for $h = 5$ or 10, by subtracting 0·55 F^2(cal.) of the twin component $(5n, k, -l-n)$. The twinning factor of 0·55 was arrived at by trial and error; I estimate its standard uncertainty at about 0·02. After correction, two reflections showed slightly negative values of F_o^2; these were included in the refinement. The weights of the adjusted reflections were reduced by the factor $\frac{1}{4}$ for $h = 0$ and by $\frac{1}{16}$ for $h = 5$ or 10 – unnecessarily, probably, since the final model shows nearly as good agreement for the adjusted reflections as for the others.

Final least-squares refinement led to an R of 0·0232 for 668 reflections (two had been removed because their twin mates were not recorded). During the last cycles, the 44 reflections with $\sin^2 \theta / \lambda^2 \geq 1·78$ ($\theta \geq 71·5°$ for Mo radiation) were given zero weight since several of them showed large residuals suggesting that the θ-2θ scan range had not encompassed the entire $K\alpha_1$-$K\alpha_2$ doublet; if these reflections are deleted from the R index, it becomes 0·0217. The GOF for 626 reflections is 1·63, but is artificially small because of the reduced weights assigned to the twinned reflections. Refinement was by full-matrix minimization of $\sum w(F_o^2 - F_c^2)^2$, with $w = [2F_o\sigma(F_o)]^{-2}$.

Attempts were made to locate the H atom, with no success: difference maps (with various $\sin \theta / \lambda$ cutoffs) showed no clear peak, and refinement of an isotropic B for an H atom placed in its logical site at $0, 0, \frac{1}{2}$ (NMKSS) led to an increase to over 10·0. NMKSS reported similar difficulties in locating the H atom. The problem of locating the H was probably exacerbated by rather severe extinction effects (see SUP 42832).

Table. 1. *Parameters of the* V *atom, space group* C2/m

The U_{ij}'s are matrix elements, with units Å^2.

x	0·26608 (3)	U_{11}	0·00607 (5)
y	0	U_{22}	0·00601 (4)
z	0·23373 (3)	U_{33}	0·00582 (4)
		U_{13}	0·00053 (3)

The final parameters are given in Table 1.* They are more precise, by factors of 5 to 10, than those reported by NMKSS for the Cm model; moreover, the U_{ij} values are not only more isotropic than those of NMKSS but, of course, are identical for all V atoms. The general description of the structure is unchanged.

NMKSS noted that their refinement of this structure was probably hampered by the presence of twins and suggested that these twins were 'less than 1 µm in width'. The sample had been ground into a sphere 0·178 (3) mm in diameter; that the twins could have survived intact this grinding is evidence that the twinning was very intimate. It is somewhat surprising, then, that the twin component was a minor – rather than an equal – contributor to the diffraction pattern.

---

* A list of observed and calculated structure factors has been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43937 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Reference

Noda, Y., Masumoto, K., Koike, S., Suzuki, T. & Sato, S. (1986). *Acta Cryst.* B42, 529–533.

The Further Geometry of Grain Boundaries in Hexagonal Close-Packed Metals

By Fu-Rong Chen* and A. H. King

Department of Materials Science and Engineering, State University of New York at Stony Brook, Stony Brook, NY 11794-2275, USA

Abstract

A technique is given for finding partial DSC vectors appropriate to crystals with more than one atom per lattice site. The DSC lattice is made up of vectors that represent displacements of one crystal with respect to the other that leave the boundary structure shifted, but not complete. A new, rapid method for finding the step vectors associated with perfect DSC dislocations is described. Partial DSC vectors and step vectors for perfect DSC dislocations in hexagonal close-packed crystals are determined. The availability of reactions between lattice partial dislocations and grain boundaries in hexagonal close-packed crystals is also assessed.

---

* Now at Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA.

Introduction

Geometrical models of the structures of grain boundaries have received a great deal of attention since the early 1970's, with considerable emphasis being placed upon understanding the principles which govern structure, and the ways in which structure influences the grain-boundary properties (Smith & Pond, 1976; Sutton, 1984). Grain-boundary geometry has been described in terms of the coincidence-site lattice (CSL), and its generalization called the O lattice (which is the lattice of possible origins of the transformation which produces crystal 2 from crystal 1). Also of importance in describing the grain-boundary geometry is the so-called DSC lattice, which is a lattice made up of vectors which represent displacements of one crystal with respect to the other which leave the boundary structure shifted, but complete: DSC vectors thus define the allowable Burgers vectors of perfect grain-boundary dislocations. The existence of DSC dislocations in high-angle grain boundaries, conserving structures of high lattice coincidence through small changes in misorientation, has been confirmed by various transmission electron microscope investigations; most of these observations were made in materials with cubic crystal structures (Bollmann, Michaut & Sainfort, 1972; Clark & Smith, 1978; Sun & Balluffi, 1982). The behavior of grain boundaries, in many cases, has also been linked to the properties of grain-boundary dislocations, although this frequently requires that further geometrical concepts be brought into consideration.

Two important geometrical features have been identified beyond the usual CSL, O lattice and DSC lattice: the first of these is the step vector associated with a DSC dislocation, which is used in determining the height of the step in the grain-boundary plane that is associated with the core of a grain-boundary dislocation. The definition of the step vector and an extensive description of its properties was given by King & Smith (1980) and step vectors for grain-boundary dislocations in cubic materials were tabulated by King (1982). Quantitative confirmation of the importance of step vectors in determining the behavior of grain boundaries has been given by Fukutomi, Kamijo & Horiuchi (1986). The second important feature is the ability of grain boundaries to absorb or transmit crystal-lattice dislocations during deformation or grain-boundary migration: this is always possible for perfect crystal-lattice dislocations, which leave only DSC dislocation residues in grain-boundary planes, but for lattice partial dislocations the reactions may be impeded by the fact that non-DSC residues may be produced, as discussed by King & Chen (1984) and Chen & King (1984) for cubic crystals.

Interest in the structure and behavior of grain boundaries in non-cubic crystals is currently increas-ing, with some emphasis on the h.c.p. structure. Various attempts have been made to provide techniques for determining the basic geometrical parameters, such as the CSL and DSC lattice vectors, for these boundaries (Bonnet, Cousineau & Warrington, 1981; Bleris, Nouet, Hagege & Delavignette, 1982), but these techniques have proven to be flawed (Chen, 1986). Definitive methodologies have, however, recently become available (Grimmer & Warrington, 1987). An important extension to the familiar work on cubic structures has been the postulation of 'constrained' CSL structures, where three-dimensional CSL's can only be formed if the value of $(c/a)^2$ is held at a rational value: boundary structures related to these CSL's have recently been observed by Chen (1986). The necessary geometry for describing the structures of the grain boundaries is therefore in place, but the 'further' geometry needed in order to correlate structure with many types of behavior is not. It is the purpose of this paper to indicate the appropriate techniques for determining this information, and to provide tabulations of the data.*

In addition to the features described above, the possibility of a new class of dislocations in the grain boundaries of h.c.p. materials arises, because of the fact that the structure has two atoms per lattice site. This provides the possibility of dislocations which cause translations equivalent to shifts between different atom sites, which are not shifts between identical lattice sites, as suggested by Smith (1980). Such dislocations would have Burgers vectors which can be summed to form DSC vectors in the same way that lattice partial Burgers vectors can be summed to form perfect ones: we therefore refer to these defects as 'partial DSC' dislocations, or PDSC dislocations, and it is of interest to determine the possible Burgers vectors for these defects.

Partial DSC Burgers vectors

For h.c.p. metals there are two atoms per lattice site in the primitive unit cell: one is at the latice site $[000]$ and the other one is at the non-lattice site $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$. If we call the unit cell containing an atom at $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ the positive unit cell and denote it as $(+)$, there is an equivalent unit cell which is rotated 60° about $[001]$ relative to the positive unit cell and containing an atom at the non-lattice site $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$: we call this the negative unit cell and denote it as $(-)$. The $(+)$ and $(-)$ unit cells can transform to each other by either

---

a rotation of 60° about [001] or a translation by the vector of $\frac{1}{3}\langle 120 \rangle$ type. Three types of partial DSC vectors (PDSC's) are formed by: (1) joining the lattice sites in crystal 2 to non-lattice sites in crystal 1 called PDSC1, (2) joining the non-lattice sites in crystal 2 to lattice sites in crystal 1 called PDSC2, (3) joining the non-lattice sites in both crystals called PDSC3. Crystals 1 and 2 can each be arranged with either a $(+)$ or a $(-)$ unit cell. The possible Burgers vectors of grain-boundary dislocations then become more varied, since the Burgers vectors may not only belong to the set of DSC lattice vectors as in b.c.c. and f.c.c. crystals but may also be PDSC's. Burgers vectors of the PDSC types described above may or may not be equal to DSC vectors, depending upon the structure of the CSL. They have the effect of transforming the structure of the CSL if they are not equal to the DSC vectors, and may not necessarily be distinct from the DSC vectors in every structure produced by such transformations. Examples of PDSC Burgers vectors are shown in Fig. 1, along with the types of transformation of the bilattice structure that they can produce. Fig. 1(a) shows the various DSC and PDSC Burgers vectors for the $\Sigma = 7$ CSL in the reference structure referred to as $(+,+)$, where both of the crystals are in the $(+)$ orientation with respect to an origin at a coincident atom site. Displacement of crystal 2 by a PDSC1 vector yields the structure shown in Fig. 1(b), which is refered to as $(-,+)$, denoting the orientations of crystals 1 and 2 with respect to origins at a coincident atom site. Relative displacements of one crystal from the $(+,+)$ structure by PDSC3 vectors yield the $(-,-)$ structure shown in Fig. 1(c): note that this structure is a mirror image of the $(+,+)$ structure, so that dislocations of the PDSC3 type may separate regions of grain boundary of identical energy. Note also that for the $(-,+)$ structure, the PDSC3 Burgers vectors are identical to the DSC Burgers vectors, so they are structure-conserving translations for this case. For starting configurations with lower symmetry than those shown here (i.e. with no atom site coincidences) there will be no 'accidental equalities' of the vectors or the structures associated with them.

A similar type of defect has been observed in diamond-cubic-structured germanium (Bacmann, Silvestre, Petit & Bollmann, 1981) and a related type of dislocation has been observed in twist grain boundaries in magnesium oxide, where the Burgers vector defines a shift between the two interpenetrating f.c.c. lattices decorated with different chemical species (Sun & Balluffi, 1982).

Partial DSC vectors can be deduced by analytical methods. There are three types of PDSC associated with transformations between different kinds of boundaries which may be denoted as structure $(+,+)$, $(+,-)$, $(-,+)$, and $(-,-)$ depending on the orientations of the unit cells of the two crystals. The

three types of PDSC are always describable as DSC vectors added to a PDSC vector within the unit cell of the DSC lattice denoted as Pdsc; just as the non-lattice sites of the h.c.p. structure can be described as lattice vectors added to a non-lattice vector $[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ or $[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ within the unit cell.

(1) PDSC1 are vectors joining lattice sites of lattice 2 to non-lattice sites of lattice 1, hence PDSC1 can be written as:

$$PDSC1 = (x_1 + t_i) - Rx_2$$
$$= (x_1 - Rx_2) + t_i$$
$$= DSC + t_i \qquad (1)$$

where x_1 and x_2 are the lattice vectors of lattice 1 and lattice 2 respectively. t_i $(i = 1, 2)$ are the non-lattice
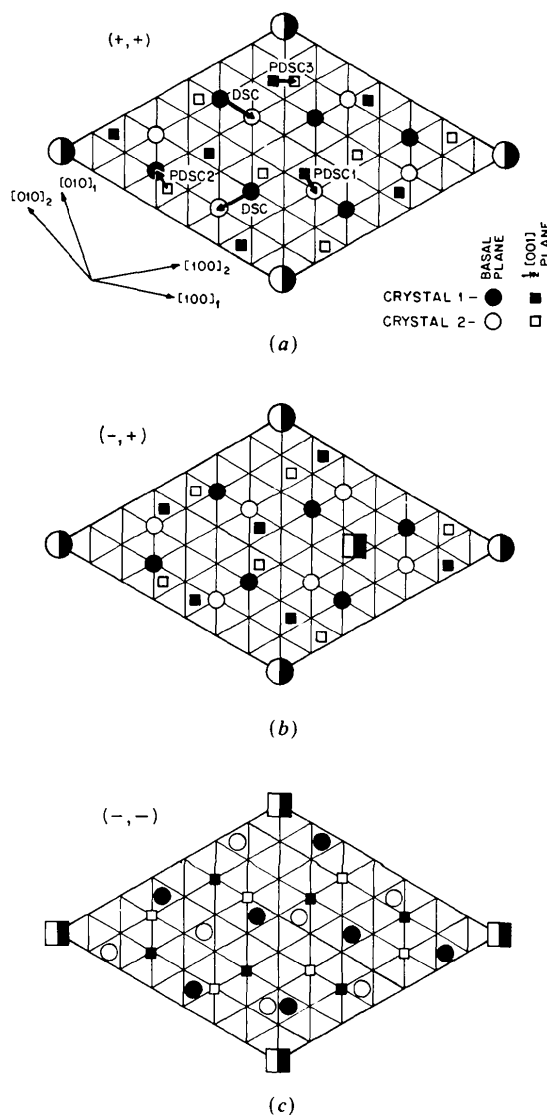

Fig. 1. Examples of the partial DSC Burgers vectors, and the structural transformations associated with them, for the $\Sigma = 7$ exact coincidence system in hexagonal close-packed crystals.

Table 1. *Partial DSC Burgers vectors for h.c.p. crystals*

The 'System' column gives the value of Σ, rotation axis and rotation angle (°). The PDSC vectors are given as columns, with each element multiplied by 2Σ, in order to provide integer values. The vectors are listed according to the types of coincidence structure (choice of origin) in which they are found, and where they are equal to the DSC vectors they are listed merely as 'DSC'.

System	(+,+)(+,-) Pdsc1	(-,+)(-,-) Pdsc1	(+,+)(-,+) Pdsc2	(+,-)(-,-) Pdsc2	(+,+) Pdsc3	(+,-) Pdsc3	(-,+) Pdsc3	(-,-) Pdsc3
(a) $(c/a)^2$ = any								
7 [001]/21·79	-8	2	-8	2	2	D	D	-8
	-10	-8	-10	-8	–	S	S	-10
	21	21	21	21	0	C	C	0
13 [001]/32·20	4	-10	4	-10	-10	D	D	4
	-10	-14	-10	-14	-14	S	S	-10
	39	39	39	39	0	C	C	0
19 [001]/13·17	-14	2	-14	2	2	D	D	-14
	-16	-14	-16	-14	-14	S	S	-16
	57	57	57	57	0	C	C	0
31 [001]/17·90	-8	14	14	-8	D	14	-8	D
	-22	-8	-8	-22	S	-8	-22	S
	93	93	93	93	C	0	0	C
37 [001]/9·43	-20	2	-20	2	2	D	D	-20
	-22	-20	-22	-20	-20	S	S	-22
	111	111	111	111	0	C	C	0
43 [001]/15·178	16	-10	-10	16	D	-10	16	D
	-10	-26	-26	-10	S	-26	-10	S
	129	129	129	129	C	0	0	C
49 [001]/16·43	4	-22	4	-22	-22	D	D	4
	-22	-26	-22	-26	-26	S	S	-22
	147	147	147	147	0	C	C	0
(b) $(c/a)^2 = \frac{12}{5}$								
9 [100]/83·62	6	-6	2	-2	8	-2	2	-8
	12	-12	4	-4	16	-4	4	-16
	-3	3	-7	7	-10	-2	2	10
12 [100]/48·19	0	0	-8	8	4	-4	4	-4
	0	0	-16	16	8	-8	8	-8
	12	-12	8	-8	-10	-2	2	10
16 [210]/75·52	-32	32	32	-32	D	32	-32	D
	8	40	40	8	S	40	8	S
	-12	-12	-12	-12	C	-12	-12	C
17 [210]/65·68	-34	34	34	-34	D	34	-34	D
	-14	20	20	-14	S	-16	-50	S
	-3	-3	-3	-3	C	-18	-18	C
19 [210/54·62]	-38	38	38	-38	D	38	-38	D
	-10	28	28	-10	S	40	2	S
	3	3	3	3	C	-12	-12	C
21a [100]/58·41	-6	6	10	-10	-2	-16	16	2
	-12	12	20	-20	-4	-32	32	4
	-9	9	1	-1	4	-10	10	-4
21b [100]/25·22	-6	6	2	-2	2	-8	8	-2
	-12	12	4	-4	4	16	16	-4
	9	-9	11	-11	-10	-2	2	10
23 [210]/42·34	-46	46	46	-46	D	46	-46	D
	-14	32	32	-14	S	44	-2	S
	-15	-15	-15	-15	C	-12	-12	C
24 [841]/82·82	36	0	-32	8	4	-4	4	-4
	0	0	-16	-32	-16	16	-16	16
	6	-24	-16	4	-10	-14	14	10
27 [310]/61·22	-6	6	2	-2	2	-8	8	-2
	-30	30	10	-10	10	-40	40	-10
	3	-3	17	-17	-10	-14	14	10
28 [100]/73·40	4	-4	4	-4	-4	D	D	4
	8	-8	8	-8	-8	S	S	8
	-6	6	-6	6	6	C	C	-6

vectors, $t_1 = [\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ for the (+,+) and (+,-) structures, and $t_2 = [\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ for the (-,+) and (-,-) structures.

(2) PDSC2 are vectors joining non-lattice sites of lattice 2 to lattice sites of lattice 1, hence PDSC2 can be written as:

$$PDSC2 = (x_1) - R(x_2 + t_i)$$
$$= (x_1 - Rx_2) - Rt_i$$
$$= DSC + (-Rt_i) \qquad (2)$$

where $t_1 = [\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ for the (+,+) and (-,+) structures, and $t_2 = [\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ for the (+,-) and (-,-) structures.

(3) PDSC3 vectors join non-lattice sites of lattice 2 to non-lattice sites of lattice 1, and hence PDSC3 can be written as:

$$PDSC3 = (x_1 + t_i) - R(x_2 + t_j)$$
$$= (x_1 - x_2) + (t_i - Rt_j)$$
$$= DSC + (t_i - Rt_j) \qquad (3)$$

where both t_i and $t_j = [\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ for the (+,+) structure and both t_i and $t_j = [\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ for the (-,-) structure. $t_i = [\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$ and $t_j = [\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$ are for the (+,-) structure; interchanging the roles of t_i and t_j gives the (-,+) structure.

The vectors t_i, $-Rt_i$, and $t_i - Rt_j$ are then resolved in the coordinates of the DSC lattice. Assuming that the components in DSC coordinates are p, q, r, the Pdsc vectors in the unit cell of the DSC lattice can be written:

$$Pdsc = PDSC - [Int\ (p)DSC1 + Int\ (q)DSC2$$
$$+ Int\ (r)DSC3] \qquad (4)$$

where Pdsc is the partial DSC within the unit cell of the DSC lattice, PDSC are any partial DSC vectors, DSC1, DSC2 and DSC3 are the basis vectors of the DSC lattice, Int (p), Int (q), and Int (r) are the three largest integers which are not greater than p, q, r, respectively.

The three types of Pdsc vectors which may be associated with the four possible kinds of structure are listed in Table 1.

Step vectors

A quick method of searching step vectors associated with each DSC basis has been developed, and this method has a significant advantage over the one proposed by Brokman (1981) in that it uses a computer program for which the input data consist only of the known coincidence geometry. In particular, it requires knowledge of the rotation matrices leading to coincidence misorientations, along with the CSL and DSC vectors: no knowledge of the internal positions of atoms in the CSL is required, as is the case for Brokman's technique. The necessary data are therefore available using the techniques given by Grimmer & Warrington (1987). The relationship between step vectors and DSC vectors is shown in

Fig. 2 and expressed as:

$$S = DSC + RX_2 \qquad (5)$$

where R is a rotation matrix corresponding to the exact coincidence orientation, and X_2 is a lattice vector in lattice 2, expressed in that coordinate system. We search for lattice vectors $[h,k,l]$ of lattice 2 that sum with DSC vectors to give three integer lattice vector components in the step vector, since the step vector must be a member of lattice 1. The range of this search is $0 \le h \le \sqrt{\Sigma}$, $-\sqrt{\Sigma} \le k \le \sqrt{\Sigma}$, $-\sqrt{\Sigma} \le l \le \sqrt{\Sigma}$, where Σ is the ratio of the volumes of the unit cells of the CSL and the crystal, as usual. If there is a vector of lattice 2 satisfying (5), the step vector associated with the DSC vector can then be expressed within the unit cell of the CSL by the following procedures:

(1) Resolve the step volume, S, into components of the CSL bases. In other words, we can write:

$$S = rCSL_1 + sCSL_2 + tCSL_3 \qquad (6)$$

where CSL_1, CSL_2, and CSL_3 are the bases of CSL, and r, s and t are the components of the step vector.

(2) The step vector in the unit cell S' then can be written:

$$S' = S - [\text{Int}\,(r)CSL_1 + \text{Int}\,(s)CSL_2 + \text{Int}\,(t)CSL_3] \qquad (7)$$

where $\text{Int}\,(r)$, $\text{Int}\,(s)$ and $\text{Int}\,(t)$ are the largest integers which are not greater than r, s and t.

(3) The smallest step vector can be selected from the eight equivalent step vectors in the unit cell.

For the coincidence systems obtained by applying Hagége & Nouet's method, the CSL and DSC bases deduced by Bonnet's method and Grimmer's theory, and step vectors determined by our technique are listed in Table 2.

Step vectors cannot be defined for partial DSC dislocations, since they are not structure-preserving defects.
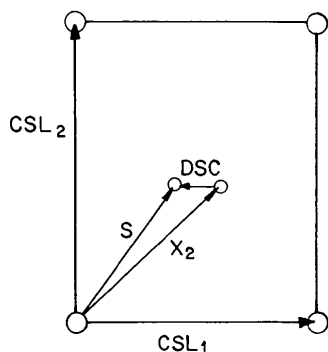

Fig. 2. Illustrating the technique used to find step vectors when the DSC and CSL vectors are known: S is the step vector, which must be a vector of lattice 1, and X_2 is a vector of lattice 2.

Table 2. *CSL, DSC and step vectors for h.c.p. crystals*

The 'System' column has the same meaning as in Table 1, and the vectors are again given as columns, but the elements are multiplied only by Σ. The first given step vector corresponds to the first given DSC vector, *etc.*

System	CSL			DSC			Step		
(a) $(c/a)^2$ = any									
7	0	2	1	2	-3	0	1	0	0
[001]/21·79	0	-1	3	-1	-2	0	1	-1	0
	1	0	0	0	0	7	0	0	0
13	0	3	4	-4	3	0	2	-1	0
[001]/32·20	0	-1	3	-3	-1	0	1	1	0
	1	0	0	0	0	13	0	0	0
19	0	3	2	3	-5	0	1	0	0
[001]/13·17	0	-2	5	-2	-3	0	1	-1	0
	1	0	0	0	0	19	0	0	0
31	0	5	1	-5	6	0	-2	-1	0
[001]/17·90	0	6	-5	-6	1	0	1	-3	0
	1	0	0	0	0	31	0	0	0
37	0	4	7	4	-7	0	1	0	0
[001]/9·43	0	-3	4	-3	-4	0	1	-1	0
	1	0	0	0	0	37	0	0	0
43	0	7	1	1	7	0	-2	-4	0
[001]/15·178	0	1	-6	-6	1	0	2	-2	0
	1	0	0	0	0	43	0	0	0
49	0	5	3	5	-8	0	-2	4	0
[001]/16·43	0	-3	8	-3	-5	0	2	2	0
	1	0	0	0	0	49	0	0	0
(b) $(c/a)^2 = \frac{12}{5}$									
9	1	1	1	1	6	-3	0	1	1
[100]/83·62	0	2	3	2	3	3	0	2	2
	0	1	-3	1	-3	-3	-1	-1	-1
12	1	2	0	2	6	-6	0	-1	-1
[100]/48·19	0	4	0	4	0	0	1	-2	-2
	0	1	3	1	-3	-3	-1	0	0
16	2	0	0	0	0	16	-1	-1	-1
[210]/75·52	1	2	2	2	6	4	-2	0	-2
	0	1	-3	1	-5	2	0	0	1
17	2	0	1	0	0	-17	-1	-1	-1
[210]/65·68	1	1	-6	1	-12	-14	2	-1	1
	0	-1	-2	-1	-5	-3	1	0	0
19	2	0	1	0	0	19	0	-1	-1
[210]/54·62	1	3	-3	3	4	6	-1	0	0
	0	1	2	1	-5	2	-1	0	-1
21a	1	0	8	1	-10	-8	-2	-1	4
[100]/58·41	0	1	16	2	1	-16	-3	-2	8
	0	-1	5	-2	-1	-5	-1	0	2
21b	1	1	2	4	1	9	0	0	0
[100]/25·22	0	3	5	8	2	-3	1	1	0
	0	3	-2	1	-5	-3	-2	0	1
23	2	0	1	0	0	23	-1	-1	0
[210]/24·34	1	4	0	4	3	8	-1	0	2
	0	1	-3	1	-5	2	1	0	0
24	1	2	2	6	-4	-2	0	-1	-2
[841]/82·82	2	0	4	0	-8	8	-2	1	1
	-1	1	-2	-3	-2	-7	-1	1	1
27	3	1	0	-5	6	-10	-1	-1	-1
[310]/61·22	1	3	1	2	3	-23	-1	-2	0
	0	1	-3	-2	-3	-4	-1	0	-1
28	1	2	2	2	-6	18	-2	0	2
[100]/73·40	0	4	4	4	-12	8	-3	1	4
	0	-3	4	-3	-5	1	1	-1	0
29	1	0	2	-4	3	-11	0	-2	0
[100]/67·71	0	1	5	-8	6	7	1	-4	1
	0	4	-9	-3	-5	-1	-1	2	1

Interactions between lattice partial dislocations and grain boundaries

It is well known that a perfect lattice dislocation may always dissociate into an integral number of grain-boundary dislocations whose Burgers vectors belong to the DSC lattice. During this process the total

Burgers vector (Bollmann, 1970; Bollmann, Michaut & Sainfort, 1972) and step height (King & Smith, 1980) must be conserved. A lattice dislocation can also be transmitted through a grain boundary by creating a lattice dislocation in the other grain and yielding a residual perfect DSC dislocation in the grain boundary. In other words, the transmission process is allowed, if the difference between the Burgers vectors of the lattice dislocations in each grain is a member of the DSC lattice. The processes of dislocation absorption and transmission by grain boundaries have been discussed in detail by Hirth & Balluffi (1973) as well as Pond & Smith (1977) and are illustrated schematically in Fig. 3.

However, during the process of deformation, Schockley partial dislocations may glide and/or sessile Frank partial dislocation loops may grow toward grain boundaries. Alternatively, the grain boundaries may migrate toward stationary dislocations during the processes of recrystallization, grain growth and diffusion-induced grain-boundary migration (DIGM). The interaction between partial dislocations and grain boundaries then becomes possible. The interactions of lattice partial dislocations with grain boundaries in f.c.c. and b.c.c. crystal systems have been discussed by King & Chen (1984) and Chen & King (1984). They found that coincidence systems whose Σ values are integral multiples of 3 exhibit significantly different behavior in the processes of partial dislocation absorption and transmission from those whose Σ values are not integral multiples of 3. This applies for both f.c.c. and b.c.c. crystal systems. Lattice partial dislocations are members of the DSC lattice only when Σ is an integral multiple of 3. In other words, the partial dislocations can only be absorbed in the $\Sigma = 3N$-related coincidence boundaries, where N is an integer. The transmission

of a partial dislocation must always yield a DSC residue, and this fact was used to check the possibilities of transmission of partial dislocations in those surveys. The results for the transmission of partial dislocations show certain patterns which are different for $\Sigma = 3N$ and $\Sigma \neq 3N$ coincidence-related boundaries.

In this research, the same techniques were applied to check the processes of absorption and transmission of partial dislocations by grain boundaries in the h.c.p. crystal system. In the h.c.p. system, the PDSC vectors are also the candidate Burgers vectors for grain-boundary dislocations; therefore, the lattice partial dislocations may be absorbed by dissociating into an integral number of DSC and/or PDSC dislocations, or transmitted by yielding a PDSC residue. In order to avoid this complication, only DSC grain-boundary dislocations are considered.

Thirty-seven lattice partial dislocations were considered as participants in the reactions with grain boundaries. Their Burgers vectors were of the types $\langle\frac{2}{3}, \frac{1}{3}, 0\rangle$, $\langle\frac{4}{3}, \frac{2}{3}, 0\rangle$, $\langle\frac{2}{3}, \frac{1}{3}, \frac{1}{2}\rangle$, $\langle\frac{4}{3}, \frac{2}{3}, 1\rangle$, $\langle\frac{2}{3}, \frac{1}{3}, 1\rangle$, $\langle\frac{10}{18}, \frac{8}{18}, \frac{3}{18}\rangle$ and $\langle 0, 0, \frac{1}{2}\rangle$.

Absorption reactions

The 37 lattice partial dislocations were resolved into a coordinate system which is defined by the three primitive DSC bases, in order to examine whether a particular absorption may be available, for all the coincidence systems given in Table 2. The results can be summarized as follows:

(1) No partial dislocation absorptions are allowed for exact coincidence-related boundaries, or for constrained coincidence-related boundaries with $(c/a)^2$ values being $\frac{5}{2}, \frac{33}{13}, \frac{51}{20}, \frac{18}{7}, \frac{13}{5}, \frac{21}{8}, \frac{27}{10}, \frac{27}{8}, \frac{17}{5}, \frac{31}{9}, \frac{7}{2}, \frac{39}{11}$.

(2) $\langle 0, 0, \frac{1}{2}\rangle$ partials can be absorbed in the even Σ value constrained coincidence systems associated with $(c/a)^2$ being $\frac{12}{5}, \frac{8}{3}, \frac{24}{7}$.

(3) $\langle\frac{2}{3}, \frac{1}{3}, 0\rangle$, $\langle\frac{4}{3}, \frac{2}{3}, 0\rangle$, $\langle\frac{2}{3}, \frac{1}{3}, \frac{1}{2}\rangle$, $\langle\frac{4}{3}, \frac{2}{3}, \frac{1}{2}\rangle$, and $\langle\frac{2}{3}, \frac{1}{3}, 1\rangle$ partial dislocations can be absorbed in the $\Sigma = 3N$ constrained coincidence systems associated with $(c/a)^2$ being $\frac{8}{3}$.

(4) $\langle\frac{10}{18}, \frac{8}{18}, \frac{3}{18}\rangle$ partial dislocations can also be absorbed in $\Sigma = 18$ with $(c/a)^2$ being $\frac{8}{3}$.

A useful rule is that lattice partial dislocations having Burgers vectors that join lattice sites to non-lattice atomic sites may always be absorbed into a grain boundary by the formation of PDSC dislocations.

Transmission reactions

The process of transmission is allowed, if the difference of the Burgers vectors of the dislocation in each grain is a member of the DSC lattice. The results are summarized in Table 3. Unlike the results for the f.c.c. and b.c.c. crystal systems, there is not a simple and reliable predictive rule for the process of
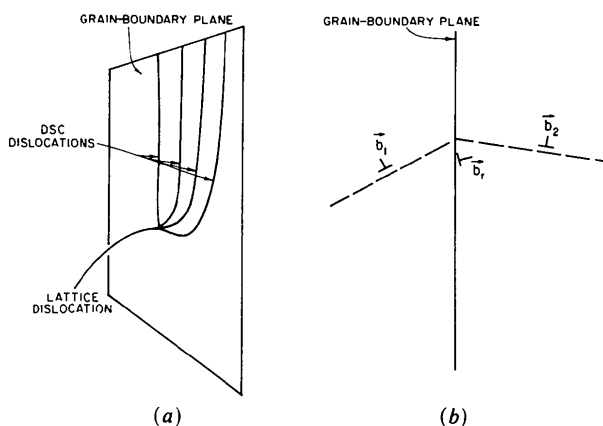

Fig. 3. Illustrating the possible reactions between crystal-lattice dislocations and grain boundaries. (a) The absorption of a dislocation by dissociation into an integral number of DSC dislocations. (b) The transmission of the dislocation leaving a DSC residue in the grain-boundary plane.

Table 3. *A summary of transmission reactions producing only DSC residues*

We give fourteen different reaction groups, each exhibiting different numbers of available reactions of various types. The coincidence systems belonging to the reaction groups are also listed below the group descriptions, with the appropriate values of c^2/a^2 given in parentheses.

Reaction type	Number of possible reactions
(a) Reaction group 1	
Perfect → perfect	18
Perfect → partial	0
Partial → perfect	0
Partial → partial	2
Total	20

$(\frac{12}{5})$: $\Sigma 9$, $\Sigma 21a$, $\Sigma 21b$, $\Sigma 27$, $\Sigma 33$, $\Sigma 39a$, $\Sigma 39b$; $(\frac{33}{13})$: $\Sigma 24$; $(\frac{51}{20})$: $\Sigma 37$; $(\frac{18}{7})$: $\Sigma 13$, $\Sigma 17$, $\Sigma 23a$, $\Sigma 29$, $\Sigma 31$, $\Sigma 35a$, $\Sigma 35b$, $\Sigma 43$, $\Sigma 47$, $\Sigma 49a$, $\Sigma 49b$; $(\frac{21}{8})$: $\Sigma 15b$, $\Sigma 39$; $(\frac{27}{10})$: $\Sigma 19$, $\Sigma 23$, $\Sigma 33b$; $(\frac{27}{8})$: $\Sigma 17$, $\Sigma 27a$, $\Sigma 41a$, $\Sigma 45b$; $(\frac{39}{11})$: $\Sigma 24$.

(b) Reaction group 2	
Perfect → perfect	18
Perfect → partial	6
Partial → perfect	6
Partial → partial	2
Total	32

$(\frac{12}{5})$: $\Sigma 12$, $\Sigma 24$, $\Sigma 36$, $\Sigma 48$.

(c) Reaction group 3	
Perfect → perfect	18
Perfect → partial	6
Partial → perfect	6
Partial → partial	594
Total	624

$(\frac{12}{5})$: $\Sigma 16$, $\Sigma 32$, $\Sigma 44$.

transmission of lattice partial dislocations in h.c.p. crystals, although, for certain values of $(c/a)^2$, $\Sigma = 2N$ and $\Sigma = 3N$ cases may fall into some particular reaction group, as illustrated by the results presented in Table 3.

As for the case of dislocation absorption, transmission or transformation reactions involving one or more lattice partials with site-switching Burgers vectors always produce PDSC dislocations in the grain-boundary plane.

References

BACMANN, J.-J., SILVESTRE, G., PETIT, M. & BOLLMANN, W. (1981). *Philos. Mag. A*, **43**, 189–200.

BLERIS, G. L., NOUET, G., HAGEGE, S. & DELAVIGNETTE, P. (1982). *Acta Cryst.* A**38**, 550–557.

BOLLMANN, W. (1970). *Crystal Defects and Crystalline Interfaces.* Berlin: Springer.

BOLLMANN, W., MICHAUT, B. & SAINFORT, G. (1972). *Phys. Status Solidi A*, **13**, 637–649.

BONNET, R., COUSINEAU, E. & WARRINGTON, D. H. (1981). *Acta Cryst.* A**37**, 184–189.

BROKMAN, A. (1981). *Acta Cryst.* A**37**, 500–506.

CHEN, F.-R. (1986). PhD Thesis, State Univ. of New York at Stony Brook.

CHEN, F.-R. & KING, A. H. (1984). *Mater. Sci. Eng.* **66**, L25–L26.

CLARK, W. A. T. & SMITH, D. A. (1978). *Philos. Mag. A*, **38**, 367–385.

FUKUTOMI, H., KAMIJO, T. & HORIUCHI, R. (1986). *Grain Boundary Structure and Related Phenomena*: Proc. JIMIS-4. Supplement to *Trans. Jpn Inst. Met.* pp. 929–936.

GRIMMER, H. & WARRINGTON, D. H. (1987). *Acta Cryst.* A**43**, 232–243.

HIRTH, J. P. & BALLUFFI, R. W. (1973). *Acta. Metall.* **21**, 929–942.

KING, A. H. (1982). *Acta Metall.* **30**, 419–427.

KING, A. H. & CHEN, F.-R. (1984). *Mater. Sci. Eng.* **66**, 227–237.

KING, A. H. & SMITH, D. A. (1980). *Acta Cryst.* A**36**, 335–343.

POND, R. C. & SMITH, D. A. (1977). *Philos. Mag.* **36**, 353–366.

SMITH, D. A. (1980). *Scr. Metall.* **14**, 715–718.

SMITH, D. A. & POND, R. C. (1976). *Int. Metall. Rev.* **21**, 61–74.

SUN, C. P. & BALLUFFI, R. W. (1982). *Philos. Mag. A*, **46**, 49–62.

SUTTON, A. P. (1984). *Int. Metall. Rev.* **29**, 377–402.

(Ni,Mg)₄ₙ₊₆Ge₂ₙ₊₁O₈₍ₙ₊₁₎, a New Structural Family Related to Olivine and Spinel

BY JACQUES BARBIER

Department of Geology, University of Western Ontario, London, Ontario N6A 5B7, Canada

Abstract

A new structural family, $(Ni,Mg)_{4n+6}Ge_{2n+1}O_{8(n+1)}$ ($n = 1, 2, 3, 4, \infty$), has been identified at atmospheric pressure in the $NiO-MgO-GeO_2$ system. Its building principle is based on regular intergrowth of n (001) olivine layers (*Pnma* setting) with one {111} cation-deficient rock-salt layer. Alternatively, individual structures are shown to contain spinel elements, the proportion of which decreases with increasing values of n. This new family therefore provides a structural transition between the olivine ($n = \infty$ end-member) and spinel structure types and may be relevant to the high-pressure olivine → spinel transformation.

1. Introduction

During the course of a re-investigation of the $NiO-MgO-GeO_2$ system at atmospheric pressure, a new