plane and C the shear modulus in the slip direction on the glide plane.

3. Parameters required for calculations
In order to make use of the above equations, values for the elastic constants, melting temperatures, and the lattice parameters are required. The elastic constants of the single-crystal Fe–Al alloys in the composition range 4 to 40 at % Al alloys have been measured by Leamy et al. [13], using the ultrasonic-pulse supersonic technique. Their data were extrapolated to obtain elastic-constant values for the Fe–50 at % Al alloy. The melting temperatures of the present alloys were taken from the Fe–Al phase diagram [14]. It was assumed that in the Fe–35 to 50 at % Al range, the B2 order is present up to the melting temperature and, therefore, T_c was taken to be the melting temperature. The lattice parameters have been measured to a high precision utilizing the powder X-ray diffraction technique [15]. The values of these parameters are given in Table I. To calculate d_v, the needed value of atomic radii ratio for FeAl was taken from [16].

4. Results and discussion
First, the calculated values of the maximum vertical displacement for rigid relative motion of two adjacent planes in the slip directions $\langle 0\,0\,1\rangle$ and $\langle 1\,1\,1\rangle$ as a function of atomic radii ratios are shown in Fig. 1. It can be seen that with increasing R_A/R_B, d_v increases appreciably for the $\langle 1\,0\,0\rangle$ slip direction while it decreases appreciably for the $\langle 1\,1\,1\rangle$ slip direction. A large difference in the d_v values for these slip directions for large R_A/R_B values plays a significant role in determining the respective dislocation mobilities. That d_v should be different for different slip directions (but same slip plane) can be qualitatively seen in Fig. 2, which depicts atomic positions on unslipped and half-slipped (1 1 0) planes in FeAl. Fig. 2a shows two layers of adjacent slip planes, the solid circles represent top layer and the dashed circles the bottom layer. When the top layer is slipped rigidly relative to the
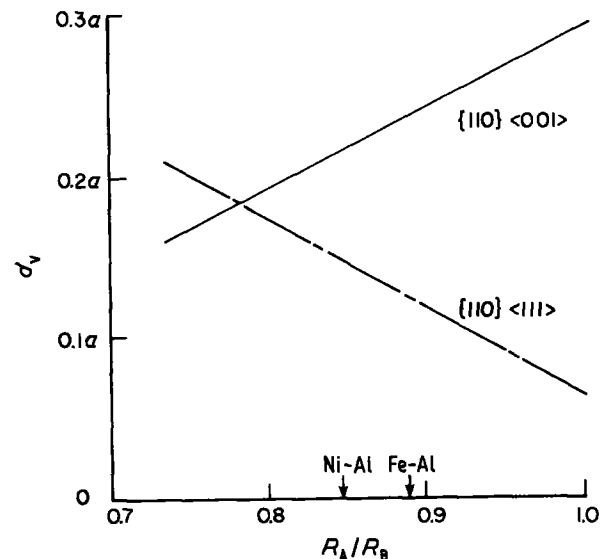

Figure 1 The maximum vertical displacement for rigid translation of two adjacent (1 1 0) atomic planes in the directions [1 1 1] and [0 0 1] as a function of atomic radii ratio for the B2 compounds.

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TABLE I Parameters required for calculations

Alloys	Room temperature elastic constant $\times 10^{12}$ (dyn cm^{-2})			Melting temperature $T_{\rm m} \simeq T_{\rm c}$ (°K)	Lattice parameter a_0, (nm)	Degree of substoichiometry, s	Zener's anisotropic factor, A
	C_{11}	C_{12}	C_{44}				
Fe–35 at % Al	1.86	1.158	1.356	1653	0.2894	0.7	3.86
Fe–40 at % Al	1.937	1.157	1.333	1613	0.2898	0.8	3.42
Fe–50 at % Al	2.085	1.225	1.265	1523	0.2909	1.0	2.94

TABLE II Energy and mobility parameters for Fe–35 at % Al

Slip system	Screw or edge dislocation	Self energy, $\times 10^{-4}$ (erg cm^{-1})	Mobility parameter, M	Md_v
$\langle 010 \rangle \{\bar{1}01\}$	S	11.36	0.48	0.12
	E	8.96	0.61	0.15
$\langle 111 \rangle \{\bar{1}10\}$	S	12.8	0.7	0.08
	E	26.7	0.32	0.04

Energy of superlattice dislocation = 9.9×10^{-4} erg cm^{-1} (screw)
= 20.0×10^{-4} erg cm^{-1} (edge)

Separation distance ω = 5.0 nm (screw)
= 10.0 nm (edge)

Antiphase-boundary energy = 105 erg cm^{-2}

TABLE III Energy and mobility parameters for Fe–40 at % Al

Slip system	Screw or edge dislocation	Self energy, $\times 10^{-4}$ (erg cm^{-1})	Mobility parameter, M	Md_v
$\langle 010 \rangle \{\bar{1}01\}$	S	11.2	0.48	0.12
	E	8.86	0.61	0.15
$\langle 111 \rangle \{\bar{1}10\}$	S	14.36	0.68	0.08
	E	25.0	0.41	0.05

Energy of superlattice dislocation = 11.34×10^{-4} erg cm^{-1} (screw)
= 19×10^{-4} erg cm^{-1} (edge)

Separation distance ω = 3.8 nm (screw)
= 8.0 nm (edge)

Antiphase-boundary energy = 150 erg cm^{-2}

TABLE IV Energy and mobility parameters for Fe–50 at % Al

Slip system	Screw or edge dislocation	Self energy, $\times 10^{-4}$ (erg cm^{-1})	Mobility parameter, M	Md_v
$\langle 010 \rangle \{\bar{1}01\}$	S	10.7	0.48	0.12
	E	9.19	0.61	0.15
$\langle 111 \rangle \{\bar{1}10\}$	S	15.2	0.7	0.08
	E	25.0	0.45	0.05

Energy of superlattice dislocation = 12.04×10^{-4} erg cm^{-1} (screw)
= 20×10^{-4} erg cm^{-1} (edge)

Separation distance ω = 3.45 nm (screw)
= 6.8 nm (edge)

Antiphase-boundary energy = 175 erg cm^{-2}

TABLE V Energy and mobility parameters for Ni–Al [4]

Slip system	Screw or edge dislocation	Self energy, $\times 10^{-4}$ (erg cm^{-1})	Mobility parameter, M	Md_v
$\langle 010 \rangle \{\bar{1}01\}$	S	9.29	0.48	0.10
	E	8.29	0.54	0.11
$\langle 111 \rangle \{\bar{1}10\}$	S	12.45	0.735	0.11
	E	26.9	0.46	0.07

Energy of superlattice dislocation = 10.2×10^{-4} erg cm^{-1} (screw)
= 20.2×10^{-4} erg cm^{-1} (edge)

Separation distance ω = 2.215 nm (screw)

Antiphase-boundary energy = 223 erg cm^{-2}

Fe (Fe) Fe

(Al) Al (Al)

Fe (Fe) Fe $\overline{1}$10 →

↓ $\searrow$ $\overline{1}\overline{1}1$

UNSLIPPED (110) 00$\overline{1}$
PLANE

(a)

Fe, Al   Fe, Al

Al, Fe

Fe, Al   Fe, Al

HALF SLIP, $\frac{1}{2}$ [00$\overline{1}$]

(b)
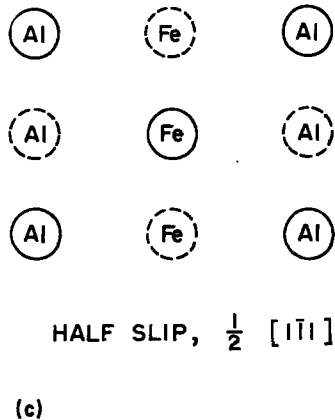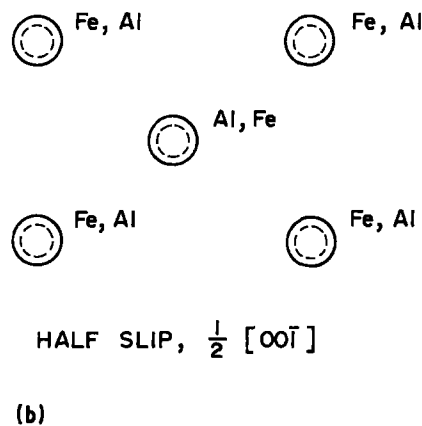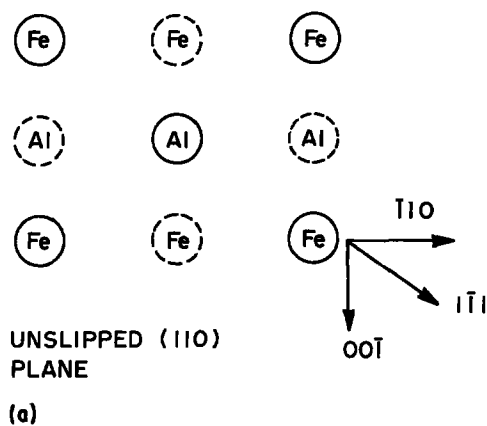
Figure 2 The half-slipped atomic position during the [0 0 1] and [1 1 1] slips of the adjacent (1 1 0) planes.

Al (Fe) Al

(Al) Fe (Al)

Al (Fe) Al

HALF SLIP, $\frac{1}{2}$ [1$\overline{1}$1]

(c)

bottom layer in the [0 0 $\overline{1}$] direction, the atoms are on top of each other in the half-slipped position; however, slip in the [1 1 $\overline{1}$] direction takes place along troughs of Fe–Al rows. Thus, the maximum vertical displacement during $\langle 1 0 0 \rangle$ slip is larger than that during $\langle 1 1 1 \rangle$ slip.

Tables II to IV present the calculated values of the energies, mobility parameters, and the product of M and d_v, respectively, for the two slip systems. In addition, in each table the calculated values of the superlattice-dislocation energy, the antiphase-boundary energy, and the equilibrium separation between the component dislocations comprising the superlattice dislocation are given. For comparison purposes the calculated values of all these parameters for NiAl, taken from [4], are presented in Table V. It should be mentioned that of all the different B2-ordered compounds investigated, the compound NiAl most nearly approaches FeAl in terms of the values of T_c and the antiphase-boundary energy.

In the case of NiAl, examination of the data in Table V reveals that $a \langle 1 0 0 \rangle$ dislocations have lower energy than the $a/2 \langle 1 1 1 \rangle$ superlattice dislocation, the difference being $\sim 10\%$ for the screw component and much larger for the edge component. Also, as indicated by the values of Md_v, there is only a small difference in the mobility of different dislocation types. Therefore, the predicted slip system in NiAl is $\langle 0 1 0 \rangle \{\overline{1} 0 1\}$ which is in agreement with the observed system [1].

It can be seen from Tables II to IV that for the Fe–Al alloys the energies of the pure edge components of the $1/2 a \langle 1 1 1 \rangle$ superlattice dislocations are much higher than those for the edge components of the $\langle 1 0 0 \rangle$ dislocations; for the screw components energy

difference for the two dislocation types is small and is a function of aluminium content. Therefore, based upon the energy difference alone, the Fe–Al alloys should, like NiAl, slip in the $\langle 1 0 0 \rangle$ directions. However, the important point here is that the values of product Md_v are $\sim 50\%$ lower for the $\langle 1 1 1 \rangle$ slip than for $\langle 1 0 0 \rangle$ slip in the Fe–Al alloys. Thus, even though the crystals may have more $\langle 1 0 0 \rangle$ type grown-in dislocations, they are not as mobile as $\langle 1 1 1 \rangle$ type dislocations. Therefore, based upon calculations summarized in Tables II and IV, the predicted room temperature slip system is $1/2 a \langle 1 1 1 \rangle \{\overline{1} 0 1\}$. This prediction is in accord with the experimentally determined system [6–11]. It should be pointed out here that the observed slip directions become $a \langle 1 0 0 \rangle$ at elevated temperatures [11].

5. Summary

In the past, the calculated values of elastic energies and parameter M have been utilized to predict slip systems in a number of B2 compounds. In the present study, the examination of these values for the Fe–Al alloys (Tables II, III and IV) reveal that slip systems can not be predicted unless the vertical displacement, d_v, is taken into account. Thus, it appears that the parameter Md_v is a better indicator of dislocation mobilities than parameter M.

Acknowledgements

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