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# THE RELATIVE STABILITY OF DISLOCATIONS EMBEDDED IN THE $\beta$ PHASE MATRIX AND IN MARTENSITE PHASES IN COPPER BASED ALLOYS.

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Abstract

Dislocations are formed during martensitic transformations in shape memory alloys. The number of dislocations (with Burgers vector $\vec{b}_\beta = a_o\langle 010\rangle$ and $\langle \bar{1}11\rangle$ line direction in the $\beta$ phase) increases when the material is subjected to thermoelastic or pseudoelastic cycles. The dislocations are accumulated in the sample and are incorporated in the corresponding growing phase. The relative energy of the dislocations when embedded in the parent phase (with respect b) one or another variant of martensite is evaluated in this work.

The crystallographic changes of the dislocations provide a primary selection rule for those martensite variants in which the dislocations have the lowest energy. In order to proceed more quantitatively a full calculation of the dislocation energies has to be performed using the anisotropic theory. In this work these calculations have been made on the basis of measured elastic constants of the $\beta$ and 2H phases of a Cu-Al-Ni alloy. It is concluded that those martensite variants are favored energetically whose basal plane contains the Burgers vector and line direction

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of the dislocations (Splitting into Shockley partials is suggested to occur).The importance of this result for the two-way shape memory (TWSM) effect is discussed,and a mechanism is proposed which can account for the multiplication of dislocations during the transformation.

## 1. INTRODUCTION

A large number of alloys based on the noble metals undergo a martensitic transformation on cooling (thermoelastic martensite) or on applying stresses (pseudoelasticity). It has been observed that dislocations are created in the material when it is subjected to transformation-retransformation cycles, either by spontaneous [1][2][3][4] or by stress induced transformation [5][6][7]. The dislocations generated by thermal cycling have been studied in detail by Rios-Jara et al.[2] in a Cu-Zn-Al alloy ($L2_1 \leftrightarrows 18R$ transformation) and by Marukawa and Kajiwara [4] in a Cu-Zn alloy ($B2 \leftrightarrows 9R$ transformation). These authors have found that most of the dislocations had <100> type Burgers vectors with <111> line directions (Indices refer to the B2 lattice).The dislocations formed after stress cycling also have been analysed by Rios-Jara et al.[2], who reported dislocations being of the same nature as those obtained by thermal cycling. A detailed study of the dislocations generated by pseudoelastically cycling a Cu-Zn-Al single crystal has been reported recently by Sade et al. [6] [7]. The study was carried out in the parent phase ($L2_1$-type) and the relationship of the dislocations with the induced variant of martensite was established. The main results, with reference to the stereographic projection of Fig.1, can be summarized as follows:

i) The dislocations were found to be accumulated in bands parallel to the trace given by the habit plane [HP] of the induced martensite variant and the basal planes. Secondary bands with traces parallel to the basal plane [BP] were observed to be

connected to the former.

ii) The Burgers vectors $\vec{b}_{\beta}$ of the dislocations were determined by the computer simulation technique. The majority of the dislocations have the Burgers vector:

$$\vec{b}_{\beta} = \pm \frac{a_{\beta}}{2} [010]$$

where $a_{\beta}$ is the lattice parameter of the $L2_1$ unit cell. These Burgers vectors correspond to a close packed direction in the basal plane after transformation to the induced variant of martensite.

iii) These dislocations were of mixed character and were composed of segments with line directions parallel to [111] and $[1\bar{1}1]$ and thus were glissile on the $(\bar{1}01)$ plane of the parent phase, or equivalently on the basal plane of the induced martensite variant.

When the material contained these dislocations is exhibited the two way shape memory (TWSM) effect [7], i.e. the most favorable variant in the subsequent spontaneous transformation was that one for which the basal plane coincided with the dislocation glide plane. This result is in agreement with the earlier conclusion of Rios-Jara and Guénin [8].However, in their case the specimen was plastically deformed until fracture occurred in the martensite phase, and at variance with the results of Sade et al [6] [7], the observed dislocations were not on the plane corresponding to the basal plane of the induced martensite (except in the vicinity of the fractured zone). Consequently, the single

variant formed by spontaneous transformation after the deformation, was not the induced variant but a different one.

In order to evaluate the possible contribution of these dislocations to the TWSM effect, Sade et al.[7] considered the changes of the Burgers vectors of the dislocations upon transformation from $\beta$ to 18R martensite and found that, they become shorter (by about 10%) when lying in the basal plane. Because of this shortening, it was suggested that the energy of the dislocations is lower when lying an the basal planes of the martensite variants derived from $(\bar{1}01)_{\beta}$ than when embedded in the parent phase or in another differently oriented 18R variant.

The arguments given by Sade et al. [7] were based on geometrical considerations, the effect of the elastic constants of one phase or the other on the dislocation energy was not taken into account. So far, the full set of elastic constants of the 18R structure (monoclinic symmetry) has not been measured. Nevertheless, the elastic constants for the 2H martensite (orthorhombic symmetry) of a Cu-Al-Ni alloy are available from the literature [9]. In this work, the energy of the dislocations embedded either in the $L2_1$ parent phase or in the 2H martensite are calculated using the anisotropic theory developped by Stroh [10]. Extension of these results to the explanations of the TWSM effect is discussed. In addition to this, the role that the interaction of a growing martensite plate with the dislocations could play in the TWSM is also considered.

## 2. CRISTALLOGRAPHIC CONSIDERATIONS

For the sake of completeness the geometrical analysis performed by Sade et al. [7] is summarised first.

The Burgers vectors of the observed dislocations are not a symmetry translation vector of the $L2_1$ parent phase. Hence, a second neighbor antiphase boundary (APB) is associated with each dislocation [6]. For the moment the ordering is disregarded and the parent phase will be considered as having a BCC structure with $a_o = \frac{a_\beta}{2}$ as lattice parameter. (The effect of the superlattice is analyzed in the Appendix).

The Burgers vectors of the dislocations in the parent phase will be then:

$$\vec{b}_\beta = \pm a_o[010]$$

Instead of taking one Burgers vector and analyzing how it changes in the different variants (or group of variants) of martensite, it is equivalent to consider the three cubic edges and study how they change in one variant of martensite.

A Burgers vector with direction $[010]_{BCC}$ lying on the $\{101\}_{BCC}$ type plane becomes shorter when this plane is transformed into the basal plane of the martensite. This is shown in Fig.2. The length of the Burgers vector($\vec{b}_o$) in the basal plane depends on the tetragonal distortion $\psi$ (with $\psi = \frac{c_f}{a_f}$ . Where $c_f$ and $a_f$ are the lattice parameters of the hypothetical FCT structure from which the 18R stacking has been derived [11]). If the condition of no volume change during the transformation is assumed to be valid [11], we obtain:

$$b_o = a_o(\sqrt{2}\ \psi)^{-1/3}$$

The parameter $\psi$ is composition dependent and the relationship with the composition was given by Ahlers [12].

The other two cubic directions lie on the $(010)_{BCC}$ plane which is transformed into the $(010)_{18R}$ plane. The $\{100\}_{BCC}$ planes become corrugated after transformation to 18R martensite. This is shown in Fig.3. The interplanar distances of these corrugated planes, $b_1$ and $b_2$, are plotted in Fig.4 together with $b_o$, as a function of $\psi$.

Refering to Fig.2, 3 and 4, two important differences between the dislocations lying on the basal plane (Fig.2) and away from it (Fig.3) should be emphasized, namely:

i) The $b_o$ (in the basal plane) is the shorter interplanar distance (by more than 10%) as compared to $b_1$ and $b_2$ (out of the basal plane).

ii) Whilst the $\vec{b}_o$ is a symmetry translation vector of the basic 18R structure (ordering is disregarded), $b_1$ and $b_2$ do not define a symmetry translation vector. Hence, dislocations with $b_1$ or $b_2$ type Burgers vectors will create stacking faults because of the misfit of the structure along the glide plane.

Although the dislocation energy depends also on the elastic constants of the martensite, the two factors mentioned above were judged to be sufficiently important suggesting that the variant of martensite whose basal plane contains the Burgers vector of the dislocations energetically will be the most favored ones with respect to the others. This earlier suggestion is confirmed in this work by a full calculation of the dislocation energy using

the anisotropic theory (see paragraph 3.3.)

There are four variants of martensite having their respective basal planes derived from the same $(101)_{BCC}$ plane [13]. Since the $[010]_{BCC}$ direction (the Burgers vector of the dislocations) is common to the $(101)_{BCC}$ and $(\bar{1}01)_{BCC}$ planes, the arguments given above still leave us eight equally favoured martensite variants. In order to proceed further we have to consider the energy of the dislocation in a more quantitative way. This will be treated in the next paragraph.

## 3.- THE ENERGY OF THE DISLOCATIONS IN THE MARTENSITE AND PARENT PHASES OF A Cu-Al-Ni ALLOY.

Since the full set of elastic constants of the 18R martensite is not known (only some combinations of them have been measured till now [14] in a Cu-Zn-Al alloy) we can approximate the problem by considering the energy of the dislocations in the 2H structure of a Cu-Al-Ni alloy, from which the nine elastic constants were measured [8]; see Table I.

In this 2H structure we can compare the energy of the dislocation with the same Burgers vector lying in the basal plane ($\vec{b}_o$, see Fig.2 b) but with different line direction lying either on the basal plane or on the prismatic type plane. Furthermore, since the elastic constants of the $L2_1$ phase, for the same Cu-Al-Ni alloy, are also known [15] (see Table I), the energy of these dislocations embedded in the 2H structure can be quantitatively compared with themselves when embedded in the $L2_1$ (or B) parent phase.

3.1 Energy of the dislocations gliding on the basal plane of the 2H structure.

3.1.1 The energy of dislocations with total Burgers vector.

The formula for evaluating the dislocation energy in an anisotropic medium has been developed by Stroh [10] (see also Hirth and Lothe [16] and Steeds [17]:

$$E = \frac{C_{44}}{4\pi} H_{ij} b_i b_j \log\left(\frac{R}{Ro}\right) \qquad (1)$$

where $H_{ij}$ is a matrix depending on the elastic constants and the dislocation line direction, $b_i$ is the component of the Burgers vector referred to the dislocation axes, and R and Ro are the conventional inner and outer cut-off radii.

The coefficients of the matrix $H_{ij}$ were calculated using the subrutine computer program ANCALC developed by Head et al. [18]. The matrix of the elastic constants and the calculation of the cosine directions were modified to be suitable for orthorhombic symmetry. For the dislocation line direction shown in Fig. 2b (derived from the $[111]_{BCC}$ line direction), with the lattice parameters of the 2H structure (in nm)[19]:

$$\begin{aligned} a &= 0.4382 \\ b &= 0.5356 \\ c &= 0.4222 \end{aligned} \qquad (2)$$

and using the elastic constants for the 2H phase given in table I, we obtained:

$$H_{ij}^{bp} = \begin{bmatrix} 1.12591 & 0 & -0.10075 \\ 0 & 1.00106 & 0 \\ -0.10075 & 0 & 0.38828 \end{bmatrix} \qquad (3)$$

From (1) the energy, $E_{ob}$, of a dislocation gliding on the basal

plane was calculated:

$$E_{ob} = 2.63 \ \frac{mJ}{m^2} \qquad (4)$$

where $R = 2.5 \times 10^{-6}$ m and $Ro = 1 \times 10^{-10}$ m have been taken, as usually (Ball and Smallman [20]).

3.1.2. The dissociation into Shockley partial dislocations.

The dislocation considered in the last paragraph can dissociate into Shockley partials if the stacking fault energy is sufficiently low (see, for example Hirth and Lothe [16]).

An estimation of the stacking fault energy when hexagonal faults are introduced in the 18R structure of Cu-Zn-Al alloys has been given by Ahlers [21]. This stacking fault energy $\gamma_{sf}$ is of the order of 5 to 10 $\frac{mJ}{m^2}$. Such a value of $\gamma_{sf}$ corresponds to a displacement (along the $\vec{a}$ direction), which conserve the long range order. This is not the case if a dissociation into $\vec{b}_o^{(1)}$ and $\vec{b}_o^{(2)}$ (see Fig.4) is assumed. When ordering is taken into account, the displacement vector $\vec{bo}^{(1)}$ will create an antiphase boundary (APB) (see the Appendix). The value of this $\gamma_{APB}$ (the antiphase boundary energy) in Cu-Zn-Al alloys can be estimated in terms of the pair interchange energy given by Ahlers [21]. For alloy compositions showing the $L2_1$ to 18R transformation (with an electron concentration of about 1.48), a range of values for $\gamma_{APB}$ from 0.3 to 19 $\frac{mJ}{m^2}$ is obtained (see the Appendix).

Adding up both contribution to the stacking fault energy, we obtain as upper limit: $\gamma = \gamma_{sf} + \gamma_{APB} \simeq 30 \ \frac{mJ}{m^2}$. Although this

value of $\gamma$ can only be regarded as an estimate, it could be useful to use it for calculating the energy of the dissociated dislocation [16] [17]:

$$E_{ob}^{d} = E_{ob}^{(1)} + E_{ob}^{(2)} + E_{ob}^{(1)(2)} + \gamma W \qquad (5)$$

where $E_{ob}^{(i)}$ is given by (1) with the corresponding $\vec{b}_o^{(i)}$ Burgers vector, $E_{ob}^{(1)(2)}$ is the interaction energy between the partials, which approximately can be taken as [17]:

$$E_{ob}^{(1)(2)} = \frac{C_{44}}{2\pi} H_{ij}^{bp} b_i^{(1)} b_i^{(2)} \log\left(\frac{R}{W}\right) \qquad (6)$$

where W is the distance between the partials which is related to $\gamma$ by :

$$W = \frac{C_{44}}{2\pi} H_{ij}^{bp} b_i^{(1)} b_j^{(2)} \frac{1}{\gamma} \qquad (7)$$

Using the coefficients of $H_{ij}$ given by (3), we obtained

$$W = 3.3 \text{ nm}$$

and

$$E_{ob}^{d} = 2.38 \frac{mJ}{m} \qquad (8)$$

It should be noticed that the value $E_{ob}^{d}$ (given by (8)) of the dissociated dislocation is by about 10% lower than the energy $E_{bp}$ of the undissociated dislocation. Hence, the decomposition into Shockley partials can indeed occur, specially if we take into account that the value of $\gamma$ can be significantly lower than that used in (5).

3.2. Energy of the dislocations gliding on a prismatic type plane.

For dislocations with Burgers vector, $\vec{b}_o$, lying on the basal plane and line directions out of the basal plane (derived from the $[\bar{1}11]_{BCC}$ or $[\bar{1}\bar{1}1]_{BCC}$, see Fig.1), as shown in Fig.5, the coefficients of the matrix $H_{ij}$ are:

$$H_{ij}^{pp} = \begin{pmatrix} 1.06875 & 0 & 0.09353 \\ 0 & 0.89545 & 0 \\ 0.09353 & 0 & 0.41539 \end{pmatrix} \qquad (9)$$

Proceeding in the same way as in paragraph 3.1.1, we obtained

$$E_{op} = 2.51 \ \frac{mJ}{m^2} \qquad (10)$$

Comparing this value of $E_{op}$ with $E_{ob}^{d}$ given by (8) we see that the dislocations gliding on the basal plane could have the lowest energy after Shockley dissociation.

3.3. The energy of the dislocations with Burgers vector out of the basal plane.

The Burgers vectors lying on the $(010)_{1BR}$ plane were assumed to have their length ($b_1$ and $b_2$) equal to the interplanar distances (see Fig.4) and direction along the normal of the respective planes (see Fig.3a).

Using the matrix $H_{ij}$ given by (3) and (9) we obtained:

For a Burgers vector with length $b_1$:

$E_{1b} = 331 \ \frac{mJ}{m}$, with line direction on the basal plane, and

$E_{1p} = 298 \ \frac{mJ}{m}$, with line direction on the prismatic type plane.

For a Burgers vector with length $b_2$:

$E_{2b} = 383 \frac{mJ}{m}$, with line direction on the basal plane

$E_{2p} = 352 \frac{mJ}{m}$, with line direction on the prismatic type plane.

Although these values can only be regarded as an estimate it is encouraging to find that they are higher as compared to the energy of the dislocations with Burgers vector $\vec{b}_o$ on the basal plane (see 3.1. and 3.2.). Moreover, since the Burgers vectors $b_1$ and $b_2$ do not posses translation symmetry the stacking fault energy associated with these dislocations should be added to the elastic energy given above.

3.4. The energy of the dislocations in the $L2_1$ phase of the Cu-Al-Ni alloy.

For dislocations having a Burgers vector $\vec{b}_\beta = \pm \frac{a_\beta}{2}\langle 010\rangle$, and a $\langle 111\rangle$ line direction, using the elastics constant of the $\beta$ phase given in Table I, and taking $a_\beta = 0.5836$ nm [19], we obtain:

$$H_{ij}^{\beta} = \begin{pmatrix} 0.66172 & 0 & 0 \\ 0 & 0.66172 & 0 \\ 0 & 0 & 0.21706 \end{pmatrix} \qquad (11)$$

and

$$E^{\beta} = 3.29 \frac{mJ}{m^2} \qquad (12)$$

The energy of the dislocations in the $\beta$ phase is larger by more than 30%, as compared to $E^d_{ob}$ and $E_{op}$ in the 2H phase.

## 4. DISCUSSION

The structural analysis made by Sade et al.[6] (summarized in paragraph 2) indicated that the 24 variants of martensite can be

divided into 3 groups of 8 variants each , with respect to the orientation relationship of every variant with a given $\vec{b}_{\beta} = \frac{a_{\beta}}{2}\langle 010\rangle$ Burgers vector. In the first group the Burgers vector lies on the basal plane, it is a symmetry translation vector of the basic 9R structure and its length shortens by about 10% as compared to $b_{\beta}$. For the second group the interplanar distance associated with the Burgers vector remains almost unchanged (as compared to that in the parent phase) but no Burgers vector with translation symmetry can be defined. Hence, faults are necessarily associated with these dislocations. For the third group, no Burgers vector with translation symmetry can be found and in addition the interplanar distance increases by about 10% after transformation to martensite.

The calculation of the elastic energy of the dislocations embedded in the martensite (section 3.1., 3.2. and 3.3.) confirms the earlier suggestion of Sade et al. [7], i.e., the dislocations with Burgers vectors out of the basal plane have a higher energy as compared to those with Burgers vector on the basal plane.

Considering now that the line direction of the dislocations in the parent phase are [111] and $[1\bar{1}1]$, the first group of the 8 most favored variants can be further divided into two subgroups: one subgroup of 4 variants in which the line directions lie in the basal planes (derived from $(\bar{1}01)_{\beta}$) and another subgroup of 4 variants which the line direction are out of the basal planes (derived from $(101)_{\beta}$).

In order to estimate the difference in the dislocation energy when lying in one or the other subgroup, we have made use of the

elastic constants for the 2H structure of a Cu-Al-Ni alloy (paragraphs 3.1. and 3.2.). Considering the dislocations with total Burgers vector, $\vec{b}_o$ (see Fig.2 b), and applying the full anisotropic theory in the computer calculation, we obtained $E_{ob} = 2.63 \frac{mJ}{m^2}$ (for dislocations with line direction on the basal plane) and $E_{op} = 2.51 \frac{mJ}{m^2}$ (line direction on a prismatic type plane). The energies of these two dislocations are almost equal. Since these values correspond to the 2H structure, it is in principle difficult to say how they could change when the 18R structure (which is of our interest) is considered. Nevertheless, the 2H and 18R structure differ only in their respective stacking sequences, the other lattice parameters and atom configurations remaining unchanged [22]. Hence, it seems reasonable to assume that the energies of the dislocations given above would not change considerably from one structure (2H) to the other (18R).

Up to now, is cannot be unambigously deduced which of the two subgroups of 4 variants are more favorable. However, for the dislocations with line direction in the basal plane there is still a further contribution to be considered. This is the dissociation into Shockley partials. The associated stacking fault energy appears to be sufficiently low (see paragraph 3.1.2.and Appendix I) so that the dissociation into Shockley partials can be really expected. So far , such a dissociation has not been studied experimentally, some difficulties in the contrast analysis could appear since the martensitic phases are normally heavily faulted.If the decomposition into Shockley partials is taken into account, we can assume that the first subgroup of 4 variants,whose

basal plane contains the Burgers vector and the line direction, is energetically the most favorable one, as compared to the other variants.

We can find a difference in relative stability between these four variants by considering the orientation of most of the dislocation bands, i.e. parallel to the habit plane of the induced variant during the training. The calculation for the Cu-Al-Ni alloy showed that the energy of the dissociated dislocation lying on the basal plane ($E^{d}_{ob} = 2.38 \frac{mJ}{m^2}$, see paragraph 3.1.2.) is lower by about 30% as compared to the same dislocation but embedded in the $\beta$ parent phase ($E_{\beta} = 3.29 \frac{mJ}{m^2}$, see paragraph 3.3.). On the other hand it is known that the 18R martensite grows first as thin plate parallel to the habit plane and then thickens. Under these conditions the maximum gain in energy at the beginning of the transformation will be obtained for martensite plates growing with the habit plane parallel to the dislocation bands. Among the four possible variants mentioned above the only one to comply with this condition is that corresponding to the induced variant during the cycling.

The arguments given above are based on the relative stability between the differently oriented variants of martensite and between those with the parent phase in a material containing dislocations. However, in order to have a complete description of the TWSM effect two other fundamental aspects need to be considered, namely: i) The nucleation of the phases and ii) The interaction of the growing martensite with the dislocations.

A theoretical frame for treating the nucleation of martensite

has been developed by Guénin and Gobin [23][24].Their approach is based on the softening of the C′ constant for some of the {110} $\langle 1\bar{1}0 \rangle$ shear systems in the vicinity of particular defects. Following this theory, Hazarabedian [25] has shown in a qualitative way that the C′ constants which become softer arround the dislocations reported here could acount for the nucleation of several variants, including the induced variant.

Concerning the interaction of a growing martensite plate with the dislocations, two aspects are to be taken into account i) The martensite grows first as a thin plate parallel to the habit plane. As suggested by Delaey et al.[26], the stress field (in the parent phase) arround the advancing tip is approximately similar to that created by a dislocation with Burgers vector $b = e\ s$, where e is the thickness of the tip and s is the amount of the macroscopic phear. The tip thickness is of the order of 1.0 to 1.5 nm [27], whilst a typical value of s for BCC to 9R transformation is $s \simeq 0.2$ [28]. Hence, the length of the effective Burgers vector is $b \simeq 0.3$ nm, which is similar to a normal dislocation. Interaction forces should exist between the tip and the existing dislocations. The component of the force along the direction in which the front advances could be attractive or repulsive. If it is attractive for one sense of the Burgers vector (of the existing dislocations) it will be repulsive for the opposite sense [16]. Since dislocations with both senses of Burgers vector (in approximatelly equal proportion) have been found in the fatigued materials [6], we can assume that the interaction of the tip with the individual dislocation is not modified on the average, by the

arrangements of dislocations in groups.

As noticed by Marukawa and Kajiwara [4], another source of internal stresses arises from the volumen change (normal to the habit plane) accompanying the transformation. Assuming that only one variant of martensite grows, this stress can be important during the longitudinal growing of the plate through the whole specimen. When the variant thickens the volume change contributes to the macroscopic shape change. Owing to the fact that the volume change (about 0.3%) as well as the initial thickness of the plate is small it seems that the interaction of this stress with the dislocations is also rather small.

ii) The second aspect refers to the thickening of the martensite plate. When the interface moves in a direction normal to the habit plane we could consider the material as a "bimetallic" solid (as first suggested by Head [29]). Here again the dislocations could be repelled or attracted by the moving interface depending on the elastic and geometric characteristics (see for example Dundurs and Sendeckyj [30]). A rigorous treatment of the interaction of a dislocation with the interface between two anisotropic media has been outlined by Barnett and Lothe [31]. Nevertheless, we could, in principle, assume that the force would be attractive if the energy of the dislocation lying outside is higher than its energy when embedded in the growing medium. Under this assumption, those variants whose the basal plane contains the Burgers vector would be attracted towards the dislocation arrangements. And conversely, the dislocations can be moved by the growing (or shrinking) martensite plate. This provides a possible mechanism for the

dislocation reproduction during the fatigue cycling, as already suggested by Sade et al.[6].

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Table I

Elastic constants [$GN/m^2$]

| Phases | $C_{11}$ | $C_{22}$ | $C_{33}$ | $C_{44}$ | $C_{55}$ | $C_{66}$ | $C_{12}$ | $C_{13}$ | $C_{23}$ | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|
| $L2_1^+$ | 143 | | | 94 | | | 124 | | | 12 |
| 2H* | 189 | 141 | 205 | 54.9 | 19.7 | 62.6 | 124 | 45.5 | 115 | 8 |

Elastic constants of the $L2_1$ and 2H phases of a Cu-Al-Ni alloy.

+ The elastic constants are referred to the cubic axes.

* The elastic constants are referred to a system parallel with the orthorhombic axes.

Appendix

It is customary to describe the $L2_1$ body centered cubic superlattice by four interpenetrating face centered cubic sublattice. The various possible atomic configurations are then expresed in term of the concentration probabilities $P_i^{\nu}$ of the $i^{th}$ component, on the four sublattices $\nu$ = I, II, III and IV (see Marcinkowski and Brown [32]).

The basal planes of the 18R structure are derived from the {110} type planes of the $L2_1$ structure ( see main text, Fig.2). The site configuration on the basal plane of our interest are shown in Fig. A-1. An antiphase boundary (APB) is already inherited from the parent phase, this corresponds to a $\vec{b}_o$ displacement vector and is schematically shown in Fig. A-2a.

We assume the $\vec{b}_o$ Burgers vector to dissociate into Shockley partials with $\vec{b}_o^{(1)}$ and $\vec{b}_o^{(2)}$ Burgers vectors respectively (see main text, Fig. 5) on the side where the stacking AB is present. The traslation vector $\vec{b}_o^{(1)}$ will transform the B′ type plane into a C′′′ type plane (see Fig. A-1, this is schematically shown in Fig.A-2b. The energy, $\gamma_2^m$, of the preexistent APB should be sustracted to the $\gamma_1^m$ energy corresponding to the APB associated with the $\vec{b}_o^{(1)}$ traslation vector. Thus the energy of interest for the Shockley dissociation will be $\gamma_{APB} = \gamma_1^m - \gamma_2^m$.

The APB energy can be evaluated by counting the number of nearest neighbor or next nearest neighbor, havinga bond energy $V_{ij}^{(k)}$, that changes from one stacking to the other.

The same procedure as that suggested by Flinn [33] and Iden [34] for binary alloy and Romero et al.[35] for ternary alloys,

for calculating the APB energies in $L2_1$ superlattices, can be followed for the martensitic phases. Thus we obtained

$$\gamma_1^m = \frac{1}{ab} \sum_{\substack{i>j \\ i,j=1,2,3}} \left[ \frac{1}{2} \left( m_{ij}^{(1)} - 3\, m_{ij}^{(2)} \right) \left( S_i T_j + S_j T_i \right) - \right.$$

$$\left. - \left( m_{ij}^{(1)} - m_{ij}^{(2)} \right) R_{ij} + m_{ij}^{(2)} \left( S_i S_j + T_i T_j \right) \right] \qquad (A1)$$

for the displacement vector: $\vec{b}_o^{(1)}$, and

$$\gamma_2^m = \frac{1}{ab} \sum_{\substack{i<j \\ i,j=1,2,3}} \left[ m_{ij}^{(1)} - m_{ij}^{(2)} \right] \left[ S_i S_j + T_i T_j - 2R_{ij} \right] \qquad (A2)$$

Where the following definitions were introduced:

$$\begin{aligned} R_{ij} &= \sum_{\nu=I}^{IV} P_i^{\nu} P_j^{\nu} \\ S_i &= (P_i^{I} + P_i^{II}) \\ T_i &= (P_i^{III} + P_i^{IV}) \end{aligned} \qquad (A3)$$

The occupation probabilities satisfy the following relations:

$$\begin{aligned} &\sum_{\nu} P_i^{\nu} = 4\, C_i \quad , \quad \nu = I,\ II,\ III \text{ and } IV \\ &\sum_{i} P_i^{\nu} = 1 \\ &\sum_{i} C_i = 1 \end{aligned} \qquad (A4)$$

Where $C_i$ is the average concentration of the ith element given in atomic per cent.

The APB energies can be now calculated for Cu-Zn-Al alloys in

both: the $L2_1$ parent phase [29] and the martensitic phases. The values of the pair interchange energies $W_{ij}^{(k)}$ (for $L2_1$) and $m_{ij}^{(k)}$ (for martensite) were given by Ahlers [20] and they are listed in Table A I.

In order to have an estimate of the APB energies of the materials exhibiting the TWSM, the occupation probabilities, given by (A4), were calculated for some of the alloy composition used by Sade et al [5], which are listed in Table A II. A perfectly ordered $L2_1$ type superlattice as suggested by Rapacioli and Ahlers [36] was assumed. Thus:

$P_{Cu}^{I} = P_{Cu}^{II} = 1$ ; $P_{Cu}^{IV} = P_{Al}^{III} = 0$; $P_{Al}^{IV} = 4\ C_{Al}$. With these occupation probabilities and the pair interchange energy of Table A I the various APB energies were obtained. The values are listed in Table A II.

It is to be notice that the APB with displacement vector $\vec{b}_{\beta}$ (and energy $\gamma_2^{\beta}$) in the parent phase lowers its energy ($\gamma_2^{m}$) when embedded in the martensite. Hence, the presence of this type APB (associated to the dislocations) could also contribute favoring the martensitic transformation.

## Figure Captions

Fig.1 : Stereographic projection showing tha habit plane [HP] and basal plane [BP] normals of the induced 18R variant, for tensile axis in the indicated unit triangle.

Fig.2 : Correspondence between : a) The $(\bar{1}01)_{BCC}$ plane and, b) The basal plane. The dislocation axes ($x_1$, $x_3$) and dislocation line direction (DLD) are indicated in both cases.

Fig.3 : Correspondence between : a) The $(010)_{BCC}$ plane and, b) The $(010)_{18R}$ plane. Only the first layer is drawn.

Fig.4 : Interplanar distances in the 18R martensite($b_0$, $b_1$ and $b_3$) relative to $a_0$, as a function of the tetragonality $\psi$.

Fig.5 : The dissociation of the Burgers vector $\vec{b}_0$ into $\vec{b}_0^{(1)}$ and $\vec{b}_0^{(2)}$.

Fig.6 : The orthorhombic unit cell, the atoms inside the cell are not drawn. The dislocation line direction (DLD) is indicated.

Fig.A1: The atomic sites arrangements on the different basal planes involved in a dissociated dislocation.

Fig.A2 :a) The antiphase boundary inherited from the $L2_1$ phase.
b) The antiphase boundary associated to the dissociation into Shockley partials.

Table A I

| Pair of elements | $L2_1$ | | Martensite | |
|---|---|---|---|---|
| | $W_{ij}^{(1)}$[k] | $W_{ij}^{(2)}$[k] | $m_{ij}^{(1)}$[k] | $m_{ij}^{(2)}$[k] |
| Cu-Al | 1345 | 825 | 1459 | 442 |
| Cu-Zn | 955 | 535 | 727 | 65 |
| Al-Zn | 0 | 200 | 0 | 0 |

Where $k = 1.38 \cdot 10^{-23}$ J is the Boltzman constant multiplied by 1K.

Pair interchange energies used for calculation of the APB energies.

Table A II

| Alloy | Composition, at % | | | APB energies $\left[\frac{mJ}{m^2}\right]$ | | | |
|---|---|---|---|---|---|---|---|
| | Cu | Zn | Al | $\gamma_1^m$ | $\gamma_2^m$ | $\gamma_1^m - \gamma_2^m$ | $\gamma_2^\beta$ |
| 1 | 0.682 | 0.155 | 0.163 | 30.3 | 30 | 0.3 | 46 |
| 2 | 0.630 | 0.260 | 0.110 | 34 | 15 | 19 | 23 |

Antiphase boundary energies for two Cu-Zn-Al alloy compositions.

The $\gamma_2^\beta$ was calculated, using the formula (2) of ref.[35].

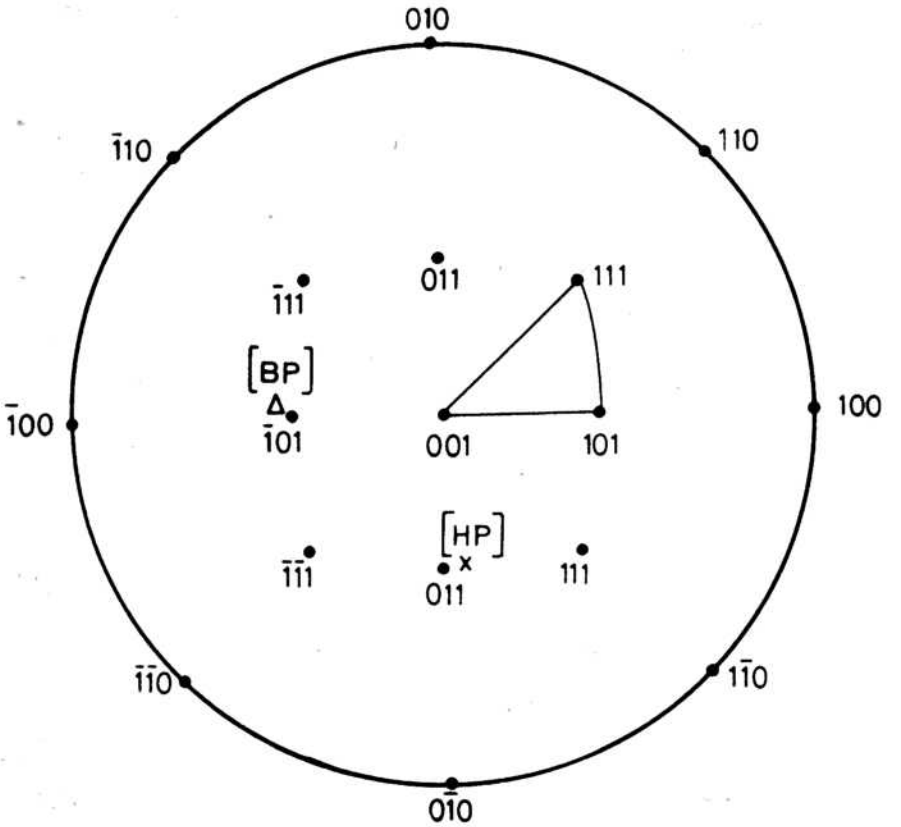

010
$\bar{1}10$
110
$\bar{1}00$
100
$\bar{1}\bar{1}0$
$1\bar{1}0$
$0\bar{1}0$
$\bar{1}11$
011
111
[BP]
$\bar{1}01$
001
101
[HP]
$\bar{1}\bar{1}1$
011
111

Figure 1

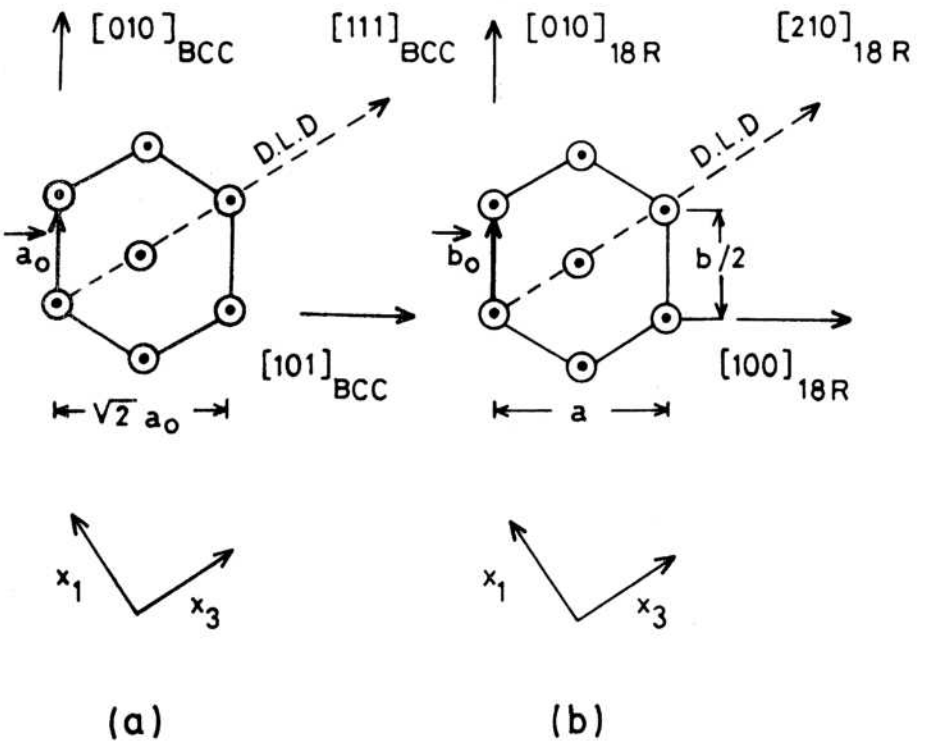



Figure 2

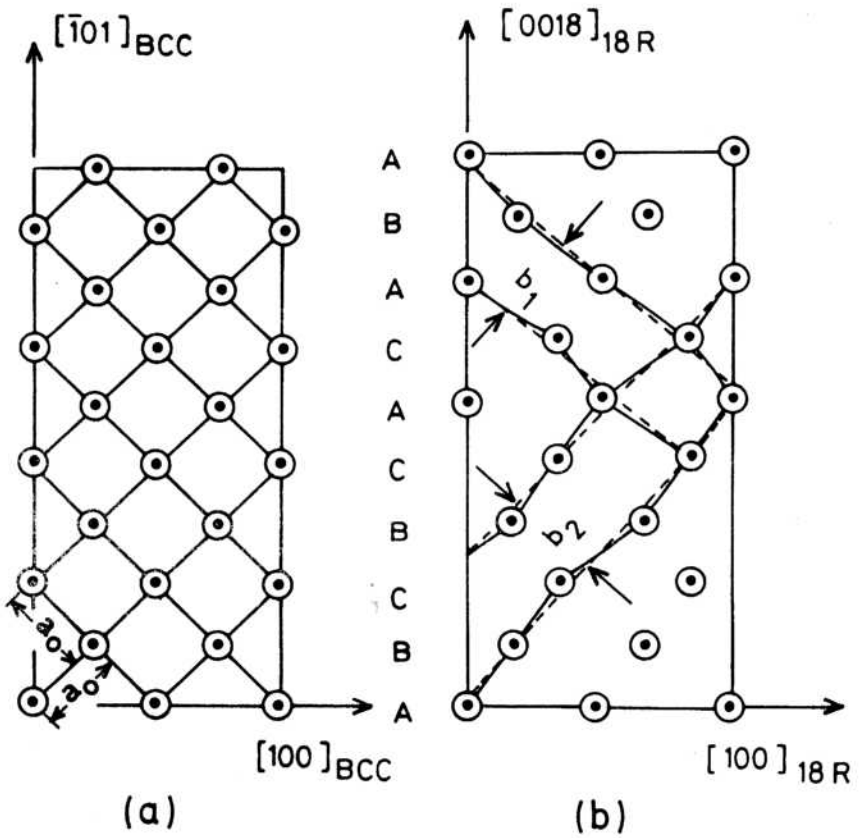



Figure 3

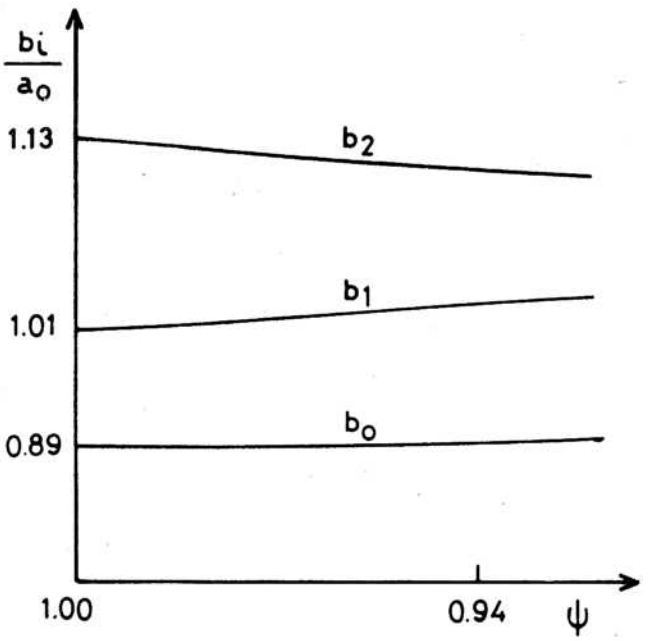



Figure 4

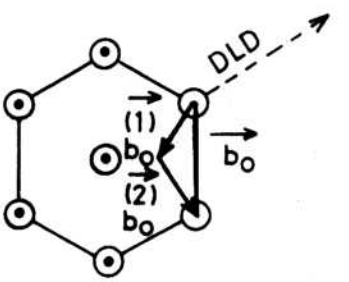
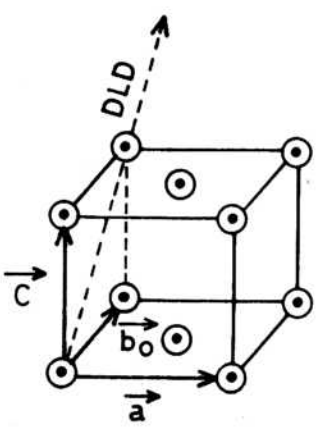



Figure 5



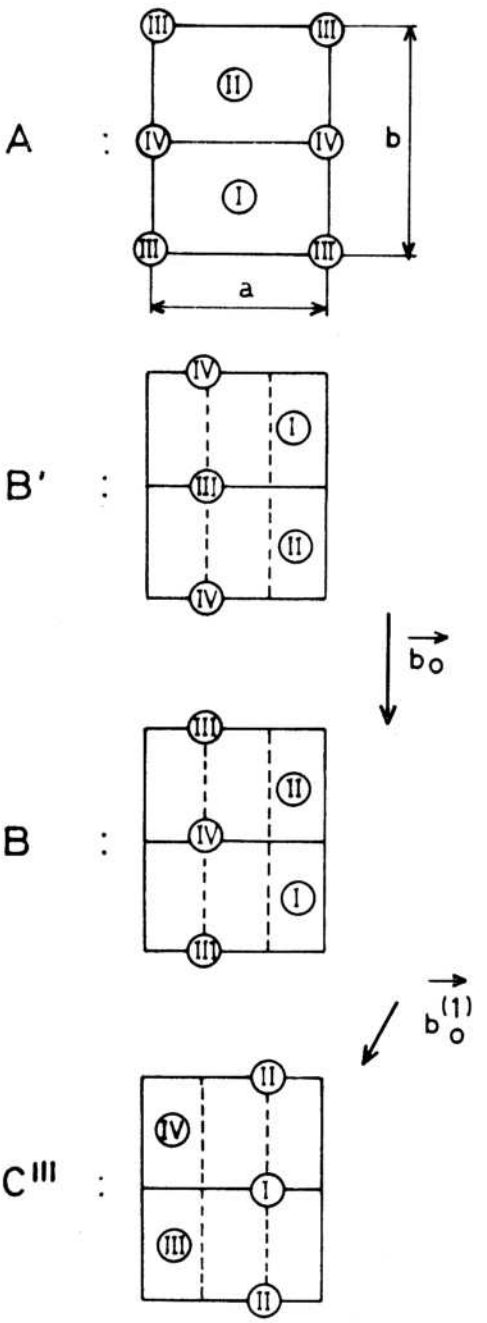

A :
III
III
II
IV
IV
b
I
III
III
a
B' :
IV
I
III
II
IV
$\vec{b}_o$
B :
III
II
IV
I
III
$\vec{b}_o^{(1)}$
$C^{III}$ :
II
IV
I
III
II

Figure 7

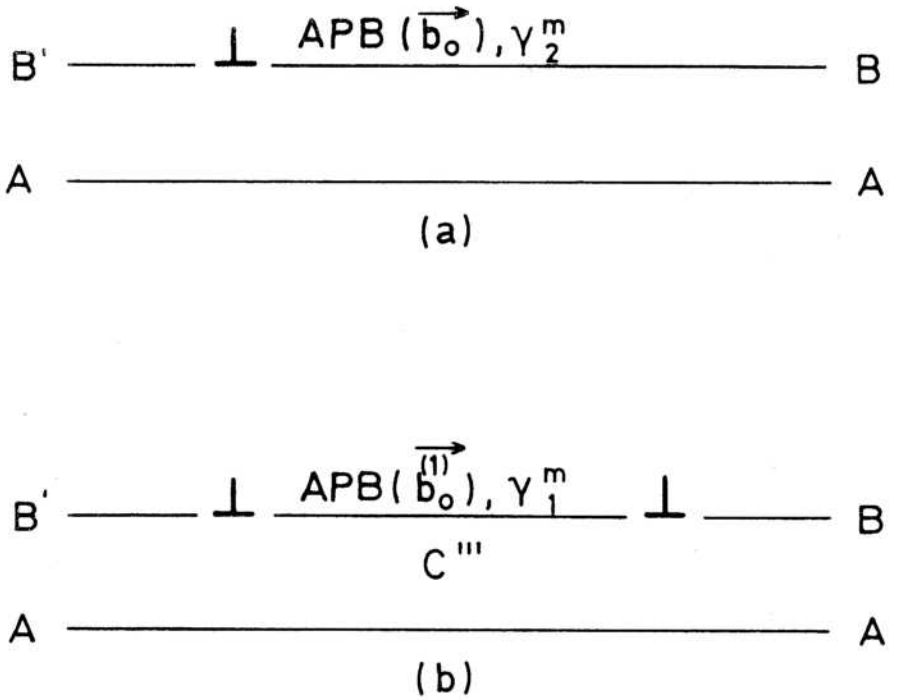



Figure 8

S.C. DE BARILOCHE, 31 MAYO 1988

SEÑOR DIRECTOR DEL CENTRO ATOMICO BARILOCHE:

De acuerdo con las normas establecidas para la publicación de trabajos (BAP 96/78), elevo para su consideración el trabajo titulado **"The relative stability of dislocations embedded in the β phase matrix and in martensite phases in Copper based alloys".**

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Vista la solicitud de publicación presentada por el Sr. Jefe de la División **Metales** del trabajo **"The relative stability of dislocations embedded in the B phase matrix and in martensite phases in Copper based alloys".**

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ARTURO LOPEZ DAVALOS
Director
Centro Atómico Bariloche

C.E.: 441.400 - 61/88

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A LA DIRECCION DEL CENTRO ATOMICO BARILOCHE:

De acuerdo a lo establecido en la Resolución de Presidencia N°1018, artículos 4° y 5°, se remite en devolución el presente expediente.

El trabajo titulado: "THE RELATIVE STABILITY OF DISLOCATIONS EMBEDDED IN THE β PHASE MATRIX AND IN MARTENSITE PHASES IN COPPER BASED ALLOYS".

producido por: F.C. Lovey, A. Hazarabedian y J.E. Garcés.

ha sido visado y se ha procedido al archivo de una copia del original en esta Comisión de Publicaciones.

Queda a cargo del organismo de origen la prosecución de los trámites del pago de gastos que origine la publicación.

Solicitamos que nos envíen 3 separatas de la publicación ya editada, a fin de que podamos ingresar este material en el catálogo general de las publicaciones de la CNEA.

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