Structure of Dislocations and Mechanical Properties of B2 Alloys

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Why is the slip direction different in different B2 alloys?

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Abstract

The dominant slip directions in different intermetallic alloys with B2 structure are different, either ⟨0 0 1⟩ or ⟨1 1 1⟩. The elastic energy of ⟨1 1 1⟩ dislocations is usually significantly higher than that of ⟨0 0 1⟩ dislocations and it is commonly assumed that ⟨1 1 1⟩ slip occurs if ⟨1 1 1⟩ dislocations can dissociate on {1 1 0} planes into ½⟨1 1 1⟩ superpartials. However, we show in this paper that ½⟨1 1 1⟩ anti-phase boundaries may not be metastable faults on {1 1 0} planes and the displacement vectors of metastable stacking-fault-like defects on these planes vary from material to material. This analysis involves calculations of {1 1 0} γ-surfaces for eight B2 alloys (CuZn, FeAl, NiAl, FeTi, CoTi, NiTi, FeGa, PdAl) using a density functional theory-based method. Since both ⟨1 1 1⟩ and ⟨0 0 1⟩ screw dislocations may possess non-planar cores if undissociated and will then control plastic properties analogously as ½⟨1 1 1⟩ screw dislocations in body-centered cubic metals, the dissociations have been analyzed for screw dislocations. Subsequently, we assume that if the width of splitting in {1 1 0} planes exceeds the Burgers vector of the corresponding dislocation, the dislocation spreads in this plane and is glissile while undissociated dislocation is sessile. The ability to glide is then regarded as the determining factor for the choice of the slip direction. If no planar spreading occurs the dominant dislocations are determined by their energy. This analysis predicts the slip directions for all alloys studied and demonstrates that an interplay of elastic anisotropy, displacement vectors of metastable stacking-fault-like defects and their energies govern the choice of the slip direction in any specific B2 alloy.

Keywords: B2 ordered alloys; Slip direction; Dislocations; γ-Surface; Elastic anisotropy

1. Introduction

In intermetallic compounds and alloys that crystallize in B2, body-centered cubic (bcc)-based, structure the shortest lattice vector is $a\langle 0\,0\,1\rangle$, where a is the lattice parameter. Hence, the ⟨0 0 1⟩ direction is expected to be the most common direction of slip. However, as seen in Table 1, which summarizes observed slip directions in alloys studied in this paper, both ⟨0 0 1⟩ and ⟨1 1 1⟩ slip directions occur but in different B2 alloys one or the other dominates. The ⟨0 0 1⟩ slip cannot operate, of course, in single crystals loaded in tension/compression along the ⟨0 0 1⟩ axis. In this case either the operating slip has the ⟨1 1 1⟩ direction and/or fracture occurs. However, in several B2 alloys (e.g. CuZn, FeAl, FeGa) the ⟨1 1 1⟩ direction dominates even for loadings when ⟨0 0 1⟩ slip may take place. This is in spite of the fact that the square of the Burgers vector of ⟨1 1 1⟩ dislocations is three times larger than that of ⟨0 0 1⟩ dislocations. One possibility is that the elastic anisotropy may affect the choice of the Burgers vector. This is discussed in Section 2 where it is shown that only in CuZn, which is very anisotropic, does the ⟨1 1 1⟩ screw dislocation have a lower energy than the ⟨0 0 1⟩ screw dislocation. This suggests that

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Table 1
Observed slip system in the eight B2 alloys studied.

Alloy	CuZn	FeAl	NiAl	FeTi	CoTi	NiTi	FeGa
Dominant slip directions	⟨1 1 1⟩	⟨1 1 1⟩	⟨0 0 1⟩ ⟨1 1 1⟩	⟨0 0 1⟩	⟨0 0 1⟩	⟨0 0 1⟩	⟨1 1 1⟩
References	[1–5]	[6–11]	[5,12–16]	[17]	[18–23]	[9,24–27]	[28]

the energy is not the only, and possibly not even the main, aspect determining which dislocations mediate the slip.

Another important factor is the dislocation mobility, which depends crucially on the dislocation core structure. The glide of dislocations can be very restricted if their cores are non-planar and thus sessile with a very high Peierls stress [29]. The best-known example is bcc metals in which the $1/2\langle 1\,1\,1\rangle$ screw dislocations possess cores spread into three $\{1\,1\,0\}$ planes of the $\langle 1\,1\,1\rangle$ zone [29–31]. On the other hand, dislocations with planar cores are usually quite mobile since their cores are glissile and their Peierls stress low. It is generally accepted that this is the case if dislocation can dissociate in their slip plane into partials separated by metastable stacking faults. A well-known example is face-centered cubic (fcc) metals with metastable stacking faults of the type $1/6\langle 1\,1\,2\rangle$.

It is commonly assumed that in B2 ordered alloys a metastable stacking fault-like planar defect on $\{1\,1\,0\}$ planes is the anti-phase boundary (APB) corresponding to the displacement $\frac{1}{2}\langle 1\,1\,1\rangle$ and thus $\langle 1\,1\,1\rangle$ dislocations can dissociate into $\frac{1}{2}\langle 1\,1\,1\rangle$ superpartials if the energy of the APB is low enough. However, as found in a number of atomistic studies [32–39], the $\frac{1}{2}\langle 1\,1\,1\rangle$ APB may not be a metastable fault on $\{1\,1\,0\}$ planes. Instead, displacements leading to metastable faults are not determined by crystallography but by details of atomic interactions and may differ significantly from $\frac{1}{2}\langle 1\,1\,1\rangle$. This is investigated in Section 3 using the concept of the γ-surface, the minima of which determine the possible metastable planar faults [29,31,40,41]. These surfaces have been calculated using a density functional theory (DFT)-based method and the metastable faults on the $(1\,\bar{1}\,0)$ plane have been found for the following B2 alloys: CuZn, FeAl, NiAl, FeTi, CoTi, NiTi, FeGa and PdAl. These metastable faults are different in different B2 alloys and thus possible splittings of both $\langle 1\,1\,1\rangle$ and $\langle 0\,0\,1\rangle$ dislocations may vary from one alloy to another. This may have a significant impact upon the choice of the slip directions in individual B2 alloy. The possible dislocation dissociations in the above-mentioned eight alloys have been analyzed using the γ-surface studies of metastable faults and anisotropic elasticity of dislocations. This investigation has been carried out for screw dislocations since in the B2 structure both $\langle 1\,1\,1\rangle$ and $\langle 0\,0\,1\rangle$ dislocations, if undissociated, may posses non-planar cores and control thus plastic properties analogously as $\frac{1}{2}\langle 1\,1\,1\rangle$ screw dislocations in bcc metals [32,34,37,38,42–45]. If the width of splitting in the $(1\,\bar{1}\,0)$ plane exceeds significantly the Burgers vector of the corresponding dislocation, the dislocation spreads in this plane and is regarded as glissile while undissociated dislocation is assumed to be sessile. We then consider that the determining factor for the slip direction is the ability of the corresponding screw dislocation to glide. In the case that no planar spreading occurs either for $\langle 0\,0\,1\rangle$ or $\langle 1\,1\,1\rangle$ dislocations the energy determines the dominant dislocations. Results of this study are presented in Section 4. This analysis demonstrates that an interplay of elastic anisotropy, displacement vectors of metastable stacking-fault-like defects, and energies of these faults govern the choice of the slip direction in any specific B2 alloy. All these aspects are controlled by the electronic structure of a given material and thus the choice of the slip systems cannot be analyzed in either purely crystallographic terms or employing considerations such as the relation between the order–disorder transition temperature and the energy of APBs [4,46].

2. Elastic properties

The elastic constants together with the lattice parameters of the B2 alloys studied in this paper were calculated using the method based on the DFT as implemented in the VASP code [47–49]. The electron–ion interactions were treated using projector-augmented wave (PAW) method [50,51] and the exchange and correlation functional was approximated by generalized gradient (GGA) [52] for all alloys apart from PdAl for which the local density approximation was used since the lattice parameter was reproduced better than when using the generalized gradient approximation. Spin-polarization was included in alloys containing Fe in order to account for possible magnetic effects. The number of **k**-points and the cut-off for the plane waves included were chosen on the basis of convergence tests. The same method was also utilized when calculating the γ-surfaces.

Table 2 summarizes the lattice constants and elastic moduli of the alloys studied and compares these results with experimentally determined values. The experimental data always correspond to the lowest temperature at which these were measured, which is in most cases well below the room temperature. An exception is NiTi which displays the bcc structure only above room temperature [53,54]. The elastic constants of NiTi are strongly dependent on temperature between 300 and 400 K and were therefore measured at 400 K, beyond which the temperature dependence is small [55,56]. The calculated lattice parameters agree with the experimental ones within 1%. The elastic moduli are in good agreement with the available measured ones considering that measurements reported by different authors commonly differ by more than 20% [57].

The anisotropy factor $A = 2C_{44}/(C_{11} - C_{12})$, listed in Table 3, shows that all the B2 alloys studied are elastically significantly anisotropic. In the framework of anisotropic

Table 2
Calculated and experimental lattice parameters a (Å) and elastic moduli (GPa).

Alloy	CuZn	FeAl	NiAl	FeTi	CoTi	NiTi	FeGa	PdAl
a (this work)	2.97	2.88	2.90	2.95	2.97	3.01	2.90	3.02
a (experiment) [58]	2.95	2.91	2.88	2.98	2.99	3.01	2.91 [55]	3.04
C_{11} (this work)	123.3	254.4	204.1	384.8	212.6	185.3	240.4	221.8
C_{11} (experiment)	119	194	199	310	203	162	NA	NA
C_{12} (this work)	107.3	136.1	133.2	102.8	169.5	149.7	150.2	160.9
C_{12} (experiment)	102	116	137	86	129	132	NA	NA
C_{44} (this work)	83.4	139.6	114.5	68.2	52.2	48.6	115.7	92.9
C_{44} (experiment)	74	133	116	75	68	71	~100	NA
References for experiments	[59]	[60]	[61]	[62]	[63]	[64]	[65]	

Table 3
Anisotropy factors A and energy factors K (J/m $\times 10^{-9}$) determining the elastic energy of corresponding dislocations per unit length (m).

Alloy	A	$K^{screw}_{\langle 111\rangle}$	$K^{edge}_{\langle 111\rangle}$	$K^{screw}_{\langle 001\rangle}$	$K^{edge}_{\langle 001\rangle}$	$K^{screw}_{\langle 111\rangle}/K^{screw}_{\langle 001\rangle}$
CuZn	10.42	0.369	1.130	0.585	0.405	0.63
FeAl	2.36	1.531	2.766	0.921	0.855	1.66
NiAl	3.23	1.028	2.152	0.766	0.671	1.34
FeTi	0.48	2.252	2.611	0.473	0.939	4.76
CoTi	2.42	0.606	1.328	0.366	0.438	1.66
NiTi	2.73	0.535	1.212	0.350	0.402	1.53
FeGa	2.56	1.218	2.388	0.774	0.750	1.57
PdAl	3.05	0.946	2.066	0.674	0.664	1.40

elasticity the energy of a dislocation per unit length is $K\ln(R/r_0)$, where K is a function of elastic moduli, the magnitude of the Burgers vector and its orientation with respect to the dislocation line; and R and r_0 are the usual outer and inner cut-off radii. (In the isotropic case $K_{iso} = \mu b^2/4\pi$ for screw dislocations, where μ is the shear modulus and b the magnitude of the Burgers vector; for edge dislocations K_{iso} is divided by $(1-\nu)$ where ν is the Poisson ratio.) The K factors for both screw and edge dislocations with the Burgers vectors $\langle 1\,1\,1\rangle$ and $\langle 0\,0\,1\rangle$ were calculated using the method described fully in Ref. [66]. The results are summarized in Table 3. It can be seen that, as expected, the energy of $\langle 1\,1\,1\rangle$ dislocations is generally larger than that of $\langle 0\,0\,1\rangle$ dislocations. An exception is the case of screw dislocations in CuZn, which is very highly anisotropic. However, in the isotropic case the ratio $K^{screw}_{\langle 1\,1\,1\rangle}/K^{screw}_{\langle 0\,0\,1\rangle} = 3$, while the anisotropic values are in all cases apart from FeTi smaller, close to 3/2. Hence the elastic anisotropy decreases in most cases the energy difference between the $\langle 1\,1\,1\rangle$ and $\langle 0\,0\,1\rangle$ dislocations. The reverse is true only for FeTi, the anisotropy of which is opposite to that of all the other alloys in that its anisotropy factor $A < 1$.

3. Displacements of metastable stacking-fault-like defects on the (1 1 0) plane

Determination of possible metastable planar faults on a given crystal plane can be done using the concept of the γ-surface that is a theoretical construct defined as follows. We cut the crystal along a chosen crystal plane and displace the upper part with respect to the lower part by a vector **u**, parallel to the plane of the cut. The fault created in this way is called the generalized single layer stacking-fault and it is not in general metastable. The energy of such a fault per unit area, $\gamma(\mathbf{u})$, can be evaluated when an appropriate description of atomic interactions is available. In our case it is the DFT-based method as employed in the VASP code. In such calculations relaxations perpendicular to the fault have to be allowed but no relaxations parallel to the fault are permitted. Repeating this procedure for various vectors **u** within the repeat cell of the selected crystal plane yields an energy-displacement surface, commonly called the γ-surface. Local minima on this surface determine the displacement vectors of all possible metastable single-layer stacking-fault-like defects, and the values of γ at these minima are the energies of these faults.

Calculations of γ-surfaces were carried out for the $(1\,\bar{1}\,0)$ plane. The distribution of A and B atoms in two adjacent $(1\,\bar{1}\,0)$ planes in an AB alloy with the B2 structure is shown in Fig. 1. The γ-surface must have an extremum for the displacement ½[1 1 1] for any description of interatomic forces. The reason is that when the generalized fault with this displacement is formed there are two mirror planes perpendicular to the fault plane, (1 1 0) and (0 0 1), and as a result the γ-surface must have vanishing first derivatives in both [1 1 0] and [0 0 1] directions and thus in any direction (see also Ref. [67]). However, this extremum need not be a minimum as often assumed. The cross-sections of the γ-surfaces along the [1 1 0] direction, which are presented for the alloys studied in Fig. 2, show that the displacement ½[1 1 1] leads to a minimum only in the case of CuZn and FeTi. For all the other alloys the minima are displaced to various positions along the [1 1 0] direction and the displacement ½[1 1 1] in fact corresponds to a maximum in this cross-section. For each of the minima shown in

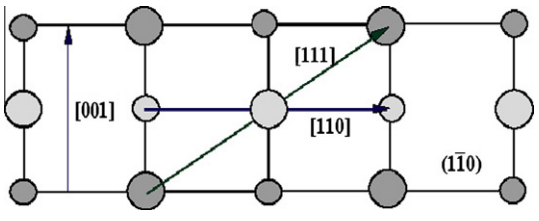

Fig. 1. Distribution of A and B atoms in two adjacent $(1\,\bar{1}\,0)$ planes in a B2 alloy. Shading differentiates the A and B atoms.

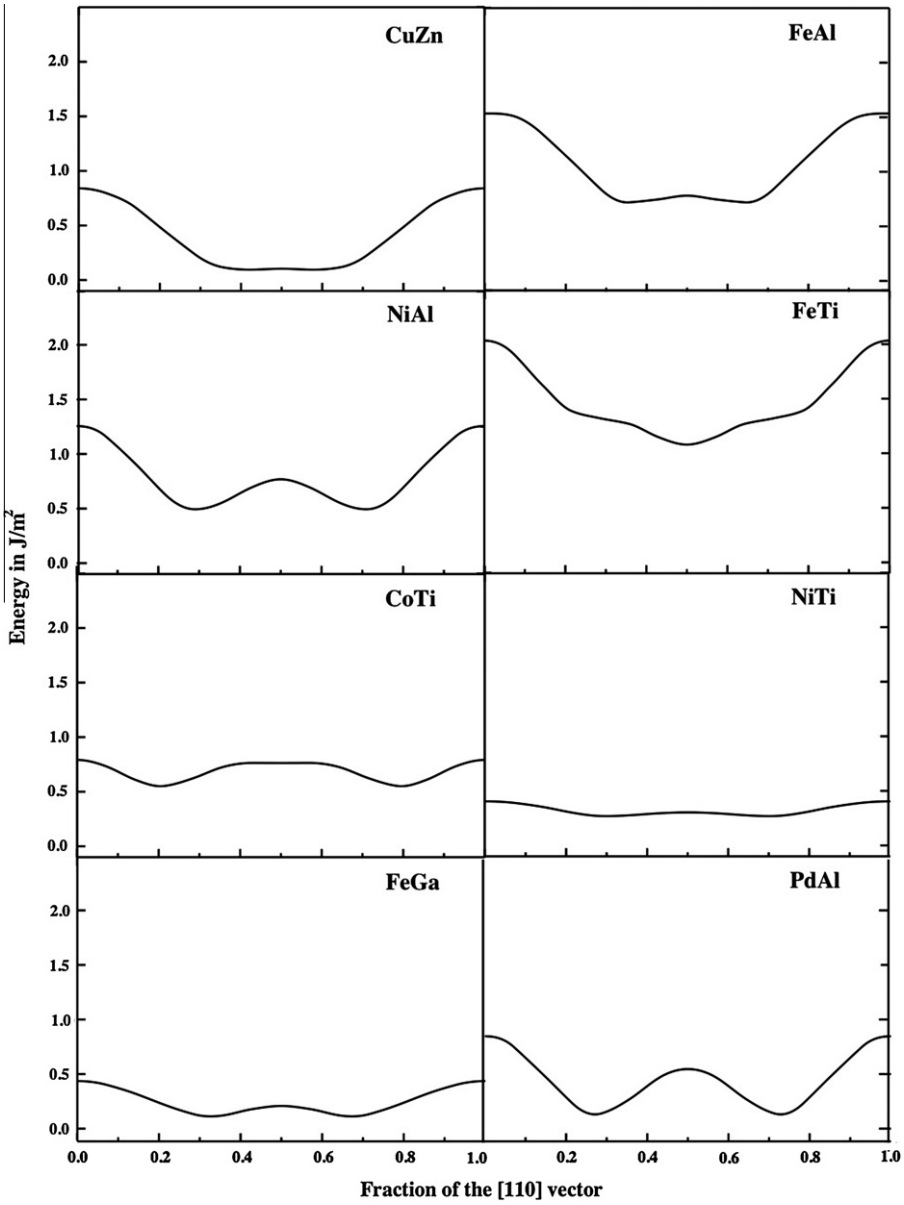

Fig. 2. [1 1 0] cross-sections of γ-surfaces for the $(1\bar{1}0)$ plane in the B2 alloys studied.

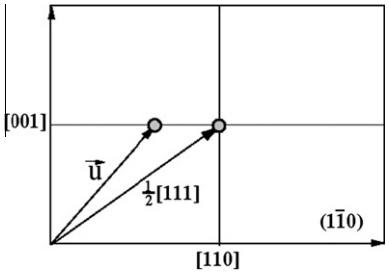

Fig. 3. Schematic picture of the position of the minimum of the γ-surface, corresponding to the displacement vector $\vec{\mathbf{u}}$, for the $(1\bar{1}0)$ plane in a B2 alloy.

Fig. 2 we carried out calculations of the cross-section of the γ-surface along the [0 0 1] direction and this proved that they are, indeed, local minima. Hence, the vectors corresponding to these minima determine displacement vectors of metastable faults on the $(1\bar{1}0)$ plane and can be written as (see Fig. 3):

$$\mathbf{u} = \frac{1}{2}[0\,0\,1] + \frac{\alpha}{2}[1\,1\,0] = \frac{1}{2}[\alpha, \alpha, 1] \quad (1)$$

where α varies between 0 and 1. When $\alpha = 1$ this fault is the usually assumed APB with the displacement ½[1 1 1]. Values of α, together with the energies of the corresponding faults, are summarized for the B2 alloys studied here in Table 4. It is important to realize that the stacking-fault-like defects characterized by these displacements cannot be anticipated on crystallographic grounds and are generally different for different B2 alloys. Similarly, displacement vectors deviating from ½[1 1 1] were found in a number of studies employing the embedded atom model (EAM)

Table 4
Displacements of metastable planar faults on the $(1\bar{1}0)$ plane, as determined by the parameter α, and energies of these faults.

Alloy	CuZn	FeAl	NiAl	FeTi	CoTi	NiTi	FeGa	PdAl
α	1	5/7	4/7	1	3/7	4/7	5/7	4/7
γ (mJ/m^2)	95	720	494	1079	553	269	138	155

[68,69] type central force potentials [32–38]. However, bonding in B2 alloys with transition metals does not have generally a purely central character and thus in these calculations the metastable faults could not be uniquely associated with specific alloys.

4. Analysis of dissociations of screw dislocations

As mentioned in the Introduction, $\langle 0\,0\,1\rangle$ and $\langle 1\,1\,1\rangle$ screw dislocations in B2 alloys may have non-planar cores. Since the Peierls stress of such dislocations is always much higher than that of dislocations with planar cores [29] their mobility is much lower. The dislocations that mediate the plastic deformation may then be those with higher mobility even if their energy is higher than those with low mobility. In calculations employing pair potentials Yamaguchi and Umakoshi [42,43] found the core of the [0 0 1] screw dislocation spread simultaneously into (1 1 0) and $(1\,\bar{1}\,0)$ planes. On the other hand, in calculations that employed an EAM potential for NiAl Schroll et al. [37,38] found that the [0 0 1] screw dislocation had a planar core confined into one of the {1 1 0} planes. At the same time the core of the screw [1 1 1] dislocation was found in this study to be spread into three {1 1 0} planes of the [1 1 1] zone, analogously to ½[1 1 1] screw dislocations in bcc metals. Tendencies to possess non-planar cores were found in other atomistic studies of $\langle 0\,0\,1\rangle$ and $\langle 1\,1\,1\rangle$ screw dislocations in B2 alloys [34,35,45]. Whether $\langle 1\,1\,1\rangle$, $\langle 0\,0\,1\rangle$ or both types of screw dislocations are having planar cores or are sessile owing to the non-planar cores, can only be studied exactly by atomistic modeling of dislocations using a description of atomic interactions that reflects fully the correct quantum mechanical nature of bonding. In principle, this can be done in the framework of the DFT but such atomistic studies of dislocations are very limited owing to the sizes of the blocks of atoms for which representative studies could be made when using periodic boundary conditions [70,71]. A very promising alternative is bond-order potentials [72] (for reviews see Refs. [73–75]) and/or multi-ion potentials [76,77] for transition metals that reflect correctly the main quantum mechanical aspects of bonding. These potentials were employed successfully in studies of dislocations in bcc transition metals [78–82] but no such potentials have been developed for B2 alloys. In analogy with dislocations in fcc materials, the nearest approximation in which planarity of the dislocations can be studied is investigation of the possible splittings of dislocations that involve metastable stacking faults. Using the results of calculations of the γ-surface (Table 4) we studied the following possible dislocation dissociations of [1 1 1] and [0 0 1] screw dislocations on the $(1\,\bar{1}\,0)$ plane that are shown schematically in Fig. 4a and b, respectively:

$$[1\,1\,1] = \mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_1 \tag{2}$$

where $\mathbf{b}_1 = \frac{1}{2}[\alpha, \alpha, 1]$ and $\mathbf{b}_2 = (1-\alpha)[1\,1\,0]$;

$$[0\,0\,1] = \mathbf{b}_1 + \mathbf{b}_3 \tag{3}$$

where $\mathbf{b}_3 = \frac{1}{2}[-\alpha, -\alpha, 1]$.

When determining the widths of splittings we regarded the partial dislocations as singular Volterra dislocations. For the splitting given by Eq. (2) the width of splitting $d_{[111]}$ is defined as the distance between the partials with the Burgers vectors $\mathbf{b}_1$ (see Fig. 5a). The force between the partials with the Burgers vectors $\mathbf{b}_1$ is equal to $F_{11}/d_{[111]}$ and between partials with the Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ $2F_{12}/d_{[111]}$. The width of splitting is then:

$$d_{[111]} = \frac{2F_{12} + F_{11}}{\gamma} \tag{4a}$$

where γ is the energy of the corresponding stacking fault-like planar defect. When $\alpha = ½$ and only two partial dislocations with Burgers vectors $\mathbf{b}_1 = ½[1\,1\,1]$ are present, the above formula applies when taking $F_{12} = 0$; $d_{[111]}$ is then the separation between the two partials. For the splitting given by Eq. (3) the width of splitting $d_{[001]}$ is defined as the distance between the partials with the Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_3$ (see Fig. 5b). The force between these two partials is $F_{13}/d_{[001]}$ and the width of splitting is then:

$$d_{[001]} = \frac{F_{13}}{\gamma} \tag{4b}$$

The values of F_{11}, F_{12} and F_{13} were calculated using the standard anisotropic elastic theory of Volterra dislocations [66] and are summarized in Tables 5 and 6. The widths of splittings calculated according to Eqs. (4a) and/or (4b) are presented in Tables 5 and 6, respectively. In these tables the widths of splittings are normalized by the magnitudes of the vectors of [1 1 1] and [0 0 1] dislocations, respectively.

5. Discussion

It is now well established that ½[1 1 1] screw dislocations control plastic behavior of pure bcc metals owing to their non-planar cores that make them much less mobile when compared with dislocations of other orientations. However, this phenomenon is much more common and, as demonstrated in a review [29], dislocations with non-planar cores are found in hexagonal close-packed materials when slip is not on the basal plane, many intermetallic compounds and even oxides and molecular crystals. Thus fcc

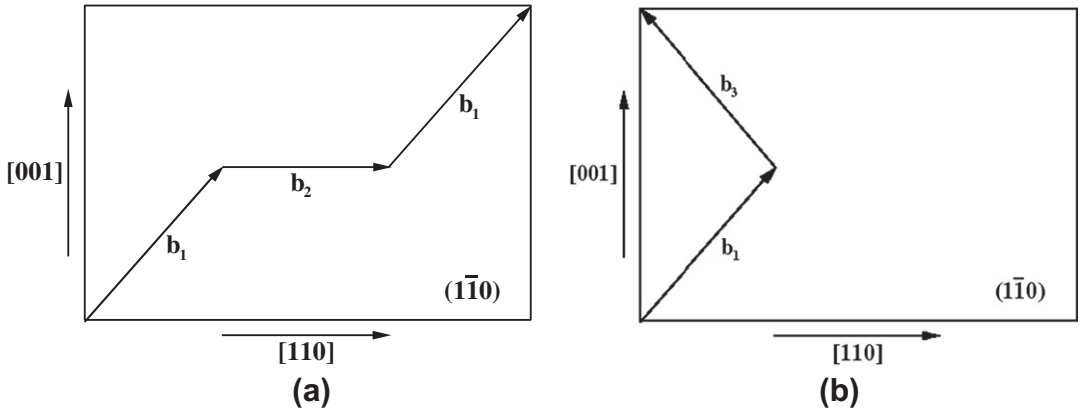

Fig. 4. Possible dissociations of dislocations on the $(1\bar{1}0)$ plane. (a) Splitting of the [1 1 1] dislocation according to Eq. (2). (b) Splitting of the [0 0 1] dislocation according to Eq. (3).

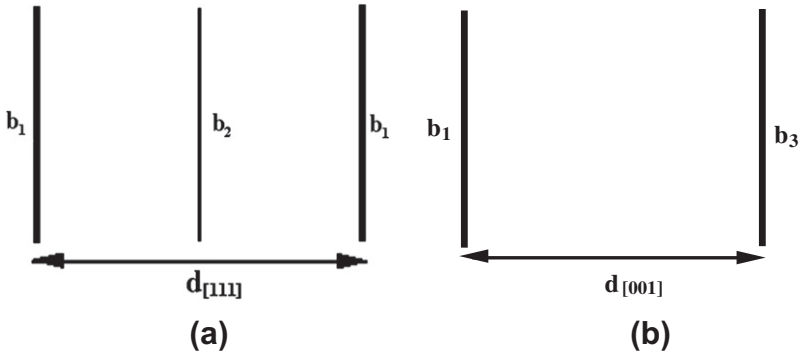

Fig. 5. Schematic picture of dislocation dissociations on the $(1\bar{1}0)$ plane. (a) Splitting of the [1 1 1] dislocation into three partials according to Eq. (2). (b) Splitting of the [0 0 1] dislocation into two partials according to Eq. (3). $d_{[111]}$ and $d_{[001]}$ define the widths of splitting in the two cases.

Table 5
Force constants F_{11} and F_{12} and the width of splitting in units of the magnitude of the Burgers vector, b, of [1 1 1] dislocations for the dissociation given by Eq. (2) (Fig. 4a).

Alloy	CuZn	FeAl	NiAl	FeTi	CoTi	NiTi	FeGa	PdAl
F_{11} (10^{-9} N)	0.184	0.527	0.307	1.126	0.166	0.161	0.420	0.285
F_{12} (10^{-9} N)	0	0.185	0.120	0	0.044	0.058	0.143	0.107
$d_{[111]}/b$	3.7	2.5	2.2	2.0	0.9	2.0	10.2	6.2

Table 6
Force constant F_{13} and width of splitting in units of the magnitude of the Burgers vector, a, of [0 0 1] dislocations for the dissociation given by Eq. (3) (Fig. 4b).

Alloy	CuZn	FeAl	NiAl	FeTi	CoTi	NiTi	FeGa	PdAl
F_{13} (10^{-9} N)	0.025	0.051	0.188	−0.720	0.105	0.059	0.035	0.143
$d_{[001]}/a$	0.9	0.2	1.3	0	0.6	0.7	0.9	3.0

crystals, in which all the dislocations are planar owing to their splitting in {1 1 1} planes that involves well-defined stacking faults, are a very special case [83]. When non-planar the core usually spreads into several crystallographic planes that all contain the direction of the dislocation line. This is the reason why screw dislocations possess non-planar cores most commonly, though not exclusively [29]. While such core structure has not yet been unambiguously observed even when employing state-of-the-art high-resolution electron microscopy [84], it has been found in practically all atomistic studies of bcc metals as well as other materials [29]. As already mentioned, atomistic calculations employing central force potentials revealed that cores of both ⟨1 1 1⟩ and ⟨0 0 1⟩ screw dislocations in B2 alloys may be non-planar and thus either one or both these dislocations may be sessile [32,34,37,38,42–45].

In this paper we make an assumption that it is the mobility of ⟨0 0 1⟩ and ⟨1 1 1⟩ screw dislocations that plays a very important, possibly decisive, role in the choice of the slip direction in a particular B2 alloy and that the

mobility increases with the planarity of the cores of screw dislocations. The energy then decides the preference for dislocations if both these dislocations possess very narrow and possibly non-planar cores. Atomistic studies of dislocation cores that take fully into account the differences in bonding in different B2 alloys are well beyond the present possibilities. For this reason we investigated the planarity of the dislocation cores approximately by analyzing possible dissociations of dislocations on {1 1 0} planes that involve stacking-fault-like defects found by the γ-surface calculations, and our results are summarized in Tables 5 and 6. These considerations lead to the following findings for the eight B2 alloys studied.

In both CuZn and FeAl the splitting of [1 1 1] screw dislocation on the $(1\bar{1}0)$ plane is significantly larger than that of the [0 0 1] screw dislocation, which is in fact smaller than one lattice spacing, and thus this dislocation has to be regarded as undissociated. The mobility assumption then predicts that the dominant slip direction is [1 1 1] in both these alloys, which is in agreement with observations [1–11]. Moreover in CuZn, owing to the large elastic anisotropy, the [1 1 1] screw dislocations are even energetically favored over the [0 0 1] dislocations. The situation is a less clear cut in NiAl. Both [1 1 1] and [0 0 1] dislocations can dissociate, albeit marginally, and, indeed, both slip directions operate in this alloy although [0 0 1] dominates [5,12–16]. The [0 0 1] slip is, of course, favored energetically as seen in Table 3. Moreover, it is likely that the partials on the $(1\bar{1}0)$ plane have screw components akin to the screw dislocation in pure bcc metals since the deviation of their Burgers vectors from ½[1 1 1] is not large and they have non-planar cores that renders them less mobile. In FeTi the [0 0 1] dislocation cannot split at all and [1 1 1] only marginally. However, as seen in Table 3 the [0 0 1] dislocation is almost five times more favored energetically owing to the unusual elastic anisotropy of this alloy and this suggests that the [0 0 1] slip direction be favored. This is, indeed, observed experimentally [17]. In NiTi neither [0 0 1] nor [1 1 1] dislocation can dissociate (the calculated widths of splitting are smaller than the corresponding Burgers vectors) and the energy favors significantly the [0 0 1] slip direction (Table 3). Indeed, [0 0 1] slip is observed [9,24–27]. In FeGa a significant splitting of the [1 1 1] screw dislocation is predicted, while the [0 0 1] dislocation is undissociated. This suggests that the [1 1 1] slip direction is favored even though the energy of the [0 0 1] dislocation is significantly lower (Table 3). Indeed, [1 1 1] slip is observed in this alloy [28]. There are no experimental data for slip directions in PdAl and the present calculations suggest that both [0 0 1] and [1 1 1] screw dislocations may split on the $(1\bar{1}0)$ plane. Hence, the prediction is that both dislocations may be mobile and the situation may be similar as in NiAl with [0 0 1] dominating.

6. Conclusions

In this study we have shown that the choice of the slip direction cannot be simply assessed according to the energy of dislocations mediating the slip. What needs to be considered is an interplay between the mobility of dislocations and their energy. The former is controlled by the type of spreading of dislocation cores and the latter by the anisotropic elasticity together with the energy of the possible planar faults on the slip plane. If the core spreads in one plane, in similar fashion to conventional splitting into partials, the dislocations are probably more mobile than if their core is narrow and most probably non-planar in the case of screw dislocations. In this paper we investigated the core spreading by calculating the widths of possible splittings with planar faults that vary from alloy to alloy and are determined by the minima of corresponding γ-surfaces. In these calculations we employed the anisotropic elasticity of Volterra dislocations to evaluate the interactions between partials. This is obviously a rather crude approximation since the cores of partials will also spread and this affects both their separation [85] and their mobility. Nevertheless, this analysis gives a reasonable first-order assessment of possible core spreading of screw dislocations in different alloys.

An outstanding example is the choice of slip directions in FeAl and CoTi [39]. In the framework of conventional thinking the APB energy in FeAl should be very similar to that of CoTi because the ordering energies in these two alloys are very similar [86]. This would suggest that the preferred slip direction is the same in both alloys. However, the favored slip direction in FeAl is ⟨1 1 1⟩ and in CoTi ⟨0 0 1⟩. As shown in the previous section, the explanation lies in the interplay of vectors of the planar faults, which are different in the two alloys, the elastic anisotropy and energies of the faults. This example, together with all the successful explanations of slip directions discussed in the previous section, shows that only an analysis that takes fully into account displacements of possible stacking fault-like defects, elastic anisotropy and energies of planar defects evaluated appropriately for a given alloy can explain the choice of slip direction. At the same time such analysis may be a first approximation for the assessment of the ductility. If at least one of the ⟨1 1 1⟩ and ⟨0 0 1⟩ dislocations has a spread core, and is therefore mobile and mediates the slip, it is likely that the alloy is ductile. On the other hand, if both these dislocations have very narrow cores and may be sessile in the screw form, the material is likely to be brittle. Recently the ductility and/or brittleness was studied for a number of rare-earth-based B2 intermetallics, some of which were found to be unusually ductile [87–89]. The explanation might be sought in the analysis similar to that made in this paper. Moreover, the analysis of this type applies not only to B2 alloys but may be similarly utilized when studying slip systems and related ductility/brittleness in any materials with a variety of potential slip systems.

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