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Dislocations in $Y_3Al_5O_{12}$

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The energies of dislocations in yttrium aluminium garnet are calculated and the likely configurations of both growth and mechanically induced dislocations in crystals grown from solution and from the melt are discussed.

1. Introduction

There is a great deal of interest in garnets as a result of their uses in magnetic, microwave and, in the case of yttrium aluminium garnet (YAG), laser devices. The perfection of these materials, particularly their dislocation structure, is of importance in its possible relation to electronic properties.

This paper concerns a theoretical study of the likely dislocation configurations in YAG–$Y_3Al_5O_{12}$. Previous studies of dislocations in melt grown crystals observed in transmission electron microscopy [1, 2], by X-ray topography [3] and by optical microscopy [4, 5] have been reported. A study of dislocations observed in crystals grown from high temperature solution has also been reported [6, 7]. This paper reviews both existing data and new calculations on dislocations in YAG which relate to the experimental observations.

2. Dislocation energies

Garnets crystallize in the cubic space group *I*a3d. Being body-centred their shortest dislocation Burgers vector (**b**) and thus the lowest energy dislocation, will be $\frac{1}{2}\langle 111\rangle$. The energy of a dislocation can be divided into two components, core energy and line tension energy. The latter is an order of magnitude larger than the former and thus dominates. The dislocation line energy is given by

$$E_1 = C\cdot|\mathbf{b}|^2\cdot K \qquad (1)$$

where C is a constant representing the spatial limits of the dislocation strain field (varying between 1.0 and 1.5), $|\mathbf{b}|$ is the modulus of the Burgers vector and K is termed the energy factor [8]. K is related to the elastic properties of the solid and has the dimensions of a buld modulus. It can easily be seen that E_1 varies primarily as a function of $|\mathbf{b}|^2$. The shortest values of $|\mathbf{b}|$ are listed in Table I and it can clearly be seen that energetically only $\mathbf{b} = \frac{1}{2}\langle 111\rangle$, $\langle 100\rangle$ and $\langle 110\rangle$ are likely. The energy factor K varies as a function of dislocation character (that is edge or screw) and has been calculated using a computer program [9] from the elastic constants [10]. The results tabulated in Table II show that K varies from a maximum for the edge component to a minimum for the screw component. It can also be seen that for the edge dislocations K varies very little. This is an indication of the high elastic isotropy of this material (the isotropy factor $A = 2C_{44}/C_{11} - C_{12} = 1.03$ [10]). Calculation of the total energies show them to be very large varying from 987 eV nm^{-1} for $\mathbf{b} = \frac{1}{2}\langle 111\rangle$ screw to 3532 eV nm^{-1} for $\mathbf{b} = \langle 110\rangle$ edge (max). (C is taken here as equal to 1.3). Thus it can be seen

TABLE I Values of $|\mathbf{b}|$ and $|\mathbf{b}|^2$

[*h k l*]	$\lvert\mathbf{b}\rvert$ (nm)	$\lvert\mathbf{b}\rvert^2$ (nm)^2
$\frac{1}{2}$[111]	1.04	1.08
[100]	1.20	1.44
[110]	1.70	2.88
$\frac{1}{2}$[113]	1.99	3.96
[210]	2.69	7.21
[211]	2.94	8.65

TABLE II Variation of K for different Burgers vectors

Burgers vector	K(screw) ($\times 10^{10}$ NM^{-2})	K(edge) ($\times 10^{10}$ NM^{-2})	
		Minimum	Maximum
$\frac{1}{2}$[111]	11.248	15.062	15.062
[001]	11.50	14.99	15.006
[110]	11.311	14.985	15.090

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TABLE III Preferred directions of growth dislocations–growth from solution

Type	Burgers vector	Growth direction	$\omega(°)$	$\phi(°)$	$\theta(°)$	Character	ΔW ($\times 10^{10}$ Nm^{-2})	($\Delta W/W$)
1a	$\frac{1}{2}[111]$	[110]	35.3	45.0	77.0	Mixed	0.073	(0.62%)
1b	$\frac{1}{2}[\bar{1}11]$	[110]	90.0	45.0	90.0	Edge	0.038	(0.26%)
1c	[001]	[110]	90.0	45.0	90.0	Edge	0.037	(0.25%)
1d	[010]	[110]	45.0	32.5	90.0	Mixed	0.071	(0.56%)
1e	$[\bar{1}\bar{1}0]$	[110]	00.0	45.0	90.0	Screw	0.064	(0.58%)
1f	$[1\bar{1}0]$	[110]	90.0	45.0	90.0	Edge	0.035	(0.24%)
1g	$[\bar{1}00]$	[110]	60.0	53.0	103.0	Mixed	0.058	(0.43%)
2a	$\frac{1}{2}[1\bar{1}1]$	[112]	61.9	15.5	31.0	Mixed	0.016	(0.12%)
2b	$\frac{1}{2}[11\bar{1}]$	[112]	90.0	45.0	35.0	Edge	0.024	(0.16%)
2c	$\frac{1}{2}[111]$	[112]	19.5	45.0	44.0	Mixed	0.054	(0.48%)
2d	[010]	[112]	65.9	30.0	45.0	Mixed	0.042	(0.30%)
2e	[001]	[112]	35.3	45.0	25.0	Mixed	0.038	(0.31%)
2f	[110]	[112]	54.7	45.0	51.0	Mixed	0.051	(0.39%)
2g	[011]	[112]	30.0	26.5	36.0	Mixed	0.049	(0.42%)
2h	$[01\bar{1}]$	[112]	73.2	61.5	26.0	Mixed	0.034	(0.24%)
2i	$[\bar{1}10]$	[112]	90.0	45.0	35.0	Edge	0.033	(0.22%)

that with these high energies the YAG lattice will not easily dislocate.

3. Growth dislocations

Methods for studying line directions of growth dislocations have been developed by Klapper [11]. He has shown that dislocations have been found to propagate in directions which minimize their line energy per unit growth length (W). The propagation of a dislocation during growth is subject to the following relation

$$W = \frac{K}{\cos\alpha} = \text{Minimum} \qquad (2)$$

where α is the angle between the growth direction normal and the dislocation line direction, L. Equation 2 can be solved using a computer program [9] to give values of α (actually two angles are needed to define L in three dimensions, for a minimum value of W).

3.1. Growth dislocations in solution grown crystals

YAG crystallizes from solution with both {110} and {112} facets. Considering the multiplicity of these forms and the three likely Burgers vectors, the orientation parameters for the 16 families of growth dislocations were determined. These are summarized in Table III. In this table ϕ and θ are the orientation parameters, representing the angles the dislocation line makes with [001] and with [010] in (001), respectively. The angle ω is that between the Burgers vector and the growth direction and describes the "uniqueness" of a particular configuration. Finally the shape of the minimum of W is shown in absolute terms and as a percentage variation ($\Delta W/W$) with ΔW calculated using points $(\phi, \theta) \pm 5°$ from (ϕ, θ) minimum. It can be seen that the minima are very flat and that some variations from W minimum can be expected, particularly for edge dislocations where the average $\Delta W/W$ is 0.23% compared with 0.42 and 0.58 for mixed and screw dislocations. Fig. 1 shows the shape of the typically flat minimum for an ω versus ϕ plot (dislocation Type 1a). It is also worth noting that only one (Type 1e) pure screw dislocation is predicted and that the mixed dis-

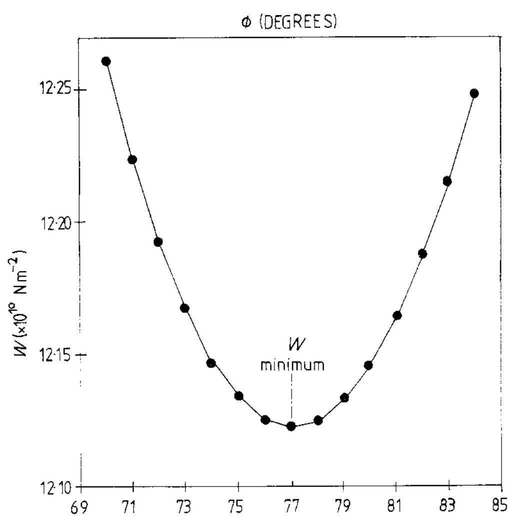

Figure 1 Shape of the minimum of the plot of the line energy per unit growth length against orientation parameter ϕ for dislocation Type 1a.

locations should be readily identifiable in practice due to their line orientation parameters not being along low index planes. These predicted configurations have been observed in practice and have enabled identification of the Burgers vectors of dislocations of mixed character in flux grown YAG [6, 7].

3.2. Growth dislocations in crystals grown from the melt

The configuration of growth dislocations in crystals prepared from the melt have been shown [12] to be similar to those observed in crystals grown from solution in that they propagate in directions to satisfy Equation 2. However there are two major differences. Firstly, YAG grows from the melt above the interface roughening transition [13] in the normally fast growing ⟨1 1 1⟩ direction. Secondly, a convex melt-growth interface is often used compared to the normally planar interface from solution. The use of the convex growth interface to control the direction of propogation of dislocations in melt grown $Gd_5Ga_3O_{12}$ (GGG) has been extensively studied both theoretically and experimentally by Schmitt and Weiss [12] but these studies have not so far been applied to YAG. Detailed calculations of the dislocation orientations have been made for this system assuming a planar (1 1 1) interface although an approximation allows the identification of dislocations in practice. The predictions based on this model are summarized in Table IV. It can be seen that a pure screw dislocation (Type 3a) is likely and this would propagate normal to the growth interface as would the edge dislocation (Type 3e). The mixed dislocations can be expected to vary by angles of the order of $\pm$ 5 to 15° from the growth normal. The geometry of these dislocations has been well confirmed in studies of (GGG) [14, 15] but has not been reported in YAG.

Garnets grown at the high temperatures employed in growth from the melt contain a high concentration of point defects (vacancies, self-interstitials and impurities). Whilst these point defects are stable at the melt temperature the crystal lattice becomes supersaturated with them during cooling. The excess point defects tend to getter to the dislocations resulting in dislocation climb and decoration. Two types of climb induced dislocations have been noted in garnet. Firstly, dislocation loops and segments have been noted in GGG [e.g. 16] due to impurity inclusions of iridium (the crucible material). The loops were often found to lie in the (1 1 1) plane. Secondly, dislocation helices have been observed by many authors [e.g. 17] in GGG. The reported character of these dislocations is that they are formed by the nucleation of second phase (excess Ga_2O_3) interstitials, the latter leading to climb. Whilst no dislocations formed by a climb mechanism have been reported in YAG the decoration of dislocations in flux grown YAG [7] by the gettering of solvent impurities has been observed.

4. Dislocations induced by plastic deformation

It is fairly clear that YAG is a brittle material at room temperature and does not undergo any plastic deformation. However, as crystal growth occurs at 1000° C (solution growth) and 1500° C (melt growth), some high temperature plastic deformation is likely due to increasing atomic vibrations and relaxations in the crystal lattice. This is supported by observations of grain boundary multiplication in YAG [4] by etch pitting techniques.

Plastic deformation has been induced in $Y_3Fe_5O_{12}$ (YIG) where the samples were compressed at a temperature of 1350° C [18]. Here dislocation loops and half segments generated predominantly by a climb mechanism were imaged in the electron microscope. The role of dislocation dissociation in plastically deformed garnet has also been studied by the same authors [19].

Whilst no tensile data is available for YAG at these elevated temperatures, it is perhaps useful to speculate on the likely slip systems. Table V shows the order of the most closely packed planes

TABLE IV Preferred directions of growth dislocation–growth from the melt

Type	Burgers vector	growth directions	ω(°)	ϕ(°)	θ(°)	Probable character
3a	$\frac{1}{2}$[1 1 1]	[1 1 1]	0.0	45.0	55.0	Screw
3b	$\frac{1}{2}$[$\bar{1}$ 1 1]	[1 1 1]	70.5	29.0	49.0	Mixed
3c	[0 0 1]	[1 1 1]	54.7	45.0	40.0	Mixed
3d	[1 1 0]	[1 1 1]	35.3	45.0	65.0	Mixed
3e	[1 1 0]	[1 1 1]	90.0	90.0	135.0	Edge

TABLE V Closely packed planes in YAG

Plane $\{hkl\}$	Reticular area (normalized)
{2 1 1}	2.45
{2 2 0}	2.83
{3 2 1}	3.74
{4 0 0}	4.00
{4 1 1}	4.24
{3 3 2}	4.69
{4 3 1}	5.01

in garnet as determined by calculations of reticular densities based on space group symmetries [20]. As plastically induced dislocations tend to have the lowest energies, the assumptions for Burgers vectors can still be regarded as valid. The combination of Burgers vectors and close packed planes (slip planes) produce the likely slip systems and these are summarized in Table VI.

5. Conclusions

Refined calculations of dislocation line energies have confirmed that dislocations with $\mathbf{b} = \frac{1}{2}\langle 1\,1\,1\rangle$, $\langle 0\,0\,1\rangle$ and $\langle 1\,1\,0\rangle$ are the most likely to occur. Dislocation line orientation parameters have been calculated subject to Klapper's criteria that growth dislocations propagate to minimize their elastic line energy. These calculated minima have been found to be flat thus indicating a likely spread of line directions for a given value of **b**. These calculations have enabled the identification of mixed dislocation in flux grown YAG. Probable slip systems for plastically deformed YAG based on these calculations have been estimated. This work comprises part of a study to understand the role of dislocations in the growth of YAG and in its mechanical properties at high temperature.

TABLE VI Probable slip systems for garnet

Slip plane	Burgers vector
(2 1 1)	$\frac{1}{2}[\bar{1}11]$ $[011]$
(1 1 0)	$\frac{1}{2}[\bar{1}1\bar{1}]$ $[001]$ $[1\bar{1}0]$
(3 2 1)	$\frac{1}{2}[\bar{1}11]$
(1 0 0)	$[010]$ $[011]$
(4 1 1)	$[01\bar{1}]$
(3 3 2)	$[\bar{1}10]$
(4 3 1)	$\frac{1}{2}[\bar{1}11]$

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