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PLASTIC DEFORMATION AND RELATED STRUCTURAL DEFECTS IN COMPOUNDS WITH GARNET STRUCTURE

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Résumé. — On étudie les possibilités de défaut de structure résultant de la déformation plastique de composés de structure grenat, en fonction de la dissociation des dislocations et des fautes d'empilement associées. La cristallographie de ces fautes conduit à en dégager deux types principaux dont l'énergie est susceptible d'être considérablement différente et de contrôler le comportement plastique. Ces conclusions sont comparées à des observations préliminaires par microscopie électronique de grenat d'yttrium et de fer (YIG) déformé plastiquement.

Abstract. — Possible structural defects induced by plastic deformation in compounds with garnet structure are examined. A special attention is paid to dislocation dissociation and associated stacking fault configurations. Crystallography considerations allow to point out two kinds of planar defects whose energies may appreciably differ and control plastic properties. These predictions are compared to preliminary electron microscope observations of plastically deformed Yttrium Iron Garnet (YIG) single crystals.

1. Garnet structure and possible dislocation dissociations. — The garnet structure is body centred ; since it corresponds to the shortest unit translation Burgers vectors dislocations with $a/2 < 111 >$ Burgers vectors are to be expected and dislocations with $a < 001 >$ Burgers may result from the attractive combination :

$$\frac{a}{2} < 111 > + \frac{a}{2} < \bar{1}\bar{1}1 > \rightarrow a < 001 > .$$

In the garnet structure the oxygen sublattice is not a close packed one, it is usually described in terms of

cation coordination polyhedra. In YIG (Yttrium Iron Garnet, $\text{Y}_3\text{Fe}_5\text{O}_{12}$, $a = 12.376 \text{ \AA}$) largest cations (Y^{3+}) occupy dodecahedral sites whereas cations Fe^{3+} are found in both octahedral and tetrahedral ones (Fig. 1).

Following Ashbee and Thomas [1] we have chosen in a previous study [2] to represent the oxygen sublattice as oxygen octahedra centred on related cations because this octahedral cation sublattice has the smallest sub-cell parameter (Fig. 2). The dissociation abilities of dislocations have been restricted to those probably yielding planar defects with lowest energy : those leaving the more dense sublattice unaffected. Possible fault vectors are therefore the unit translation vectors of the octahedral cation sublattice, they destroy the perfect packing of the other cation sublattices and

FIG. 1. — Cation distribution in one octant of the unit cell.
● dodecahedral cation. ○ tetrahedral cation. △ octahedral cation.

FIG. 2. — Oxygen octahedra in one octant of the unit cell.

affect the oxygen one since oxygen octahedra do not correspond exactly in such translations. These planar defects may result from the impingement of domains where order has been differently nucleated as well as from dislocation dissociation. The simplest dissociations are :

$$\frac{a}{2} \langle 111 \rangle \rightarrow \frac{a}{4} \langle 111 \rangle + \frac{a}{4} \langle 111 \rangle$$

$$a \langle 001 \rangle \rightarrow \frac{a}{2} \langle 001 \rangle + \frac{a}{2} \langle 001 \rangle .$$

Related stacking faults are fundamentally different. No tetrahedral and dodecahedral cations correspond in an $a/4 \langle 111 \rangle$ resulting in an increase in coulombic energy in these sublattices (electrostatic faults, γ_e , EF). On the contrary tetrahedral and dodecahedral cations correspond in $a/2 \langle 001 \rangle$ which results, in YIG, in an exchange of cations with same valency (order faults, γ_o , OF) (Fig. 3). One can reasonably predict the latter defect (OF) to be less energetical.

FIG. 3. — Correspondence of cations in an $a/2 \langle 001 \rangle$ translation.

The stacking fault energy also depends on the fault plane, then off all possible but simple dissociations (Fig. 4) three dissociations are mainly expected [2] :

$$\frac{a}{2} \langle 111 \rangle \rightarrow \frac{a}{4} \langle 111 \rangle + \frac{a}{4} \langle 111 \rangle$$

in any plane containing $\langle 111 \rangle$ (1)

$$a \langle 001 \rangle \rightarrow \frac{a}{2} \langle 001 \rangle + \frac{a}{2} \langle 001 \rangle$$

in any plane containing $\langle 001 \rangle$ (2)

$$a \langle 001 \rangle \rightarrow \frac{a}{4} \langle 111 \rangle + \frac{a}{2} \langle 001 \rangle +$$

$$+ \frac{a}{4} \langle \bar{1}\bar{1}\bar{1} \rangle \text{ in } \{ \bar{1}\bar{1}0 \} . \quad (3)$$

FIG. 4. — Possible dissociations of $a/2 [111]$ and $a [001]$ Burgers vectors in the (110) plane.

2. Possible experimental evidence of dissociation. — Depending on the relative energies of the stacking faults resulting from dislocation dissociations one can expect three experimental situations :

— $\gamma_o \ll \gamma_e$, γ_e large.

Reaction (2) may lead to widely dissociated $a \langle 001 \rangle$ dislocations. Since dislocation self energies are not very different ($3 \frac{a^2}{4}$ for $\frac{a}{2} \langle 111 \rangle$ and a^2 for $a \langle 001 \rangle$), a widely dissociated $a \langle 001 \rangle$ dislocation may be energetically more favourable than an undissociated $a/2 \langle 111 \rangle$ one. Plastic deformation would then be controlled by such $a \langle 001 \rangle$ dislo-

FIG. 5. — $\gamma_o < \gamma_e$, expected node.

cations as observed in some ordered alloys where dislocations with shortest Burgers vector do not control plastic deformation.

— $\gamma_0 < \gamma_e$, γ_e and γ_0 low enough to allow resolvable dissociation. $a < 001 >$ are more dissociated than $a/2 < 111 >$ ones. A triple node may be formed without partial recombination following the reaction (Fig. 5):

$$\frac{a}{2} < 111 > + \frac{a}{2} < \bar{1}\bar{1}1 > \rightarrow a < 001 >$$

$$\text{or : } \begin{cases} \frac{a}{4} < 111 > + \frac{a}{4} < \bar{1}\bar{1}1 > \rightarrow \frac{a}{2} < 001 > \\ \frac{a}{4} < 111 > + \frac{a}{4} < \bar{1}\bar{1}1 > \rightarrow \frac{a}{2} < 001 > \end{cases}$$

Plastic deformation should be controlled by $a/2 < 111 >$ dislocations.

— $\gamma_0 > \gamma_e$.

As far as dislocation with $a < 001 >$ Burgers vector are concerned dissociation (3) is probably the most favourable one. Indirect evidence of this property should be given by the observation of extended triple nodes (Fig. 6) unless $a/2 < 111 >$ dislocations were not splitted in $\{110\}$ planes.

FIG. 6. — $\gamma_0 > \gamma_e$, expected node.

3. Transmission electron microscopy observations. —

TEM investigations have been carried out on plastically deformed YIG single crystals. Experimental procedure have been given elsewhere [3]. Large loops (L) and hexagonal meshed networks (Fig. 7) are the most frequently observed defects. The dislocation

FIG. 7. — Dislocations A, B and C have $a/2 < 111 >$ Burgers vectors, dislocations D and E have $a < 001 >$ ones [3].

network is formed with $a/2 < 111 >$ dislocations (A, B, C) and $a < 001 >$ ones (D, E), the latter appearing as junction segments [3]. It seems therefore that $a/2 < 111 >$ is the probable slip direction. However in the electron microscope, the situation in YIG at 100 kV is approximately the same as that in metals at 1 MV, i.e. many beam dynamical conditions, high resolution experiments have not been successfully carried out till now and we are not able to conclude concerning dislocation dissociation.

FIG. 8. — Sub-grain boundary resulting from plastic deformation.

FIG. 9. — Stacking faults observed in plastically deformed YIG.

Dislocation loops have $a/2 < 111 >$ Burgers vectors, they have been found to be in $\{111\}$ planes.

Narrower dislocations networks also result from plastic deformation and seem to give better resolution conditions (Fig. 8).

Planar defects were observed in specimens deformed

at several temperatures in the range 1 350-1 200 °C. They are bound by partial dislocations (Fig. 9), some of them (a, b) have been found to lie in $\{110\}$ planes, however the number of different imaging conditions was too limited to allow an unambiguous determination of the displacements vectors.

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