nuclei can both lead to binding relative to the promolecule.

Nevertheless the value of analyses of $\Delta\rho$ in terms of binding alone must be questioned. It is clear from our analyses on N_2 and F_2 that major sources of binding are large sharp changes in density close to the nuclei. The deformation density in the centre of the bond, or far beyond the nuclei, plays little or no role in binding the nuclei. This does not imply, however, that broad topographical features are unimportant in chemical bonding. The broad topographical characteristics of the density are determined by the requirements of antisymmetry in the wavefunction, modulated by polarization terms that minimize the energy. These broad features make significant contributions to the binding energy, which is fundamental to chemical bonding.

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Geometrical Representation of the Algebraic Properties of Crystallographic Slip Systems

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Abstract

Highly symmetrical crystalline materials usually possess a sufficient number of equivalent slip systems to accommodate a given plastic strain, *i.e.* to identify five components in a second-rank tensor. A direct geometrical representation would thus require a five-dimensional space when applied to any superabundant set of slip systems. However, such a difficulty can be avoided: a three-dimensional polyhedron of appropriate crystallographic symmetry is found to provide a correct description of all interdependence relationships between the glide systems. As an example, this isomorphism is used here in the effective selection of active slips.

The accommodation of a given plastic strain in polycrystalline materials may involve a number of different mechanisms (depending on dislocation motions) and their possible combinations such as slip or twin-

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Table 1. *Identification of the twelve strain tensors* $\mathbf{u}_k$

$$\mathbf{u}_1=\frac{1}{\sqrt{6}}\begin{pmatrix}-1&-1&-1\\1&1&1\\0&0&0\end{pmatrix}\qquad \mathbf{u}_2=\frac{1}{\sqrt{6}}\begin{pmatrix}1&1&1\\0&0&0\\-1&-1&-1\end{pmatrix}$$

$$\mathbf{u}_3=\frac{1}{\sqrt{6}}\begin{pmatrix}0&0&0\\-1&-1&-1\\1&1&1\end{pmatrix}\qquad \mathbf{u}_4=\frac{1}{\sqrt{6}}\begin{pmatrix}-1&-1&1\\1&1&-1\\0&0&0\end{pmatrix}$$

$$\mathbf{u}_5=\frac{1}{\sqrt{6}}\begin{pmatrix}1&1&-1\\0&0&0\\1&1&-1\end{pmatrix}\qquad \mathbf{u}_6=\frac{1}{\sqrt{6}}\begin{pmatrix}0&0&0\\-1&-1&1\\-1&-1&1\end{pmatrix}$$

$$\mathbf{u}_7=\frac{1}{\sqrt{6}}\begin{pmatrix}-1&1&-1\\-1&1&-1\\0&0&0\end{pmatrix}\qquad \mathbf{u}_8=\frac{1}{\sqrt{6}}\begin{pmatrix}1&-1&1\\0&0&0\\-1&1&-1\end{pmatrix}$$

$$\mathbf{u}_9=\frac{1}{\sqrt{6}}\begin{pmatrix}0&0&0\\1&-1&1\\1&-1&1\end{pmatrix}\qquad \mathbf{u}_{10}=\frac{1}{\sqrt{6}}\begin{pmatrix}-1&1&1\\-1&1&1\\0&0&0\end{pmatrix}$$

$$\mathbf{u}_{11}=\frac{1}{\sqrt{6}}\begin{pmatrix}1&-1&-1\\0&0&0\\1&-1&-1\end{pmatrix}\qquad \mathbf{u}_{12}=\frac{1}{\sqrt{6}}\begin{pmatrix}0&0&0\\1&-1&-1\\-1&1&1\end{pmatrix}$$

ning inside individual crystallites as well as edge accommodations along grain boundaries (de Fouquet, 1975).

Slip has been identified as the effective accommodation mechanism for grains of high crystallographic symmetry. This situation occurs in cubic materials providing a sufficient number of equivalent degenerate glide systems. For both b.c.c. and f.c.c. lattices, the slip direction has been found to correspond respectively to the dense ⟨111⟩ and ⟨110⟩ rows. However, some controversy remains in slip-plane determinations especially in the case of b.c.c. structures where ⟨110⟩, ⟨112⟩ and ⟨123⟩ perpendicular directions have been observed at high temperatures (Kroupa, 1968).

The following discussion is restricted for convenience to the superabundant set of twelve glides representing the {111}⟨110⟩ slip systems in f.c.c. crystals. In any one of the twelve slip coordinate systems, the corresponding basic unitary strain $\mathbf{u}_k$ and its symmetrical part $\mathbf{e}_k$ ($k=1, 12$) are given by the second-rank tensors

$$\mathbf{u}_k=\begin{pmatrix}0&0&0\\0&0&1\\0&0&0\end{pmatrix},\qquad \mathbf{e}_k=\frac{1}{2}\begin{pmatrix}0&0&0\\0&0&1\\0&1&0\end{pmatrix}. \qquad (1)$$

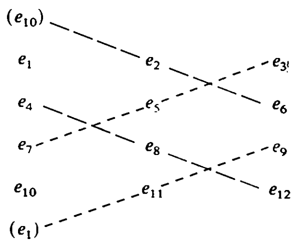
The remaining antisymmetrical part allows the prediction of the pure rotational effects of the grains and hence the texture formation.

The use of a convenient Euler matrix for every glide brings the above expressions into the [100], [010], [001] crystal coordinate system, a specific identification of the twelve strain tensors $\mathbf{u}_k$ being given in Table 1. Further simple calculations then determine both antisymmetrical and symmetrical components. In a similar way, identical results are also obtained for b.c.c. crystals and {110}⟨111⟩ slip systems since

$$(\mathbf{u}_{ij})_k^{\text{b.c.c.}}=(\mathbf{u}_{ji})_k^{\text{f.c.c.}}. \qquad (2)$$

Hence, the twelve $\mathbf{e}_k$ tensors (Royer, Mohr & Tavard, 1978) can be used to represent indistinctly pure deformation in both b.c.c. and f.c.c. materials, since an interchange between the glide direction and the normal to the slip plane in {111} ⟨110⟩ f.c.c. and {110} ⟨111⟩ b.c.c. systems does not affect the expressions of the pure deformation tensors $\mathbf{e}_k$.

Table 2. *Interdependence relationships: the twelve-element algebraic modulus*



The above set is found superabundant, *i.e.* five independent systems are sufficient here to reproduce any pure deformation. Their simplest interdependence relationships are listed below as

$$\begin{aligned}
\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3&=0, & \mathbf{e}_1+\mathbf{e}_9+\mathbf{e}_{11}&=0,\\
\mathbf{e}_4+\mathbf{e}_5+\mathbf{e}_6&=0, & \mathbf{e}_2+\mathbf{e}_6+\mathbf{e}_{10}&=0,\\
\mathbf{e}_7+\mathbf{e}_8+\mathbf{e}_9&=0, & \mathbf{e}_3+\mathbf{e}_5+\mathbf{e}_7&=0,\\
\mathbf{e}_{10}+\mathbf{e}_{11}+\mathbf{e}_{12}&=0, & \mathbf{e}_4+\mathbf{e}_8+\mathbf{e}_{12}&=0,
\end{aligned} \qquad (3)$$

and

$$\begin{aligned}
\mathbf{e}_1+\mathbf{e}_4&=\mathbf{e}_7+\mathbf{e}_{10},\\
\mathbf{e}_2+\mathbf{e}_8&=\mathbf{e}_5+\mathbf{e}_{11},\\
\mathbf{e}_3+\mathbf{e}_{12}&=\mathbf{e}_6+\mathbf{e}_9.
\end{aligned} \qquad (4)$$

A useful graph (Table 2) has already been used in preliminary attempts to describe this twelve-element algebraic modulus, *i.e.* to supply a symbolic representation of (3) and (4).

Furthermore, the following set of six basic tensors $\mathbf{v}_J$ (Table 3) can be verified as simultaneously having null projections on eight of the $\mathbf{e}_k$ systems. The four remaining ones [as listed below in (5)] are then equal in magnitude:

$$\begin{aligned}
&(\text{I}) && \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_{10}, \mathbf{e}_{11};\\
&(\text{II}) && \mathbf{e}_1, \mathbf{e}_3, \mathbf{e}_7, \mathbf{e}_9;\\
&(\text{III}) && \mathbf{e}_2, \mathbf{e}_3, \mathbf{e}_5, \mathbf{e}_6;\\
&(\text{IV}) && \mathbf{e}_4, \mathbf{e}_5, \mathbf{e}_7, \mathbf{e}_8;\\
&(\text{V}) && \mathbf{e}_4, \mathbf{e}_6, \mathbf{e}_{10}, \mathbf{e}_{12};\\
&(\text{VI}) && \mathbf{e}_8, \mathbf{e}_9, \mathbf{e}_{11}, \mathbf{e}_{12}.
\end{aligned} \qquad (5)$$

Table 3. *Basic tensors* $\mathbf{v}_J$

$$\mathbf{v}_1=\frac{\tau\sqrt{6}}{2}\begin{pmatrix}0&0&0\\0&1&1\\0&1&1\end{pmatrix}\qquad \mathbf{v}_2=\frac{\tau\sqrt{6}}{2}\begin{pmatrix}1&0&1\\0&0&0\\1&0&1\end{pmatrix}$$

$$\mathbf{v}_3=\frac{\tau\sqrt{6}}{2}\begin{pmatrix}1&1&0\\1&1&0\\0&0&0\end{pmatrix}\qquad \mathbf{v}_4=\frac{\tau\sqrt{6}}{2}\begin{pmatrix}0&0&0\\0&1&-1\\0&-1&1\end{pmatrix}$$

$$\mathbf{v}_5=\frac{\tau\sqrt{6}}{2}\begin{pmatrix}1&0&-1\\0&0&0\\-1&0&1\end{pmatrix}\qquad \mathbf{v}_6=\frac{\tau\sqrt{6}}{2}\begin{pmatrix}1&-1&0\\-1&1&0\\0&0&0\end{pmatrix}$$

This specific property was used to simplify Bishop's geometrical description of the multidimensional plastic yield surface (Bishop, 1953). Indeed, convenient combinations of $\mathbf{v}_J$ reproduce the twenty-eight Bishop stress states.

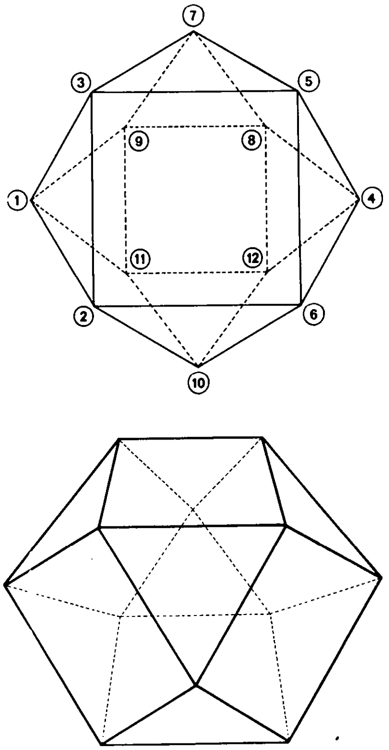


Fig. 1. Geometrical representation of the interdependence relationships.

Table 4. *Selection of pairs of active glide systems, classification of geometrically equivalent combinations*

1-2, 1-3, 1-9, 1-11, ...
1-7, 1-10, ...
1-5, 1-6, 1-8, 1-12, ...
1-4, (2-8, 3-12, 5-11, 6-9, 7-10)

However, a more efficient representation of the above properties was found, depicted in three-dimensional space by the eight triangular and six square faces of a regular polyhedron, which obviously possesses cubic symmetry (Fig. 1). The square faces of this tetareskaidecahedron correspond here to the $\mathbf{v}_J$ basic tensor properties. Furthermore, (3) and (4) result from a convenient linkage between three or four corresponding corners.

This isomorphism allows the geometrical properties of a given set of independent active slip systems as used in relaxed Taylor models of plastic deformation (Van Houtte, 1982; Tavard & Royer, 1984) to be pointed out. It also helps to classify the $\binom{12}{n}$ possible combinations between n glides ($n = 1, 5$) in symmetrically equivalent configurations (Kocks, Canova & Jonas, 1983). In the example shown in Table 4, the geometrically equivalent combinations of two active glides are built up systematically from those symmetry properties exhibited in Fig. 1.

While this three-dimensional representation is here employed for multidimensional tensor properties it may of course be extended to any other species of crystallographic slips.

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