Dissociation of $1/2 < 112 >$ perfect dislocations and nature of slip dislocations in ordered Ni₃V

G. Vanderschaeve, B. Escaig

► To cite this version:

G. Vanderschaeve, B. Escaig. Dissociation of $1/2 < 112 >$ perfect dislocations and nature of slip dislocations in ordered Ni₃V. Journal de Physique Lettres, 1978, 39 (6), pp.74-77. 10.1051/jphyslet:0197800390607400 . jpa-00231446

HAL Id: jpa-00231446

<https://hal.science/jpa-00231446>

Submitted on 1 Jan 1978

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Classification
Physics Abstracts
61.70J

DISSOCIATION OF $\frac{1}{2} \langle 112 \rangle$ PERFECT DISLOCATIONS AND NATURE OF SLIP DISLOCATIONS IN ORDERED Ni_3V

G. VANDERSCHAEVE and B. ESCAIG

Laboratoire de Structure et Propriétés de l'Etat Solide (*)
Université des Sciences et Techniques de Lille, B.P. 36, 59650 Villeneuve d'Ascq, France

(Reçu le 27 décembre 1977, accepté le 7 février 1978)

Résumé. — Les observations en microscopie électronique dans l'alliage ordonné Ni_3V montrent que les dislocations parfaites de vecteur de Burgers $\frac{1}{2}[\bar{1}\bar{1}2]$ sont dissociées en trois partielles $\frac{1}{6}[\bar{1}\bar{1}2]$ limitant une paire de fautes d'empilement intrinsèque-extrinsèque dont on a pu déduire une évaluation des énergies de fautes d'empilement (ces fautes sont celles qui n'introduisent pas de mauvaises liaisons entre premiers voisins). Sous l'effet d'une contrainte, ces paires ont tendance à émettre des partielles $\frac{1}{6}[\bar{1}\bar{1}2]$ qui propagent la déformation dans cette structure.

Abstract. — Electron microscopy observations show that in the ordered alloy Ni_3V , perfect $\frac{1}{2}[\bar{1}\bar{1}2]$ dislocations are dissociated into three $\frac{1}{6}[\bar{1}\bar{1}2]$ partial dislocations bounding an intrinsic-extrinsic pure stacking fault pair (i.e. without any wrong first neighbour bonds); from this an evaluation of stacking fault energies can be deduced. Furthermore, such pairs should extend under stress and produce $\frac{1}{6}[\bar{1}\bar{1}2]$ partials as the slip dislocations in this crystal structure.

1. Introduction. — DO_{22} ordered Ni_3V is an example of a long period ordered alloy with $M = 1$, i.e. with periodic antiphase boundaries every $M(001)$ planes. Due to the periodic shift, the unit cell in the $\{111\}$ glide plane ⁽¹⁾ is rectangular (Fig. 1) and the shortest lattice translations in this plane are $\frac{1}{2}[\bar{1}\bar{1}2]$ and $[\bar{1}\bar{1}0]$, or, using the Thompson notation $3\text{C}\delta$ and 2AB respectively.

This paper reports the particular configuration of $3\text{C}\delta$ dislocations, the lowest energy perfect dislocations in this lattice, as observed by electron microscopy. They are shown to be dissociated into three parallel $\text{C}\delta$ partials, bounding an intrinsic-extrinsic stacking fault pair; such faults do not change the first neighbour bond lengths between adjacent layers. An evaluation of stacking fault energies is deduced, in the ratio $\gamma_E/\gamma_I \simeq 2$. Furthermore, such pairs should extend under stress, and produce $\text{C}\delta$ partials as the slip dislocations in this crystal structure.

2. Stacking faults and partial dislocations. — Due to the long period along one cube axis, the stacking sequence involves six $\{111\}$ close-packed planes :

$$\dots A_1 B_1 C_1 A_2 B_2 C_2 A_1 \dots$$

(*) Laboratoire associé au C.N.R.S. n° 234.

⁽¹⁾ For the sake of simplicity, we use throughout this paper disordered face-centred cubic notations for indexing crystallographic planes and directions.

FIG. 1a. — Structure of ordered Ni_3V with long period along $[001]$.

FIG. 1b. — (111) close packed plane.

As previously reported [1], a $\text{C}\delta$ dislocation in a domain with long period along $[001]$ is leading a stacking fault (without any wrong first neighbour bonds), while $\text{A}\delta$ and $\text{B}\delta$ are limiting a *complex fault* (stacking plus order fault). Therefore it is expected that the perfect 3 $\text{C}\delta$ dislocation would dissociate into two partials separated by an intrinsic stacking fault according to the reaction :

with the new stacking sequence

introducing no wrong first neighbour bonds between adjacent layers. Formally, a more stable configuration is obtained by developing a $\text{C}\delta$ loop in the adjacent plane (Fig. 2a). For the long range elastic field of the $(2 \text{C}\delta, \delta\text{C})$ doublet is equivalent to the one of a single $\text{C}\delta$ dislocation at a distance of a few inter-atomic spacings and beyond, so that a $\text{C}\delta$ triplet is produced, introducing an intrinsic-extrinsic fault pair.

FIG. 2a. — Structure of the intrinsic-extrinsic stacking fault pair.

3 $\text{C}\delta$ dislocations are probably formed during order annealing by recombination of two CA and CB dislocations gliding on the same, or neighbouring, planes. Although they repel each other elastically, the reaction is still favourable because it reduces the width of the high energy order fault they leave behind, so that 3 $\text{C}\delta$ dislocations should be at least as numerous as 2 AB pairs. Figure 2b sketches the product $(2 \text{C}\delta, \delta\text{C})$ obtained when CA and CB dislocations meet on the same plane. When they join on two adjacent planes, it is easy to see (Fig. 2c) that only one atomic layer, C_1' , is shifted in a wrong position relative to the layer above (A_2), and below

FIG. 2b. — Two ways of recombining CA and CB dislocations on the same glide plane to obtain 3 $\text{C}\delta$ dislocation (/ / / / stacking fault; = = = = order fault; x x x x complex fault).

FIG. 2c. — Configuration of CA and CB dislocations gliding on two adjacent planes. Nucleating and moving a CB/BC dipole sweeps out the double order fault.

FIG. 2d. — Detailed geometrical configuration produced by the cross-slip of CB on (a) plane, $2 \text{C}\delta = \delta\text{A} + \text{CB}$ and $\text{CB} + \delta\text{C} = \delta\text{B}$.

FIG. 2e. — Final relaxed configuration when the partial lines are parallel to the CB (or CA) direction. Notice the complex fault between δA and δB partial.

(B_1). This configuration is probably never observed for the double order faulted interface can be swept out simply by moving a CB/BC dipole (nucleated during order annealing) all along it, resulting in the relaxed configuration of figure 2a since : $\text{CB} + \delta\text{A} = 2 \text{C}\delta$, and $\text{BC} + \delta\text{B} = \delta\text{C}$. Finally, no pairing is obtained when CA and CB dislocations slip more than one atomic layer apart, in the simple approximation of the nearest neighbour interaction between Ni and V atoms.

Moreover, further stabilization of the partial core $(2 \text{C}\delta, \delta\text{C})$, figure 2a, is expected when the partial line is parallel to CB (or CA) directions. For the CB part can then be exchanged by cross-slipping on

an (a) plane, figure 2d, from the 2 $C\delta$ group of partials ($2 C\delta \rightarrow \delta A + CB$, with δA and CB perpendicular, thus only weakly interacting, see figure 2b) to the attractive δC partial ($\delta C + CB = \delta B$). Detailed inspection of atomic order shows, figure 2d, that if a C_1 layer is turned into a C'_1 layer by moving CB to the right on a (d) plane, then moving CB on an (a) plane at an acute angle turns back the C'_1 layer to the C_1 one. Thus, the configuration of figure 2e results, with partials parallel to the CB (or CA) directions. This is not to be confused with configuration 2c, where the layer C'_1 is left behind, shifted in a wrong position. For example, if partials δA and δB were assumed to be pushed under a stress to the right in figure 2e, then a configuration like that in figure 2d would follow, trailing a wrong atomic layer like C'_1 . Since such double order faults are expected to be of a higher energy than stacking faults, an extension of the latter, by the stress is much more plausible, keeping the ($\delta A, \delta B$) doublet blocked straight along the CB (or CA) direction while the δC partials carry out the plastic slip further on. We show below electron micrographs which fully support this mechanism.

3. Electron microscopy observations. — Figure 3 is a typical example of configurations observed in the undeformed material. It shows that 3 $C\delta$ dislocations are dissociated into three $C\delta$ partials; all the examples are found to be screw in character, which will be

FIG. 3. — Intrinsic-extrinsic stacking fault pair as observed by electron microscopy in undeformed material (see text).

discussed below. The probable configuration is therefore the one shown in figure 2a.

The intrinsic-extrinsic nature of stacking fault pairs is established from micrographs 3a and 3b. On figure 3a notice that the nature of outer fringes of the two ribbons is opposite; examination of the dark field picture in figure 3b shows the nature of the narrower ribbon to be extrinsic, according to the method of Gevers *et al.* [2]. Figure 3c shows on the diffraction pattern that $[001]^*$ is not extinguished; therefore the long period has to be along $[001]$ (see reference [1c]). All the dislocation images vanish for $g = [2\bar{2}0]^*$ (Fig. 3d) and $g = [\bar{1}31]^*$ (Fig. 3e), so that the Burgers vector of the partials is parallel to $[\bar{1}12] = C\delta$. Finally, figure 3f shows an example of dark field picture, taken with $g = [\bar{1}13]^*$ ($g \cdot b = +1$ for each partial) used to determine an order of magnitude of stacking fault energies from the weak beam images.

Notice that we never observe intrinsic-extrinsic pairs bounded by either $A\delta$ or $B\delta$ dislocations in this $[001]$ domain. This is strong support for the mechanism invoked here, i.e. the dissociation of dislocations involves only a *pure* stacking fault, without any wrong first neighbour bonds. On the other hand, it has been proved elsewhere [1c] that the propagation of these dislocations controls deformation in the material.

Similar intrinsic-extrinsic pairs are found in the deformed material, and are shown in figure 4. The narrower fault ribbon here is also extrinsic, as determined by the dark field picture (Fig. 4a). Notice the straight character of the trailing partial, parallel to direction $[10\bar{1}] = BC$, at the edge of the extrinsic fault, in agreement with the model represented in figure 2e for the ($\delta A, \delta B$) partial. The S shape of the leading $C\delta$ partial might be due to the backward motion from the intrinsic fault trailing behind, when unloading; some pinning process having probably occurred during it.

FIG. 4. — Intrinsic-extrinsic stacking fault pair in deformed material. The narrower fault ribbon is the extrinsic one. Notice that the trailing partial bounding this fault is parallel to $[10\bar{1}]$.

4. Discussion. — As pointed out above, all the observed 3 $C\delta$ dislocations are found to be screw in the undeformed material. We propose that this

is due to a minimum in total elastic energy of the CA and CB dislocations, recombining during annealing to give a 3 C δ dislocation. This can be readily proved

by considering the elastic energy of two parallel dislocations gliding in the same plane (for example, see ref. [3]) :

$$E = A \{ (\mathbf{b}_1 \cdot \mathbf{t})^2 + (\mathbf{b}_2 \cdot \mathbf{t})^2 + (1 - \nu)^{-1} [(\mathbf{b}_1 \times \mathbf{t})^2 + (\mathbf{b}_2 \times \mathbf{t})^2] \} + \\ + B \{ (\mathbf{b}_1 \cdot \mathbf{t})(\mathbf{b}_2 \cdot \mathbf{t}) + (1 - \nu)^{-1} (\mathbf{b}_1 \times \mathbf{t})(\mathbf{b}_2 \times \mathbf{t}) \}.$$

The first term is the self energy of the two dislocations, whereas the second term is the interaction energy; $\mathbf{b}_1$ and $\mathbf{b}_2$ are the Burgers vectors of the two interacting dislocations, $\mathbf{t}$ is the unit line vector, ν the Poisson modulus and A and B are well known positive constants. With $\theta = (\mathbf{t}, \text{C}\delta)$,

$$E(\theta) = \frac{Ab^2}{2(1 - \nu)} (4 - \nu - 2\nu \cos^2 \theta) + \\ + \frac{Bb^2}{4(1 - \nu)} (2 + \nu - 4\nu \cos^2 \theta)$$

which is a minimum for a screw dislocation ($\theta = 0$ or $\theta = \pi$) of the 3 C δ type.

On the other hand, the measurement of widths in intrinsic-extrinsic pairs on weak beam images gives estimates of the stacking fault energies. From measurements of image peak separations of five isolated dislocations in different slip planes and taking into account the usual corrections for inclined dislocations, the following true partial separations are obtained

$$6 \leq r_E \leq 10 \text{ nm}; \quad 17 \leq r_I \leq 23 \text{ nm}$$

for extrinsic and intrinsic ribbons respectively (in order to minimize surface effects, the image peak

separations have been measured in the centre of the foil; the true partial separation is calculated according to Cockayne *et al.* [4]). Using the simple relations $\gamma_I = (\mu b^2/2\pi)(r_I^{-1} + (r_I + r_E)^{-1})$ and

$$\gamma_E = (\mu b^2/2\pi)(r_E^{-1} + (r_I + r_E)^{-1})$$

valid for screw character, and taking for the shear modulus the value $\mu = 7.4 \times 10^4$ MPa known for pure nickel as a substitute for the unknown elastic constants of Ni_3V , one evaluates

$$19 \leq \gamma_I \leq 24 \text{ mJ/m}^2 \quad \text{and} \quad 36 \leq \gamma_E \leq 45 \text{ mJ/m}^2.$$

These relatively small values, compared to the stacking fault energy of pure nickel, are in good agreement with previous results indicating that adding vanadium reduces γ considerably [5]. The ratio γ_E/γ_I is surprisingly large, about 2, compared to values around unity for other crystals. Although similar values for the ribbon widths were obtained on several independent dislocations, non equilibrium widths due to solute atom pinning are of course possible.

Acknowledgments. — Financial support of the D.G.R.S.T. is gratefully acknowledged.

References

- [1] a) VANDERSCHAEVE, G., ESCAIG, B., *Phys. Status Solidi* (a) **20** (1973) 309;
b) VANDERSCHAEVE, G., *J. Physique Colloq.* **35** (1974) C7-47;
c) VANDERSCHAEVE, G., SARRAZIN, T., *Phys. Status Solidi* (a) **43** (1977) 459.
- [2] GEVERS, R., ART, A., AMELINCKX, S., *Phys. Status Solidi* **3** (1963) 1563.
- [3] HIRTH, J. P., LOTHE, J., in *Theory of dislocations* (Mac Graw Hill), Book Company, p. 110, 137.
- [4] COCKAYNE, D. J. H., RAY, I. L. F., WHELAN, M. J., *Phil. Mag.* **20** (1969) 1265.
- [5] DELEHOUEE, L., DERUYTTERE, A., *Acta Metall* **15** (1967) 727; ISHIDA, K., *Phil. Mag.* **32** (1975) 663.