Superlattice dislocations in the L12 ordered structure of Cu2NiZn
Wegen, G.J.L. van der; Bronsveld, P.M.; Hosson, J.Th.M. De

Published in:
Philosophical Magazine A

DOI:
10.1080/01418618308245218

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
1983

Link to publication in University of Groningen/UMCG research database

Citation for published version (APA):
https://doi.org/10.1080/01418618308245218

Copyright
Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

Take-down policy
If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): http://www.rug.nl/research/portal. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.
Superlattice dislocations in the L12 ordered structure of Cu2NiZn

By G. J. L. Van der Weg, P. M. Bronsveld and J. Th. M. De Hosson

Rijksuniversiteit Groningen, Materials Science Centre,
Department of Applied Physics, Nijenborgh 18,
9747 AG Groningen, The Netherlands

[Received 23 June 1982 and accepted 10 September 1982]

ABSTRACT

Dissociation criteria for superlattice dislocations on {111} planes have been applied to the ordering alloy Cu2NiZn. The calculations showed that the splitting of a superlattice dislocation into two superlattice Shockley partials, with Burgers vector of type 1/3a<211>, bounding a superlattice intrinsic stacking fault (SISF), is energetically less favourable than the splitting into two unit dislocations, with Burgers vector of type 1/2a<110>, separated by an antiphase boundary (APB). This theoretical prediction is in agreement with the type of superlattice dislocation observed in the electron microscope. It is rather difficult to predict a priori whether each unit dislocation is split into two Shockley partials separated by a complex stacking fault (CSF) because the cut-off parameters for the dislocation cores are not known with sufficient accuracy. The splitting into two Shockley partials could not be resolved in the electron microscope, which means that either the separation between the Shockley partials is less than about 0.7 nm, or the twofold dissociation is energetically more favourable than the fourfold one.

Values for the APB energy have been calculated from the observed separations of the unit dislocations, constituting superlattice dislocations, in Cu2NiZn single crystals quenched from several temperatures. The results are in agreement with theoretical predictions.

§ 1. INTRODUCTION

Deformation of L12 ordered alloys proceeds by the glide of superlattice dislocations. The glissile superlattice dislocation on a \(\langle111\rangle\) plane can take any one of the four configurations shown in fig. 1, depending on the relative magnitudes of the fault energies. Configuration (a) represents a superlattice dislocation dissociated into two unit dislocations with Burgers vector \(1/2a_{0}\langle110\rangle\) separated by an antiphase boundary (APB). It is well known that in f.c.c. materials a unit dislocation can split into two Shockley partials with Burgers vectors of type \(1/6a_{0}\langle211\rangle\), separated by a stacking fault. The splitting of a unit dislocation into two Shockley partials may also occur in the ordered L12 alloys, resulting in configuration (b). In this case the two Shockley partials are separated by a stacking fault and an APB, forming a so-called complex stacking fault (CSF). Configuration (b) of a superlattice dislocation has already been described in detail by Marcinkowski, Brown and Fisher (1961) and has been imaged in Cu3Au by Sastry and Ramaswami (1976). A third dissociation scheme is shown in fig. 1 (c), where a superlattice dislocation is split into two superlattice Shockley partials, having a Burgers vector of type \(1/3a_{0}\langle211\rangle\), bounding a so-called superlattice intrinsic stacking fault (SISF). Dissociation scheme (c)
is expected to occur only in ordered structures with a very large APB energy and a relatively low SISF energy (e.g. Zr3Al). Each superlattice Shockley partial might split into three ordinary Shockley partials separated by a CSF and an APB, respectively, as illustrated in fig. 1 (d). Configurations (c) and (d) have been discussed by Kear, Giamei, Silcock and Ham (1968), whereas all four dissociation schemes are compared with each other by Suzuki, Ichihara and Takeuchi (1979) and by Yamaguchi, Paidar, Pope and Vitek (1982). Yamaguchi et al. (1982) state that configuration (d) is very unlikely to occur, since the very high APB energy (at least a hundred times larger than the SISF energy), which is necessary to make configuration (d) more favourable than (a) or (b), results in a self-energy of the sixfold dissociation (d) which is larger than the self-energy of the twofold dissociation (c) in fig. 1.

Different configurations of the superlattice dislocations are expected in Cu2NiZn because two different types of ordered structure can exist in this alloy. At high temperature Cu2NiZn possesses an f.c.c. disordered structure. Below the first critical temperature for ordering, $T_{c1} = 774$ K (Van Der Wegen, De Rooy, Bronsveld, De Hosson 1981 a), a modified L12 structure exists in which the Zn atoms occupy one of the four interpenetrating simple cubic sublattices, while the Cu and Ni atoms are still randomly distributed over the remaining three sublattices. Below a second critical temperature, $T_{c2} = 598$ K, a modified L10 structure exists in which the Cu and Ni atoms each occupy their own sublattice. Since the critical temperature for ordering of the alloy Cu2NiZn is not high, it can be expected that its APB energy is not large and hence the dissociation scheme (b) is assumed to occur.

The mechanical properties of Cu2NiZn have been measured as a function of both the state of order and the deformation temperature to reveal the principal dislocation processes occurring during deformation of the alloy (Van Der Wegen,
Bronsveld and De Hosson 1981 b, 1982 a). Values for the stacking-fault energy and for the APB energy are necessary to interpret the observed mechanical behaviour. The stacking-fault energy has already been determined from observations of extended dislocation nodes in disordered Cu$_2$NiZn (Van Der Wegen, Bronsveld and De Hosson 1980). In § 2 dissociation criteria for superlattice dislocations on \{111\} planes in Cu$_2$NiZn are given, and in § 4 values for the APB energy of L1$_2$ ordered Cu$_2$NiZn, which have been determined from observations on superlattice dislocations (§ 3), are described and discussed.

§ 2. DISSOCIATION CRITERIA FOR SUPERLATTICE DISLOCATIONS ON \{111\} PLANES IN L1$_2$ ORDERED Cu$_2$NiZn

The total energy for each dissociation scheme in fig. 1 can be calculated to predict the most favourable configuration in the ordered alloy Cu$_2$NiZn. Suzuki et al. (1979) compared dissociation schemes (a) and (c) using isotropic elasticity theory, taking into account the fault energies, the self-energies and the interaction energies of the dislocations. They deduced the following criteria for the total energy of both dissociation schemes ($E_a$ and $E_c$ respectively):

\[
\frac{E_{\text{APB}}}{E_{\text{SIF}}} \leq 1.9\frac{d_s}{b} \Rightarrow E_a \leq E_c
\]

for a screw superlattice dislocation, and

\[
\frac{E_{\text{APB}}}{E_{\text{SIF}}} \leq 1.1\left(\frac{d_e}{b}\right)^{2/7} \Rightarrow E_a \leq E_c
\]

for an edge superlattice dislocation, where $d_s$ is the separation of the two unit dislocations (constituting a screw superdislocation of scheme (a)), $d_e$ is the corresponding separation in an edge superlattice dislocation and $b$ is the magnitude of the Burgers vector of the unit dislocation. Theoretical values of about 80 mJ m$^{-2}$ for $E_{\text{APB}}$, 5.1 nm for $d_s$ and 9.6 nm for $d_e$ have been calculated by De Groot, Bronsveld and De Hosson (1979). The stacking-fault energy is 32 mJ m$^{-2}$ and the lattice parameter is equal to 0.3634 nm. Substituting these values in eqns. (1) and (2) results in an energy for dissociation scheme (a) which is less than for scheme (c) for the screw as well as for the edge superlattice dislocation. Hence dissociation scheme (c) is not expected to occur in Cu$_2$NiZn.

To distinguish between the twofold dissociation (scheme (a)) and the fourfold dissociation (scheme (b)) of the superlattice dislocation, anisotropic elasticity theory is used to calculate the total energy of both configurations ($E_a$ and $E_b$, respectively):

\[
E_a = 2E_{\text{el unit}}^{\text{unit}} + E_{12} + E_1 r,
\]

and for the symmetrical configuration (b) of fig. 1:

\[
E_b = 4E_{\text{el partial}}^{\text{partial}} + 2E_{12} + 2E_{13} + E_{14} + E_{23} + E_1(r - 2r_1) + 2(\gamma + E_2)r_1,
\]

where $E_{\text{el unit}}^{\text{unit}}$ is the elastic self-energy of a unit dislocation, $E_{\text{el partial}}^{\text{partial}}$ is the elastic self-energy of a Shockley partial and $E_{ij}$ represents the interaction energy among dislocations $i$ and $j$. $E_1$ and $E_2$ are the APB energy outside and inside the stacking-fault region (as defined in fig. 2 (a)), and $\gamma$ is the stacking-fault energy. Equation (3) can be rewritten as

\[
E_a = C_\theta \left[ \ln \left( \frac{R}{\epsilon_a} \right) + \ln \left( \frac{R}{\tau} \right) \right] + E_1 r,
\]
Symmetrical and asymmetrical configurations of the four Shockley partials constituting a superlattice dislocation in the modified L1₀ structure. (a)–(c) discussed in the text.

where ε₀ is a cut-off parameter and 2R is the diameter of a crystal containing one superlattice dislocation. The separation of both unit dislocations r is obtained by minimizing $E_a$ in eqn. (5) with respect to r, which yields

$$r = C \theta/E_1.$$  

In a similar way eqn. (4) can be rewritten as

$$E_b = 2A \theta \left[ \ln \left( \frac{R}{\epsilon_b} \right) + \ln \left( \frac{R}{r-r_1} \right) \right] + 2B \theta \left[ \ln \left( \frac{R}{r_1} \right) + \ln \left( \frac{R}{r-r_1} \right) \right]$$

$$+ E_1(r-2r_1) + 2(\gamma + E_2)r_1.$$  

The separations of the Shockley partials are obtained by minimizing $E_b$ in eqn. (7) with respect to $r-r_1$ and $r_1$, leading to

$$r-r_1 = 2(A \theta + B \theta)/E_1$$  

and

$$r_1 = 2B \theta/(2\gamma + 2E_2 - E_1).$$
Superlattice dislocations in the L1_2 ordered structure of Cu_2NiZn

for a screw ($\theta = 0^\circ$) and an edge ($\theta = 90^\circ$) superlattice dislocation. For $\theta = 30^\circ$ and $\theta = 60^\circ$ superlattice dislocations minimization of $E_b$ yields

$$r - r_1 = (A_\theta + 4B_\theta)/E_1;$$

and $r_1$ is given by eqn. (9). The coefficients $A_\theta$, $B_\theta$ and $C_\theta$, which are combinations of the energy factors $K_i$ (Foreman 1955), are given in table 1 for several values of $\theta$ (the angle between the total Burgers vector and the dislocation line direction).

Table 1. Relations between $A_\theta$, $B_\theta$ and $C_\theta$, and the energy factors $K_i$, for several $\theta$ values; $b_p = \frac{1}{6}\sqrt{6}a_0$, $b = \frac{1}{2}\sqrt{2}a_0$, $a_0$ = lattice parameter.

<table>
<thead>
<tr>
<th>$\theta$</th>
<th>$A_\theta$</th>
<th>$B_\theta$</th>
<th>$C_\theta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0°</td>
<td>$\frac{b_p^2}{2\pi} \left( \frac{K_1 + K_2 + 3K_3}{12 + 6 + 4} \right)$</td>
<td>$\frac{b_p^2}{2\pi} \left( \frac{K_1 - K_2 + 3K_3}{12 - 6 + 4} \right)$</td>
<td>$\frac{b}{2\pi} (K_3)$</td>
</tr>
<tr>
<td>30°</td>
<td>$\frac{b_p^2}{2\pi} \left( \frac{3K_2 + K_3}{4 + 4} \right)$</td>
<td>$\frac{b_p^2}{2\pi} (K_2)$</td>
<td>$\frac{b}{2\pi} \left( \frac{K_2 + 3K_3}{4 + 4} \right)$</td>
</tr>
<tr>
<td>60°</td>
<td>$\frac{b_p^2}{2\pi} \left( \frac{K_1 + K_2 + 3K_3}{12 + 6 + 4} \right)$</td>
<td>$\frac{b_p^2}{2\pi} \left( \frac{K_1 + K_2}{6 + 3} \right)$</td>
<td>$\frac{b}{2\pi} \left( \frac{K_1 + K_2 + K_3}{4 + 2 + 4} \right)$</td>
</tr>
<tr>
<td>90°</td>
<td>$\frac{b_p^2}{2\pi} \left( \frac{3K_2 + K_3}{4 + 4} \right)$</td>
<td>$\frac{b_p^2}{2\pi} \left( \frac{3K_2 - K_3}{4 - 4} \right)$</td>
<td>$\frac{b}{2\pi} (K_2)$</td>
</tr>
</tbody>
</table>

The energy factors $K_i$ can be expressed in terms of the elastic constants, as described by Steeds (1973). Appropriate values for the elastic constants of Cu_2NiZn have been measured by ultrasonic methods. For the outer cut-off parameter $R$ in eqns. (5) and (7), the average separation between the superlattice dislocations divided by two can be substituted. Cu_2NiZn specimens deformed up to 7% in tension contain superlattice dislocations with an average separation ranging from 0.4 to 0.1 µm. Therefore, $R$ was taken to be 0.1 µm in the calculations. The core energy of dislocations can be included in eqns. (5) and (7) by taking suitable values for the cut-off parameters $\epsilon_a$ and $\epsilon_b$. Brown (1964) suggests that the value of the cut-off parameter should equal the Burgers vector of the dislocation, i.e. $\epsilon_a = b$ and $\epsilon_b = 2b_p$, where $b$ and $b_p$ are the Burgers vectors of a unit dislocation and a Shockley partial. Using values for the APB energies between 50 and 100 mJ m^-2 and a stacking-fault energy of 32 mJ m^-2, $E_a$ and $E_b$ have been calculated for different combinations of the parameters, as shown in table 2 for a screw and an edge superlattice dislocation. From this table one would conclude that the twofold dissociation of a screw superlattice dislocation requires less energy than the fourfold dissociation, whereas the opposite is true for an edge superlattice dislocation. Further, to investigate the influence of $R$, a value of 1.0 µm was also considered. However, from table 2 it can be concluded that the dissociation scheme to be expected is not sensitive to the exact values of the APB energies and the parameter $R$. Nevertheless, it is very sensitive to the
Table 2. Total energy of a superlattice dislocation with the twofold dissociation $E_a$ and the fourfold dissociation $E_b$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$R$ (µm)</th>
<th>$E_a = E_b$ (J m⁻²)</th>
<th>$E_a$ (GJ m⁻¹)</th>
<th>$E_b$ (GJ m⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Screw</td>
<td>0.1</td>
<td>0.05</td>
<td>4.62</td>
<td>4.82</td>
</tr>
<tr>
<td></td>
<td>0.1</td>
<td>0.10</td>
<td>4.97</td>
<td>5.20</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>0.05</td>
<td>6.92</td>
<td>7.11</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>0.10</td>
<td>7.27</td>
<td>7.50</td>
</tr>
</tbody>
</table>

values chosen for the cut-off parameters $\epsilon_a$ and $\epsilon_b$. Taking $\epsilon_a = \epsilon_b \approx b_p$, the fourfold dissociation is energetically more favourable than the twofold dissociation for a screw as well as for an edge superlattice dislocation. The same result is obtained by taking $\epsilon_a = \epsilon_b = 0.116$ nm for a screw and $\epsilon_a = \epsilon_b = 0.128$ nm for an edge superlattice dislocation. These values for the cut-off parameters of unit dislocations have been obtained from atomistic calculations. Hence it is rather difficult to predict a priori which dissociation scheme, (a) or (b), will be appropriate for a superlattice dislocation in Cu₃NiZn.

In the modified L₁₀ structure, one symmetrical (fig. 2 (a)) and two asymmetrical configurations (figs. 2 (b) and 2 (c)) of the superlattice dislocations are possible. For the modified L₁₂ structure, $E_1$ is identical to $E_2$, and hence only one configuration for the superlattice dislocations is possible. The separations of the four Shockley partials in the symmetrical configuration are given by eqns. (8), (9) and (10). For the asymmetrical configurations of the modified L₁₀ structure a relation similar to eqn. (7) can be deduced, resulting in similar formulae for the separations of the Shockley partials as a function of the fault energies. A superlattice dislocation will extend over several APB domains. Each of these APB domains can have its 'tetragonal' axis of the modified L₁₀ structure (Vrijen, Bronsveld, Van Der Veen and Radelaar 1976) in any cubic direction of the f.c.c. lattice. Therefore, symmetrical as well as asymmetrical parts will be present along the superlattice dislocation line. Since the length of each part (i.e. the APB domain size) is of the same order of magnitude as the separation between the unit dislocations, the configuration of the superlattice dislocation imaged in the modified L₁₀ structure will appear as the average of the three configurations illustrated in fig. 2. Therefore, only superlattice dislocations in the modified L₁₂ structure have been analysed experimentally in this work.

§ 3. Experimental procedure

Single crystals of Cu₃NiZn were grown by the strain anneal method, which produced small but very homogeneous crystals. The various treatments of the crystals are listed in table 3, together with their compositions as determined by atomic absorption spectroscopy. The single crystals were deformed in such a direction that one slip system is activated more than any other. Thin slices parallel to the primary slip plane were cut by spark erosion, and subsequently thinned electrochemically to a thickness of about 150 µm. The crystals, which
Table 3. Properties and data of the single crystals.

<table>
<thead>
<tr>
<th>$T_{\text{anneal}}$ (K)</th>
<th>623</th>
<th>723</th>
<th>723, 763</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_{\text{anneal}}$ (hour)</td>
<td>164</td>
<td>115</td>
<td>72/2</td>
</tr>
<tr>
<td>Deformation axis</td>
<td>[213]</td>
<td>[314]</td>
<td>[154]</td>
</tr>
<tr>
<td>Schmid factor</td>
<td>0·46</td>
<td>0·47</td>
<td>0·47</td>
</tr>
<tr>
<td>Shear strain (%)</td>
<td>13</td>
<td>7</td>
<td>9</td>
</tr>
<tr>
<td>Composition (at.%)</td>
<td>Cu</td>
<td>Ni</td>
<td>Zn</td>
</tr>
<tr>
<td></td>
<td>50·1</td>
<td>49·9</td>
<td>47·5</td>
</tr>
<tr>
<td></td>
<td>25·4</td>
<td>24·6</td>
<td>27·0</td>
</tr>
<tr>
<td></td>
<td>24·5</td>
<td>25·5</td>
<td>25·5</td>
</tr>
</tbody>
</table>

were annealed for 164 hours at 623 K and subsequently deformed to a resolved shear strain of 0·13, received an additional heat treatment at 623 K for 75 min to reveal the extent of reduction in internal stress and the extent to which the discontinuous shear APB transforms into the diffuse APB under thermal equilibrium, as described by Brown (1959). The disc-type specimens were prepared in the same way as described by Van Der Wegen et al. (1980). The thin foils were examined in a JEOL 200 CX electron microscope operating at 200 kV and in a Philips EM 300 electron microscope operating at 100 kV.

The superlattice dislocations were imaged in dark field using the weak-beam technique (Cockayne 1972). Each unit dislocation constituting a superlattice dislocation or a superlattice dislocation dipole which has been identified appeared to be of type $1/2a_0\langle110\rangle$. The slip plane was identified by observing the dislocation separation upon tilting the foil. The Burgers vector of a dislocation can be determined using the criterion that a dislocation is invisible if $g \cdot b = 0$ while $g \cdot (b \land u)$ is sufficiently small ($\ll 0·5$; Cockayne 1972), where $g$ is the diffraction vector, $b$ the Burgers vector and $u$ the unit vector along the dislocation line. Ambiguities, which may arise from using the invisibility criterion, can be solved by making use of the image characteristics, especially their asymmetry (Marukawa 1979).

We have applied $g=2\bar{2}0$, with $b=1/2a_0[110]$, giving $g \cdot b = 2$ for each dislocation. At first sight it would seem to be an advantage to use $g=20\bar{2}$, so that $g \cdot b = 1$ for each dislocation. However, for $g \cdot b = 2$ the intensity of dislocation contrast is larger than when using $g \cdot b = 1$. In the former case a higher value of $s_g$ can be used for imaging the dislocation.

The image of a dislocation will be narrower, and hence will reveal more detail, the larger the deviation from the Bragg position (characterized by $s_g$). However, the larger the value of $s_g$, the smaller the intensity of the image, and the longer the exposure time necessary to image the dislocation on an electron micrograph. Long exposure times require a high stability, mechanically as well as electrically, of the electron microscope. Hence, there is an optimum in operating the electron microscope to reveal as much detail as possible, using the weak-beam technique.

Figure 3 shows an example of a weak-beam image of a superlattice dislocation in $\text{Cu}_2\text{NiZn}$. The observed separation of the imaged dislocation lines
Weak-beam image of a superlattice dislocation in a Cu$_3$NiZn single crystal annealed at 623 K for 164 hours, deformed in compression to a shear strain of 0.13; projection plane = slip plane = (111), $\mathbf{b} = 1/2a_0[011]$, $\mathbf{g} = 022$, $s_g = +0.17$ nm$^{-1}$.

Computed intensity profile of an edge-type superlattice dislocation in Cu$_3$NiZn. Separation of the cores = 6 nm. $I_0$ = primary beam intensity. $I_B$ = background intensity.

have been obtained from a microdensitometer scan perpendicular to the dislocation line direction. Such intensity profiles of superlattice dislocation images have been compared with intensity profiles computed from two-beam dynamical theory using the column approximation (Howie and Basinski 1968, Amelinckx, Gevers and Van Landuyt 1978). The displacements of the atoms.
caused by the presence of the superlattice dislocation, have been calculated from anisotropic linear elasticity theory. An example of such a computed intensity profile for an edge-type superlattice dislocation in Cu$_2$NiZn is shown in fig. 4. The actual separations of the dislocation cores have been calculated from the observed images of superlattice dislocations by performing these computer simulations.

The image peak separations ($\Delta_{\text{obs}}$) are considerably greater than $\Delta$ (see fig. 4). $\Delta_{\text{obs}}$ depends, for a given $\Delta$, on dislocation depth and foil thickness, as well as on $s_g$. Since not too small a value of $s_g$ was taken, and the thickness of the foil was larger than 20 nm, $\Delta$ could be obtained from $\Delta_{\text{obs}}$ with an accuracy of $\pm 0.5-1$ nm (Cockayne 1972). However, it should be emphasized that this value is smaller than the actual scatter in the imaged separations because of inhomogeneities and internal stress fields.

§ 4. RESULTS AND DISCUSSION

Deformation of the single crystals due to shear strains (see table 3) results in dislocation densities of about $4 \times 10^9$ cm$^{-2}$. The majority of dislocations (roughly 80%) appear as superlattice dislocation dipoles. These dipoles have been identified by using the contrast characteristics as described by Bell, Roser and Thomas (1964). Figure 5 shows a weak-beam image of such a superlattice dislocation dipole (at A), together with two superlattice dislocations. Hence, only a small fraction of the available dislocations appear as isolated superlattice dislocations, which can be used to obtain the APB energy. Many of these isolated superlattice dislocations have been imaged using the weak-beam technique. The fourfold dissociation as illustrated in fig. 1 (b) has not been observed in Cu$_2$NiZn (see, for example, figs. 3 and 5). This means that either the separation between the Shockley partials is less than about 0.7 nm, or that the twofold dissociation is energetically more favourable than the fourfold one.

Fig. 5

Weak-beam image of a superlattice dislocation dipole (at A) and two superlattice dislocations in a Cu$_2$NiZn single crystal annealed at 623 K for 164 hours, deformed 13% in compression and aged at 623 K for 75 min, projection plane = slip plane = (111), $b = 1/2a_0[0\bar{1}1]$, $g = 0\bar{2}2$, $s_g = +0.23$ nm$^{-1}$. 
Fig. 6

Separation of unit dislocations as a function of their character $\theta$ in a Cu$_2$NiZn single crystal, annealed for 164 hours at 623 K and subsequently deformed to a shear strain of 0.13. 

(a) Not aged (b) aged for 75 min at 623 K. The full curves are calculated from anisotropic linear elasticity theory.

The separation of the unit dislocations as a function of the character of the dislocations is depicted in fig. 6 (a) for the Cu$_2$NiZn alloy, which has been annealed for 164 hours at 623 K to obtain the modified L1$_2$ structure with a long-range order parameter $S''$ close to unity (Van Der Wegen et al. 1981 a). The full curves in fig. 6 are computed from anisotropic elasticity theory. An APB energy of $97 \pm 17$ mJ m$^{-2}$ can be obtained from fig. 6 (a) for the unaged sample. Similar results for the aged sample are illustrated in fig. 6 (b), leading to an APB energy of $88 \pm 29$ mJ m$^{-2}$. A value for the APB energy for Cu$_2$NiZn has been calculated using effective interatomic potentials of the transition metals which are computed within the framework of the pseudopotential approximation, based on a transition metal potential of the Heine–Abarenkov–Shaw type (De Groot et al. 1979). The experimentally determined APB value of 97 mJ m$^{-2}$ agrees very well with the $ab$ initio calculated value of 94 mJ m$^{-2}$. 
Separation of unit dislocations as a function of their character in a Cu$_2$NiZn single crystal. (a) Annealed at 723 K for 115 hours and subsequently deformed to a shear strain of 0.07; (b) annealed at 723 K for 72 hours and at 763 K for 2 hours and subsequently deformed to a shear strain of 0.09. The full curves are calculated from anisotropic linear elasticity theory.

Values of the ordering energies $W_{ij} = V_{ij} - \frac{1}{2}(V_{ii} + V_{jj})$, where $V_{ij}$ represents the pair interaction energy between atoms $i$ and $j$, have been obtained for Cu$_2$NiZn from calculated cohesive energies (De Hosson 1981). From these ordering energies a value for the APB energy of 85 mJ m$^{-2}$ can be computed, which is also in good agreement with the experimental value. Ageing the sample after deformation results in a slight decrease in the APB energy and a substantial increase in the scatter of the observed separations. These features can be explained by the continuous transformation of the discontinuous shear APB into the diffuse APB under thermal equilibrium, as described by Brown (1959).

The separation of the unit dislocations as a function of their character is shown in fig. 7 (a) for the Cu$_2$NiZn alloy, which has been annealed at 723 K for 115 hours to obtain an intermediate degree of long-range order. From this
figure an APB energy of $62 \pm 6 \text{ mJ m}^{-2}$ can be deduced using anisotropic linear elasticity. Similar results for a Cu$_2$NiZn single crystal which has been annealed at 723 K for 72 hours, and subsequently for 2 hours at 763 K, are depicted in fig. 7 (b), leading to an APB energy of $43 \pm 7 \text{ mJ m}^{-2}$. The latter single crystal was annealed at 723 K for a long period to grow large APB domains (Van Der Wegen et al. 1981 b) and then at 763 K for only 2 hours to obtain an approximately equilibrium degree of long-range order and to preserve a swirl APB domain structure. Annealing at 763 K for a longer period results in the formation of cube-shaped APB domains (Van Der Wegen et al. 1981 b), indicating a change in ordering energies. In that case the change in APB energy cannot be ascribed solely to a change in long-range order. To translate an alteration in APB energy as a function of the quench temperature into a change in long-range order, one has to keep the same domain morphology. For the modified L1$_2$ structure, the APB energy is related to the degree of long-range order $S''$ by

$$E_{\text{APB}} = (S'')^2 E_{\text{APB}}^1,$$  \hspace{1cm} (11)

where $E_{\text{APB}}^1$ is the APB energy for the modified L1$_2$ structure (i.e. no Cu–Ni ordering) with $S'' = 1$ (i.e. Zn perfectly ordered). Assuming that the long-range order parameter $S''$ is close to unity at 623 K, one can calculate the corresponding values at 723 and 763 K from eqn. (11) as $0.80 \pm 0.11$ and $0.67 \pm 0.11$, respectively. These long-range order parameters are given in table 4, together with the results of neutron diffraction experiments on single crystals of Cu$_2$NiZn (Van Der Wegen, Helmholdt, Bronsveld and De Hosson 1982 b). The values of the long-range order parameter obtained from the separations of the partials in the superlattice dislocations in Cu$_2$NiZn are in good agreement with data from other L1$_2$ structures.

<table>
<thead>
<tr>
<th>Table 4. Values for the long-range order parameter $S''$ of Cu$_2$NiZn.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$ (K)</td>
</tr>
<tr>
<td>--------</td>
</tr>
<tr>
<td>623</td>
</tr>
<tr>
<td>723</td>
</tr>
<tr>
<td>763</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 5. Calculated values of $r_1$ (in nm) using experimental values for the APB and stacking-fault energies (in mJ m$^{-2}$).</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$ (K)</td>
</tr>
<tr>
<td>--------</td>
</tr>
<tr>
<td>623</td>
</tr>
<tr>
<td>723</td>
</tr>
<tr>
<td>763</td>
</tr>
</tbody>
</table>
If the unit dislocations of a superlattice dislocation are split into two Shockley partials separated by a CSF (see fig. 1 (b)), then their separation can be calculated from eqn. (9), assuming that the CSF energy is the sum of the APB energy and the stacking-fault energy. The results are given in table 5.

For the screw ($\theta = 0^\circ$) superlattice dislocations, this separation is too small to be resolved by the weak-beam technique. However, for the other types, especially the edge ($\theta = 90^\circ$) superlattice dislocations, the splitting into two Shockley partials could be resolved. Hence, either the twofold dissociation is energetically more favourable than the fourfold dissociation, or the CSF energy is larger than the sum of the APB energy and the stacking-fault energy. The latter possibility is supported by atomistic calculations (J. Th. M. De Hosson and V. Vitek 1981, private communication), indicating that the sum of the APB energy and the SISF energy is smaller than the calculated CSF energy.

Fig. 8

Dislocation microstructure in polycrystalline Cu$_2$NiZn annealed at 593 K for 23 hours and deformed 3% in tension. Bright-field strong-beam image; projection plane = (110).

Superlattice dislocations in Cu$_2$NiZn have already been observed by Kurdyumov and Chupyatova (1967). They report separations between the unit dislocations ranging from 15·0 to 17·0 nm. These observed separations are much larger because the strong-beam imaging technique has been applied and because no distinction between superlattice dislocations and superlattice dislocation dipoles has been made. The majority of the imaged dislocations are probably of the latter type, judging from their size. The reported preference for screw dislocations is supported by the present work, as can be seen, for example, in fig. 8. However, evidence for {100} cross-slip of these screw superlattice dislocations has not been found, in agreement with the observed mechanical behaviour of Cu$_2$NiZn (Van Der Wegen et al. 1982 a).
§ 5. Conclusions

Dislocation configurations have been described in the ordered alloy Cu$_2$NiZn. From the observed distances between the dislocations, values of the APB energy have been calculated for different quench temperatures. The experimentally determined APB energy for the fully ordered L1$_2$ structure of Cu$_2$NiZn is in good agreement with the theoretical predictions of De Groot et al. (1979). The long-range order parameter $S^*$ computed from the experimental APB values behaves similarly to those reported for other L1$_2$ structures. The transformation of a discontinuous shear APB into a diffuse APB under thermal equilibrium, as suggested by Brown (1959), is confirmed to occur also in Cu$_2$NiZn. The twofold dissociation of a superlattice dislocation in Cu$_2$NiZn is more likely than the fourfold dissociation, provided the CSF energy roughly equals the sum of the APB energy and the stacking-fault energy.

Acknowledgments

Particular thanks are due to Mr. H. J. Bron, Mr. J. Harkema and Mr. U. B. Nieborg for technical assistance. The work reported was carried out as part of a project on ordering in ternary alloys of the Foundation for Fundamental Research on Matter (F.O.M.-Mt VI-B) at Utrecht and was also made possible by financial support from the Netherlands Organization for the Advancement of Pure Research (Z.W.O.) at The Hague. The neutron diffraction experiments were carried out by Dr. R. Helmholdt by means of the four-circle neutron diffractometer at the HFR reactor at Petten, and were partially supported by the Netherlands Foundation for Chemical Research (S.O.N.).

References

Brown, N., 1959, Phil. Mag., 4, 693.