Stacking Faults in Double Hexagonal Close-packed Crystals

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SUMMARY

Possible deviations in the regular ...ABACA... sequence of stacking (0004) close-packed planes in the double hexagonal close-packed (d.h.c.p.) structure have been considered. Six intrinsic and one extrinsic type stacking faults have been suggested. The schemes of stacking sequences have been usefully considered in terms of the configurational symbols suggested by Jagodzinski. Extending the Hirth and Lothe procedure, estimates of theoretical fault energies are given in terms of the number of pairs of planes of separation N *which are not in the scheme of perfect structure sequence. Relative fault energies have been arrived at reckoning only the first and second nearest neighbour interactions for three ideal situations:*
(a) the transformation energy of d.h.c.p. structure to either f.c.c. or h.c.p. structure is the same; (b) d.h.c.p. $\rightleftharpoons$ f.c.c. transformation occurs; and (c) d.h.c.p. $\rightleftharpoons$ h.c.p. transformation occurs.

ZUSAMMENFASSUNG

Mögliche Abweichungen von der regelmäßigen Stapelfolge ... ABACA ... von dichtest gepackten (0004)-Ebenen in der doppelhexagonalen (dhcp) Struktur wurden untersucht. Sechs intrinsische und ein extrinsischer Stapelfehler werden vorgeschlagen. Ein Schema der Stapelfolgen wird an Hand der von Jagodzinski vorgeschlagenen Konfigurationssymbole aufgestellt. Unter Erweiterung des Hirth–Lothe-Verfährens wurden Abschätzungen der theoretischen Stapelfehlerenergien durchgeführt; dabei wurde die Zahl N *der Trennebenenpaare, die nicht in die richtige Stapelfolge passen, berücksichtigt. Relative Stapelfehlerenergiewerte wurden gefunden, indem für drei ideale Fälle nur die Wechselwirkung zwischen nächsten und übernächsten Nachbarn berücksichtigt wurde: a) Die Umwandlungsenergien von einer doppelhexagonalen in entweder eine flächenzentrierte oder hexagonale Struktur sind gleich, b) dhcp $\rightleftarrows$ fcc-Umwandlung findet statt und c) dhcp $\rightleftarrows$ hcp-Umwandlung tritt auf.*

RÉSUMÉ

Des perturbations possibles dans l'empilement régulier de plans compacts (0004), dans l'ordre ...ABACA... qui caractérise la structure hexagonale compacte double (h.c.d.), ont été examinées. Six types de défauts d'empilement intrinsèques et un type de défaut extrinsèque sont proposés. Pour schématiser les différents ordres d'empilement des plans, les symboles de configuration introduits par Jagodzinski ont été utilisés avec profit. Moyennant une généralisation de la méthode de Hirth et Lothe, on peut donner une estimation de l'énergie théorique des défauts en fonction du nombre de paires de plans d'espacement N *qui ne sont pas disposés dans l'ordre de la structure parfaite. Des valeurs relatives de l'énergie de défaut ont été obtenues en ne tenant compte que des interactions entre premiers et seconds voisins; elles ont conduit aux trois résultats suivants:*
(a) l'énergie de transformation de la structure h.c.d. en structure c.f.c. et en structure h.c. est la même; (b) la transformation h.c.d. $\rightleftarrows$ c.f.c. est possible et (c) la transformation h.c.d. $\rightleftarrows$ h.c. est possible.

1. INTRODUCTION

Much work is available concerning stacking faults in f.c.c. and h.c.p. structures. These close-packed structures are conveniently looked upon as resulting from stacking of identical hexagonal nets of atoms with the three possible stacking positions denoted as A, B and C. B and C positions are displaced with respect to A by $\pm S$ respectively, where S is a vector of the type $a/6\langle\bar{1}\bar{1}2\rangle$ in the f.c.c. structure and $a/3\langle10\bar{1}0\rangle$ in the h.c.p. structure. The f.c.c. and h.c.p. structures are formed respectively by stacking of (111) and (0002) close-packed planes in the sequences ...ABCA... and ...ABA... respectively. Stacking faults in these structures represent deviations from the perfect schemes, the condition of close packing, however, not violated. Possible types of stacking fault have been given in terms of the operator notation[1], namely Δ and ∇ to denote translations of $+S(A\rightarrow B\rightarrow C\rightarrow A)$ and $-S(A\rightarrow C\rightarrow B\rightarrow A)$ respectively. Nabarro[2] has suggested the use of configurational symbols[3] for describing the faulted sequences of close-packed structures. In this notation close-packed planes are designated c or h depending on whether the neighbours on either sides of these planes correspond to cubic ($A\overset{c}{B}C$) or hexagonal ($A\overset{h}{B}A$) close packing. Frank[4] has identified a basic distinction between two types of fault, namely intrinsic and extrinsic. In intrinsic faults the perfect stacking scheme of each half of the crystal extends to the fault plane, while in extrinsic faults the fault plane does not belong to the crystal structure on either side of it. Christian and Swann[5] have reviewed the work on classification of stacking faults, their quantitative measurement and implication in mechanical behaviour of f.c.c. and h.c.p. metals and alloys. Hirth and Lothe[6] have indicated a useful method for estimating theoretical stacking-fault energy for the different types of fault in f.c.c. and h.c.p. structures on the basis of violations of atom-pair bonds using the hard-sphere model with the assumption of central forces.

The present work is concerned with the double hexagonal close-packed (d.h.c.p.) structure. The d.h.c.p. structure is formed by repetition of the (0004) close-packed planes in the sequence ...ABACA..., which in the operator notation is $\ldots\Delta\nabla\nabla\Delta\ldots$ and in the configurational notation is $\ldots\overset{h}{A}\overset{c}{B}AC\ldots$ Rare-earth metals americium, cerium, lanthanum, neodymium and praseodymium crystallise in d.h.c.p. structure[7]. Jayaraman[8] has noticed a general tendency in f.c.c. metals to transform first to the d.h.c.p. structure under high pressure. An h.c.p. $\rightarrow$ d.h.c.p. transformation under high pressure has also been observed[9]. Many intermediate phases[10,11] are known to be of the d.h.c.p. type. Following the procedures established for f.c.c. and h.c.p. structures, we enumerate in this paper the possible stacking faults in the d.h.c.p. structure and the Burgers vectors of the partial dislocations bounding the faults. The theoretical fault energies have been estimated on the basis of a modified Hirth and Lothe procedure.

2. DISLOCATIONS IN THE D.H.C.P. STRUCTURE

We list in Table 1 possible dislocations and their Burgers vectors in d.h.c.p. structure shown in Fig. 1 (a). Ideal c/a ratio of $\sqrt{\frac{32}{3}}$ has been assumed for calculation of b^2 values. Imperfect dislocations attached to stacking faults and composite dislocations with marginal stability, *i.e.* whose energy is equal to the sum of energies of the two component dislocations, have been included. In analogy with Thompson tetrahedron[12] for the f.c.c. structure and the bipyramid and the double tetrahedron respectively suggested by Berghezan *et al.*[13] and Damiano[14] for the h.c.p. structure, a double tetrahedron is shown in Fig. 1(b) in which possible dislocations in the d.h.c.p. structure can be conveniently illustrated. It may be noticed that the base of the tetrahedron in Fig. 1(b) has sides whose lengths are double the lattice vectors in the basal plane.

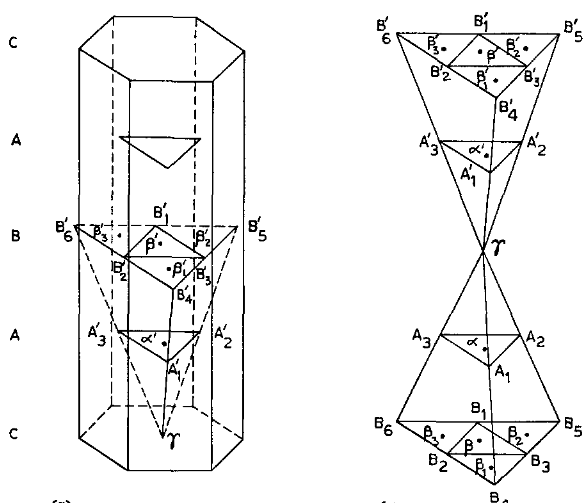

Fig. 1. Notation for Burgers vectors of dislocations in d.h.c.p. structure.

TABLE 1: DISLOCATIONS IN THE D.H.C.P. STRUCTURE

Dislocation	*Notation in Fig.* 1 *for b*	*Miller–Bravais notation for b*	b^2
Perfect	$B_1B'_1$	$\langle 0001 \rangle$	$\frac{32}{3}a^2$
	$B'_1B'_2$	$\frac{1}{3}\langle \bar{1}2\bar{1}0 \rangle$	a^2
	$B_1B'_2$	$\frac{1}{3}\langle \bar{1}2\bar{1}3 \rangle$	$\frac{35}{3}a^2$
Shockley	βB_1	$\frac{1}{3}\langle \bar{1}010 \rangle$	$\frac{1}{3}a^2$
Frank	$\alpha\beta$	$\frac{1}{4}\langle 0001 \rangle$	$\frac{2}{3}a^2$
	$\gamma\beta$	$\frac{1}{2}\langle 0001 \rangle$	$\frac{8}{3}a^2$
	$\alpha'\beta$	$\frac{3}{4}\langle 0001 \rangle$	$6a^2$
Frank + Shockley	$\alpha B_1(\alpha\beta+\beta B_1)$	$\frac{1}{12}\langle \bar{4}043 \rangle$	a^2
	$\gamma B_1(\gamma\beta+\beta B_1)$	$\frac{1}{6}\langle \bar{2}023 \rangle$	$3a^2$
	$\alpha' B_1(\alpha'\beta+\beta B_1)$	$\frac{1}{12}\langle \bar{4}049 \rangle$	$\frac{19}{3}a^2$
Frank + Perfect	$\alpha\beta_1(\alpha\beta+\beta\beta_1)$	$\frac{1}{12}\langle 4\bar{8}43 \rangle$	$\frac{5}{3}a^2$
	$\gamma\beta_1(\gamma\beta+\beta\beta_1)$	$\frac{1}{6}\langle 2\bar{4}23 \rangle$	$\frac{11}{3}a^2$
	$\alpha'\beta_1(\alpha'\beta+\beta\beta_1)$	$\frac{1}{12}\langle 4\bar{8}49 \rangle$	$7a^2$
Shockley + Perfect	$\beta B'_1(\beta B_1+B_1B'_1)$	$\frac{1}{3}\langle \bar{1}013 \rangle$	$11a^2$
	$\beta B_5(\beta B_1+B_1B_5)$	$\frac{2}{3}\langle \bar{1}100 \rangle$	$\frac{4}{3}a^2$
	$\beta B'_2(\beta B_1+B_1B'_2)$	$\frac{1}{3}\langle \bar{2}203 \rangle$	$12a^2$

3. STACKING FAULTS IN THE D.H.C.P. STRUCTURE

It is convenient to typify each fault by the virtual process that leads to its formation. The process so defined also naturally leads to the type of partials bounding the fault. Basically there are three operations, *viz.* glide, removal and insertion of layers of close-packed planes. Removal and insertion of up to three layers can be considered for the d.h.c.p. structure. When the operations of removal and insertion cause violation of close-packing conditions, the initial operation is followed by glide by $\pm \boldsymbol{S}$. In terms of partial dislocations, faults resulting from glide are bounded by Shockley partials ($\pm \boldsymbol{S}$) and those arising on account of removal or insertion of one ($\mp \frac{1}{4}\boldsymbol{F}$), two ($\mp \frac{1}{2}\boldsymbol{F}$) and three ($\mp \frac{3}{4}\boldsymbol{F}$) layers by Frank partials. Here $\boldsymbol{F}$ is the vector [0001]. Where removal and insertion are combined with glide the bounding dislocation is a composite of Frank and Shockley partials.

In Table 2 are listed the various operations and the faults. It is very useful to adopt the configurational notation. When a fault occurs there are interruptions in the regular ... ch ch ... sequence of the perfect d.h.c.p. structure. In the last column of Table 2 are given the number of interruptions of the first kind, namely when c is not followed by h or when h is not followed by c layer, as well as the number of interruptions of the second kind, namely when chc or hch sequences do not occur. A notation for faults is also suggested in terms of c and h layers that do not form part of a continuous ... ch ch ... sequence, similar to the notation in terms of Δ's and ∇'s.

Only those faults are further discussed in this paper which lead to a minimum number of interruptions of the stacking rule in any operation. When the number of interruptions of the first kind happen to be equal for two or more faults, those that lead to the smallest number of interruptions of the second kind are considered. It is also clear that two different operations can lead to the same fault, *e.g.* removal of two layers (No. 5 in Table 2) and insertion of two layers (No. 4(a) in Table 2) lead to Intrinsic–hh fault. In all, the following six intrinsic and one extrinsic type fault are considered important:

1. Intrinsic–c
2. Intrinsic–h
3. Intrinsic–ch
4. Intrinsic–cc
5. Intrinsic–hh
6. Intrinsic–ccc
7. Extrinsic–hcc

It is also possible to see from Table 2 that the configurational notation is preferable to the operator notation. Unlike in the f.c.c. and h.c.p. structures, interchange of Δ for ∇ or vice versa do not mean the same fault. The ultimate structure that results on successive introduction of any fault is also immediately indicated by the present notation. Thus Intrinsic–c fault transforms the d.h.c.p. structure to f.c.c. structure, Intrinsic–h fault to the h.c.p. structure. The stacking fault resulting from shear, if successively repeated, brings back the original structure. This is clear from the notation ch.

4. ESTIMATION OF THEORETICAL FAULT ENERGY

In the f.c.c. and h.c.p. structures, an Nth neighbour pair of planes in the perfect crystal can only be either like or unlike, *e.g.* in the perfect f.c.c. structure the second nearest neighbour planes can only be unlike (A–C, B–A) while in the perfect h.c.p. structure like (A–A, B–B). A distortional energy ψ_N may therefore be associated with every pair of planes of separation N which is not in the proper sequence. Hirth and Lothe have given expressions for the fault energy in terms of ψ_N multiplied by the number of such pairs of planes. For the d.h.c.p. structure, however, the second nearest neighbour planes in the per-

TABLE 2: STACKING FAULTS IN D.H.C.P. STRUCTURE*

Operation	Bounding partial	Faulted sequence: Roman letter notation	Faulted sequence: Operator notation	Type of fault: Intrinsic (I) or Extrinsic (E)	Type of fault: Operator notation	Type of fault: Configurational notation	No. of interruptions of the stacking rule: Interruptions of the 1st kind	No. of interruptions of the stacking rule: Interruptions of the 2nd kind
1	2	3	4	5	6	7	8	9
1. Glide	$\pm\boldsymbol{S}$	B A C A B A C A B A C A ↓ ↓ ↓ ↓ ↓ ↓ ↓ h c h c c h h c h c h c B A C A B∣C B C A C B C	∇∇ΔΔ∣Δ∇ΔΔ∣∇∇Δ	I	Δ∇ΔΔ	ch	2	4
2. Insertion of single layer	$+\frac{1}{4}\boldsymbol{F}$	h c h c c c h c h c h C A B A‖B‖C A B A C A B	ΔΔ∇∣ΔΔΔΔ∇∣∇ΔΔ	E	ΔΔΔΔ∇	hcc	3	5
3. Removal of single layer	$-\frac{1}{4}\boldsymbol{F}$	h c h c c c h c h c h B A C A B∣C A B A C A B	∇∇ΔΔ∣ΔΔΔ∣∇∇ΔΔ	I	ΔΔΔ	ccc	3	4
4. (a) Insertion of two layers	$+\frac{1}{2}\boldsymbol{F}$	h c h c h h c h c h c C A B A C∣A∣C∣A B A C A	ΔΔ∇∇Δ∣∇Δ∣Δ∇∇Δ	I	∇Δ	hh	2	3
(b) -do-	-do-	h c h c c h c c h c h c C A B A C‖B∣C∣A B A C A	ΔΔ∇∇∣∇Δ∣ΔΔ∇∇Δ	E	∇Δ	chcc	2	4
5. Removal of two layers	$-\frac{1}{2}\boldsymbol{F}$	h c h c h h h c h c h c C A B A C A∣C A B A C A	ΔΔ∇∇Δ∣∇Δ∣Δ∇∇Δ	I	∇Δ	hh	2	3
6. (a) Insertion of three layers	$+\frac{3}{4}\boldsymbol{F}$	h c h c c c c h c h c h C A B A C‖B A C∣A B A C	ΔΔ∇∇∣∇∇∇∣ΔΔ∇∇	I	∇∇∇	ccc	3	4
(b) -do-	-do-	h c h c h h c c h h c h C A B A C∣A∣C B∣A B A C	ΔΔ∇∇Δ∣∇∇∇∣Δ∇∇	E	∇∇∇	hcchh	3	6
(c) -do-	-do-	h c c h h c h h c h c h B A C‖B C B∣A B A C A B	∇∇∣∇Δ∇∇Δ∇∇∣ΔΔ	E	∇Δ∇∇Δ∇∇	chhch	3	6
(d) -do-	-do-	h c c c h h h h c h c h B A C‖B A B∣A B A C A B	∇∇∣∇∇Δ∇Δ∇∇∣ΔΔ	E	∇∇Δ∇Δ∇∇	cchhh	3	7
7. Removal of three layers			Leads to violation of close packing					

TABLE 2: (*continued*)

<table>
<tr><th rowspan="2">Operation</th><th rowspan="2">Bounding partial</th><th colspan="2">Faulted sequence</th><th colspan="3">Type of fault</th><th colspan="2">No. of interruptions of the stacking rule</th></tr>
<tr><th>Roman letter notation</th><th>Operator notation</th><th>Intrinsic (I) or Extrinsic (E)</th><th>Operator notation</th><th>Configurational notation</th><th>Interruptions of the 1st kind</th><th>Interruptions of the 2nd kind</th></tr>
<tr><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td><td>6</td><td>7</td><td>8</td><td>9</td></tr>
<tr><td>8. (a) Insertion of single layer followed by glide</td><td>$+\frac{1}{4}\boldsymbol{F} \pm \boldsymbol{S}$</td><td>A C A B A|A|C A B A C A
↓ ↓ ↓ ↓ ↓ ↓ ↓
c h c h c c h c h c h c
A C A B A C|B C A C B C</td><td>∇ΔΔ∇∇|∇|ΔΔ∇∇Δ</td><td>I</td><td>∇</td><td>c</td><td>1</td><td>2</td></tr>
<tr><td>(b) -do-</td><td>$+\frac{1}{4}\boldsymbol{F} \mp \boldsymbol{S}$</td><td>A C A B A|A|C A B A C A
↓ ↓ ↓ ↓ ↓ ↓ ↓
c h c h h h h c h c h c
A C A B A|B A B C B A B</td><td>∇ΔΔ∇|Δ|∇ΔΔ∇∇Δ</td><td>I</td><td>Δ</td><td>hhh</td><td>3</td><td>4</td></tr>
<tr><td>9. Removal of single layer followed by glide</td><td>$-\frac{1}{4}\boldsymbol{F} \pm \boldsymbol{S}$</td><td>A C A|A C A B A C A B A
↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓
c h c h h c h c h c h c
A C A B A|B C B A B C B</td><td>∇ΔΔ∇|ΔΔ∇|∇ΔΔ∇</td><td>I</td><td>ΔΔ∇</td><td>h</td><td>1</td><td>2</td></tr>
<tr><td>10. (a) Insertion of two layers followed by glide</td><td>$+\frac{1}{2}\boldsymbol{F} \pm \boldsymbol{S}$</td><td>A B A C A|A C|B A C A B
↓ ↓ ↓ ↓ ↓ ↓ ↓
c h c h c h c c c h c h
A B A C A B A C|B A B C</td><td>Δ∇∇ΔΔ|∇∇|∇∇ΔΔ</td><td>I</td><td>∇∇</td><td>cc</td><td>2</td><td>3</td></tr>
<tr><td>(b) -do-</td><td>-do-</td><td>A B A C|C B|A B A C A B
↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓
c h c h h c h h c h c h
A B A C A|C|B C B A B C</td><td>Δ∇∇Δ|∇∇|Δ∇∇ΔΔ</td><td>E</td><td>∇∇</td><td>hchh</td><td>2</td><td>4</td></tr>
<tr><td>(c) -do-</td><td>-do-</td><td>A C A B|B C|A C A B A C
↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓
c h c c c c h h c h c h
A C A B|C A|B A B C B A</td><td>∇ΔΔ|ΔΔΔ∇ΔΔ|∇∇</td><td>E</td><td>ΔΔΔ∇ΔΔ</td><td>ccch</td><td>4</td><td>6</td></tr>
<tr><td>11. Removal of two layers followed by glide</td><td></td><td></td><td colspan="6">Not considered because removal of two layers does not violate close-packing condition</td></tr>
</table>

TABLE 2: (*continued*)

Operation	*Bounding partial*	*Faulted sequence*: *Roman letter notation*	*Faulted sequence*: *Operator notation*	*Type of fault*: *Intrinsic (I) or Extrinsic (E)*	*Type of fault*: *Operator notation*	*Type of fault*: *Configurational notation*	*No. of interruptions of the stacking rule*: *Interruptions of the 1st kind*	*No. of interruptions of the stacking rule*: *Interruptions of the 2nd kind*
1	2	3	4	5	6	7	8	9
12. (a) Insertion of three layers followed by glide	$+\frac{3}{4}F \pm S$	A B A C|C A C|A B A C A ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ c h c h c h h c h c h c A B A C A B A|B C B A B	Δ∇∇ΔΔ∇|ΔΔ∇|∇Δ	I	ΔΔ∇	h	1	2
(b) -do-	-do-	A B A C|C A C|A B A C A ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ c h c c h h h c h c h c A B A C|B C|B C A C B C	Δ∇∇|∇Δ∇|ΔΔ∇∇Δ	E	∇Δ∇	chh	3	5
(c) -do-	-do-	B A C|C A B|A B A C A B ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ h c c h c h h h c h c h B A C|B C A|C A C B C A	∇∇|∇ΔΔ∇Δ∇∇|ΔΔ	E	∇ΔΔ∇Δ∇∇	chchh	3	5
(d) -do-	-do-	C A B A|A C B|C A B A C ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ h c h c c c h c c h c h C A B A C|B A|B C A C B	ΔΔ∇∇|∇∇Δ|ΔΔ∇∇	E	∇∇Δ	cchcc	3	5
(e) -do-	-do-	A C A B A|A C A|C A B A ↓ ↓ ↓ ↓ ↓ ↓ ↓ c h c h h h h h h c h c A C A B A|B A|B A B C B	∇ΔΔ∇|Δ∇Δ|∇ΔΔ∇	E	Δ∇Δ	hhhhh	5	6
13. (a) Removal of three layers followed by glide	$-\frac{3}{4}F \pm S$	A B A C|C A B A C A B A ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ c h c h c c h c h c h c A B A C A B|C B A B C B	Δ∇∇ΔΔ|Δ|∇∇ΔΔ∇	I	Δ	c	1	2
(b) -do-	-do-	A C A B A|A C A B A C A ↓ ↓ ↓ ↓ ↓ ↓ ↓ c h c h h h h c h c h c A C A B A|B A B C B A B	∇ΔΔ∇|Δ|∇ΔΔ∇∇Δ	I	Δ	hhh	3	4

* Full vertical lines indicate the position where the insertion or removal of close-packed planes has occurred, dotted lines indicate the position of the fault and full horizontal lines the configurational notation for the fault. Arrows indicate glide.

fect crystal itself can be either like (A–A) or unlike (B–C). There may thus be an excess like or unlike second nearest neighbour pair of planes in different faults implying opposite kind of fault energies. This and related anomalies are overcome if the close-packed planes are identified by the configurational symbols. We can then represent the interaction energy of like Nth neighbour pairs of planes by S_N and of unlike pairs by D_N. The configurations of planes in the pair are given in the superscript. Thus in the perfect structure the first, second, third and fourth neighbour interaction energies are respectively D_1^{ch} or D_1^{hc}, S_2^{cc} or D_2^{hh}, D_3^{ch} or D_3^{hc} and S_4^{cc} or S_4^{hh}. Consideration of symmetry and stability of the structure suggest that

$$D^{ch}_{4N-3} = D^{hc}_{4N-3} \tag{1}$$

$$S^{cc}_{4N-2} = D^{hh}_{4N-2} \tag{2}$$

$$D^{ch}_{4N-1} = D^{hc}_{4N-1} \tag{3}$$

$$S^{cc}_{4N} = S^{hh}_{4N} \tag{4}$$

When a fault occurs, some layers change their position and configuration and consequently the interaction energies, *e.g.* D_1^{ch} may become either D_1^{cc} or D_1^{hh}. The distortional energy ψ_N is the difference of the interaction energy in the faulted structure from that in the perfect structure. It is obvious that in contrast with the treatment of Hirth and Lothe, the distortional energy is no longer the same for all pairs of planes of same separation N which are not in the proper sequence and the total distortional energy is not a simple multiple of ψ_N. In terms of the S's and D's, we define the distortional energies as follows (N ranges from 1 to ∞ except for ψ''_{4N-3}, ψ'''_{4N-3} and ψ''''_{4N-3} where the range is from 2 to ∞):

$$\psi_{4N-3} = D^{cc}_{4N-3} - D^{ch}_{4N-3} \tag{5}$$

$$\psi'_{4N-3} = D^{hh}_{4N-3} - D^{ch}_{4N-3} \tag{6}$$

$$\psi''_{4N-3} = S^{cc}_{4N-3} - D^{ch}_{4N-3} \tag{7}$$

$$\psi'''_{4N-3} = S^{ch}_{4N-3} - D^{ch}_{4N-3} \tag{8}$$

$$\psi''''_{4N-3} = S^{hh}_{4N-3} - D^{ch}_{4N-3} \tag{9}$$

$$\psi_{4N-2} = D^{cc}_{4N-2} - D^{hh}_{4N-2} \tag{10}$$

$$\psi'_{4N-2} = S^{hh}_{4N-2} - D^{hh}_{4N-2} \tag{11}$$

$$\psi''_{4N-2} = D^{ch}_{4N-2} - D^{hh}_{4N-2} \tag{12}$$

$$\psi'''_{4N-2} = S^{ch}_{4N-2} - D^{hh}_{4N-2} \tag{13}$$

$$\psi_{4N-1} = S^{cc}_{4N-1} - D^{ch}_{4N-1} \tag{14}$$

$$\psi'_{4N-1} = D^{hh}_{4N-1} - D^{ch}_{4N-1} \tag{15}$$

$$\psi''_{4N-1} = D^{cc}_{4N-1} - D^{ch}_{4N-1} \tag{16}$$

$$\psi'''_{4N-1} = S^{ch}_{4N-1} - D^{ch}_{4N-1} \tag{17}$$

$$\psi''''_{4N-1} = S^{hh}_{4N-1} - D^{ch}_{4N-1} \tag{18}$$

$$\psi_{4N} = D^{cc}_{4N} - S^{cc}_{4N} \tag{19}$$

$$\psi'_{4N} = D^{ch}_{4N} - S^{cc}_{4N} \tag{20}$$

$$\psi''_{4N} = S^{ch}_{4N} - S^{cc}_{4N} \tag{21}$$

$$\psi'''_{4N} = D^{hh}_{4N} - S^{cc}_{4N} \tag{22}$$

The fault energy γ can now be written by adding the appropriate distortional energy terms. We give below the fault energies (I and E in suffix to γ refer to Intrinsic and Extrinsic faults respectively) as also γ_{TC} and γ_{TH} which represent respectively the d.h.c.p. → f.c.c. and d.h.c.p. → h.c.p. transformation energies per layer. The limits for the summation are always $N = 1$ to ∞.

$$\begin{aligned}\gamma_{I-c} = \psi_1 + \Sigma\,[&2N\psi''_{4N-2} + (2N-2)\psi'''_{4N-2} \\ &+ (N-1)\psi'_{4N-1} + 2N\psi''_{4N-1} \\ &+ N\psi''''_{4N-1} \\ &+ 2N\psi''_{4N} + 2N\psi'''_{4N} \\ &+ (2N+1)\psi_{4N+1} + 2N\psi'_{4N+1}]\end{aligned} \tag{23}$$

$$\begin{aligned}\gamma_{I-h} = \psi'_1 + \Sigma\,[&(2N-2)\psi''_{4N-2} + 2N\psi'''_{4N-2} \\ &+ 2N\psi'_{4N-1} + (2N-1)\psi''_{4N-1} \\ &+ 2N\psi''_{4N} + 2N\psi'''_{4N} \\ &+ 2N\psi_{4N+1} + (N+1)\psi'_{4N+1} \\ &+ N\psi'''_{4N+1}]\end{aligned} \tag{24}$$

$$\begin{aligned}\gamma_{I-ch} = \psi_1 + \psi'_1 + \Sigma\,[&(2N-2)\psi_{4N-2} \\ &+ (N-1)\psi'_{4N-2} \\ &+ 2\psi''_{4N-2} + 2\psi'''_{4N-2} \\ &+ \psi'_{4N-1} + 2\psi''_{4N-1} \\ &+ (2N-2)\psi'''_{4N-1} + \psi''''_{4N-1} \\ &+ (2N-1)\psi_{4N} + 2\psi''_{4N} \\ &+ 2\psi'''_{4N} + (2N-1)\psi''''_{4N} \\ &+ 2\psi_{4N+1} + 2\psi'_{4N+1} \\ &+ 2N\psi'''_{4N+1}]\end{aligned} \tag{25}$$

$$\begin{aligned}\gamma_{I-cc} = 2\psi_1 + \Sigma\,[&(2N-1)\psi_{4N-2} + 2\psi''_{4N-2} \\ &+ 2\psi''_{4N-1} + 2N\psi'''_{4N-1} \\ &+ 2N\psi_{4N} + 2\psi'''_{4N} \\ &+ 2\psi_{4N+1} + 2N\psi''_{4N}]\end{aligned}$$

$$\gamma_{\mathrm{I-hh}} = 2\psi'_1 + \Sigma[(2N-1)\psi'_{4N-2} + 2\psi'''_{4N-2} + 2\psi'_{4N-1} + 2\psi'''_{4N} + 2N\psi''''_{4N} + 2\psi'_{4N+1}] \qquad (27)$$

$$\gamma_{\mathrm{I-ccc}} = 3\psi_1 + \Sigma[2\psi_{4N-2} + (4N-2)\psi''_{4N-2} + (2N-1)\psi_{4N-1} + 2\psi''_{4N-1} + 2\psi'''_{4N-1} + (2N-2)\psi''''_{4N-1} + 2\psi_{4N} + (4N-2)\psi''_{4N} + 2\psi'''_{4N} + 2\psi_{4N+1} + (2N-1)\psi'_{4N+1} + 2N\psi''_{4N+1}] \qquad (28)$$

$$\gamma_{\mathrm{E-hcc}} = 2\psi_1 + \psi'_1 - \psi_2 + 2\psi''_2 + \Sigma[2\psi_{4N-2} + (4N-4)\psi''_{4N-2} + 2\psi'''_{4N-2} + (2N-2)\psi_{4N-1} + (2N-1)\psi'_{4N-1} + 2\psi''_{4N-1} + 2\psi'''_{4N-1} + 2\psi_{4N} + (4N-2)\psi''_{4N} + 2\psi'''_{4N} + \psi''''_{4N} + 2\psi_{4N+1} + \psi'_{4N+1} + (2N-1)\psi''_{4N+1} + 2\psi'''_{4N+1} + (2N-1)\psi''''_{4N+1}] \qquad (29)$$

$$\gamma_{\mathrm{TC}} = \Sigma[\psi_{6N-5} + \psi_{6N-4} + \psi_{6N-3} + \psi_{6N-2} + \psi_{6N-1} + \tfrac{1}{2}\psi_{6N}] \qquad (30)$$

$$\gamma_{\mathrm{TH}} = \Sigma[\psi'_{2N-1} + \psi'_{4N-1}]\,. \qquad (31)$$

5. COMPARISON OF FAULT ENERGIES

We shall consider only the first and second neighbour interactions in order to be able to compare the fault energies for the following three idealised situations:

1. $\gamma_{\mathrm{TC}} = \gamma_{\mathrm{TH}}$ and $\gamma_{\mathrm{I-c}} = \gamma_{\mathrm{I-h}}$

which gives

$$\psi_1 = \psi'_1, \quad \psi_2 = \psi'_2, \quad \psi''_2 = \psi'''_2\,,$$

2. $\gamma_{\mathrm{TC}} \gg \gamma_{\mathrm{TH}}$ and $\gamma_{\mathrm{I-c}} \gg \gamma_{\mathrm{I-h}}$

which gives

$$\psi'_1 = \psi'_2 = \psi'''_2 = \infty\,,$$

3. $\gamma_{\mathrm{TC}} \ll \gamma_{\mathrm{TH}}$ and $\gamma_{\mathrm{I-c}} \ll \gamma_{\mathrm{I-h}}$

which gives

$$\psi_1 = \psi_2 = \psi''_2 = \infty\,.$$

$\gamma_{\mathrm{TC}} \gg \gamma_{\mathrm{TH}}$ and $\gamma_{\mathrm{TC}} \ll \gamma_{\mathrm{TH}}$ correspond respectively to cases where d.h.c.p.$\rightleftharpoons$h.c.p. and d.h.c.p.$\rightleftharpoons$f.c.c. transformations occur. In Table 3 are listed the fault energies for the above three cases.

When $\gamma_{\mathrm{TC}} = \gamma_{\mathrm{TH}}$ and Intrinsic–c and Intrinsic–h faults have equal energy, this energy is one-half the energy associated with Intrinsic–ch faults. Faults consequent to removal and insertion of single layers, namely Intrinsic–ccc and Extrinsic–hcc respectively, have the highest energy. Faults arising on account of insertion of two layers with or without glide, namely Intrinsic–cc and Intrinsic–hh respectively, have the same energy, which, interestingly enough, is lower than that of the fault due to insertion of single layer. When $\gamma_{\mathrm{TC}} \ll \gamma_{\mathrm{TH}}$ Intrinsic–c faults and when $\gamma_{\mathrm{TH}} \ll \gamma_{\mathrm{TC}}$ Intrinsic–h faults have minimum energy.

In an actual situation, however, as observed by Gallagher[15], formation barriers may restrict the amount of faulting of various types which in no way should be taken to imply that the corresponding energies are in the same ratio as observed numbers of faults. The picture appears to be clear only with regard to Intrinsic–ch faults requiring only nucleation of a Shockley partial dislocation. These must be present in deformed d.h.c.p. crystals. It is difficult to predict the barriers for faults which require insertion or removal of close-packed planes.

TABLE 3: STACKING FAULT ENERGIES IN THE D.H.C.P. STRUCTURE

Fault	*Fault energy*		
	$\gamma_{\mathrm{TC}} \ll \gamma_{\mathrm{TH}}$	$\gamma_{\mathrm{TC}} \gg \gamma_{\mathrm{TH}}$	$\gamma_{\mathrm{TC}} = \gamma_{\mathrm{TH}}$
1. Intrinsic–c	$\psi_1 + 2\psi''_2$	∞	$\psi_1 + 2\psi''_2$
2. Intrinsic–h	∞	$\psi'_1 + 2\psi'''_2$	$\psi_1 + 2\psi''_2$
3. Intrinsic–ch	∞	∞	$2\psi_1 + 4\psi''_2$
4. Intrinsic–cc	$2\psi_1 + \psi_2 + 2\psi''_2$	∞	$2\psi_1 + \psi_2 + 2\psi''_2$
5. Intrinsic–hh	∞	$2\psi'_1 + \psi'_2 + 2\psi'''_2$	$2\psi_1 + \psi_2 + 2\psi''_2$
6. Intrinsic–ccc	$3\psi_1 + 2\psi_2 + 2\psi''_2$	∞	$3\psi_1 + 2\psi_2 + 2\psi''_2$
7. Extrinsic–hcc	∞	∞	$3\psi_1 + \psi_2 + 4\psi''_2$

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