

$$dH(y) = \frac{1}{2\sqrt{\pi}\sigma} [\exp(-y^2/4\sigma^2)] [1 + (2\sigma^2 - y^2)/4d^2] dy. \quad (7)$$

In this case the variance of the difference is $2\sigma^2$. As long as $\sigma \ll d$ the correction term is negligible and for all practical purposes the distribution $dH(y)$ can be treated as normal.

In calculating the distributions we have assumed that the atomic coordinates of the actual crystal structure are uncorrelated normal variates with small isotropic errors. In practice this condition is often rather well met and at least in these cases the distribution of interatomic distances is normal to a good approximation. The difference between two independently determined interatomic distances is then normally distributed to an even better approximation than the distances themselves [cf. equations (6) and (7)]. We therefore conclude that in most, if not all cases crystallographically independent molecular geometries can be compared using the powerful method of normal probability plot analysis, as suggested by De Camp (1973).

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On symmetric variations of fault energies. By A. G. CROCKER and P. D. BRISTOWE, *Department of Physics, University of Surrey, Guildford GU2 5XH, England*

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The distribution of interatomic distances across unrelaxed stacking faults is shown to be independent of the sense of the fault vector if the shear plane is perpendicular to an n -fold axis or if the shear direction is parallel to an n -fold axis. Hence the unrelaxed energies of such faults, calculated using pair potentials, are symmetric with respect to the sense of the shear.

In a recent computer simulation study of generalized stacking faults in body-centred cubic crystals (Bristowe, Crocker & Norgett, 1974) it was found that the unrelaxed energy of the faults was independent of the sense of the shear direction. The faults were all on (112) planes and the displacements were in $\pm[1\bar{1}\bar{1}]$ directions. In addition the interatomic pair potential used to evaluate their energy terminated between second and third nearest neighbours. The aim of the work was to determine the structure and energy of the faults which arise on allowing the atoms to relax, subject to the pair potential, from their initial sheared positions to equilibrium configurations. However, the symmetric variation of the unrelaxed energy has also proved to be of interest. This energy is the sum of the pair interactions between atoms which, for a given potential $\phi(r)$, are defined by the interatomic spacings r . Thus a symmetric variation of fault energy indicates that positive and negative rigid-body shears produce identical distributions of distorted bond lengths. This is illustrated for the special case of the b.c.c. fault in Fig. 1. It suggests the following general problem which will be the subject matter of the present note: Given a crystal which undergoes a rigid-body shear on a plane $h_i = (h_1 h_2 h_3)$ in a direction $u^i = [u^1 u^2 u^3]$ under what conditions are the distributions of distorted bond lengths for positive and negative shears identical?

Consider first a bond defined by the lattice vector $p^i = [p^1 p^2 p^3]$ in the undistorted crystal. If the shear plane h_i cuts this bond the vector becomes $p^i \pm au^i$ in the faulted crystal. Here a is a parameter defining the magnitude of the displacement and the two signs correspond to the two senses

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References

- ABRAHAMS, S. C. & KEVE, E. T. (1971). *Acta Cryst.* A27, 157–165.
 ALBERTSSON, J., GRENTHE, I. & HERBERTSSON, H. (1973). *Acta Cryst.* B29, 2839–2844.
 DE CAMP, W. H. (1973). *Acta Cryst.* A29, 148–150.
 KENDALL, M. G. & STUART, A. (1961). *The Advanced Theory of Statistics*, Vol. 2, pp. 227–229. New York: Hefner.
 KENDALL, M. G. & STUART, A. (1963). *The Advanced Theory of Statistics*, Vol. 1, 2nd ed., p. 263. New York: Hefner.
 OSKARSSON, Å. (1974). To be published.
 TEMPLETON, D. H. (1959). *Acta Cryst.* 12, 771–773.

of the shear. The length of the bond is thus changed from $l = (p^i p^i c_{ij})^{1/2}$ to

$$l^\pm = [(p^i p^i + a^2 u^i u^i \pm 2ap^i u^i) c_{ij}]^{1/2}$$

where c_{ij} is the direct metric tensor. Clearly $l^+ \neq l^-$ and thus if the collected bond lengths for opposite shears are to be identical another vector q^i must exist which gives rise to distorted bond lengths L^\pm satisfying $L^\pm = l^\mp$ for all values of a . For this to occur p^i and q^i must be crystallographically equivalent variants r_1^i and r_2^i , of a particular vector form r^i ,

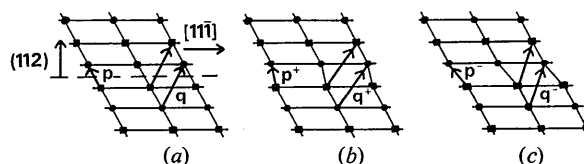


Fig. 1. Faults on a (112) plane in a b.c.c. crystal projected on to a (1 $\bar{1}$ 0) plane, atoms represented by circles and squares lying in adjacent (1 $\bar{1}$ 0) planes. The nearest-neighbour bonds $p = \frac{1}{2}[1\bar{1}\bar{1}]$ and $q = \frac{1}{2}[111]$ shown in the perfect crystal (a) are decreased in length and increased in length respectively by the shear in the $[11\bar{1}]$ direction shown in (b). These changes in length of p and q in (b) are exactly equal to the changes in length of q and p respectively arising from the equal and opposite shear shown in (c). Note that the fault plane intersects two bonds parallel to q but only one parallel to p for each atom in the interface. However in this projection the vector p may also be considered to represent the nearest-neighbour bond $\frac{1}{2}[\bar{1}\bar{1}1]$ so that equal numbers of bonds are in fact extended and contracted.

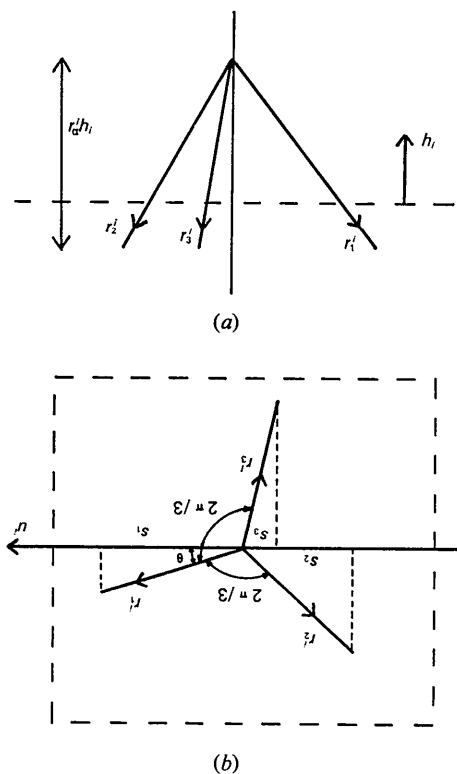


Fig. 2. Relationships between a triad of bond vectors r_α^i ($\alpha = 1, 2, 3$) related by a three-fold axis, which is perpendicular to a fault plane h_i . Diagram (a) shows h_i (broken line) in section and demonstrates that $r_\alpha^i h_i$ is constant for the three vectors. Diagram (b) shows a plan view of h_i and indicates that the projections of the vectors r_α^i on the plane h_i make angles of θ , $\theta + 2\pi/3$ and $\theta + 4\pi/3$ with u^i . In addition their projections on u^i have lengths s_α such that $\sum s_\alpha = 0$.

which satisfy $r_1^i u^j c_{ij} = -r_2^i u^j c_{ij}$. Matched pairs of this kind must of course arise for all possible variants r_α^i of r^i . In addition, as indicated in Fig. 1 for the b.c.c. fault, for each r_α^i there will be $r_\alpha^i h_i$ parallel bonds which cross the fault for each atom in the plane h_i . Hence to obtain identical distributions of bond lengths for opposite shears the condition

$$\sum_{\alpha} (r_\alpha^i h_i) (r_\alpha^i u^j c_{ij}) = 0 \quad (1)$$

must be satisfied for all lattice vectors r^i .

There are two groups of solutions of equation (1). The first arises when the shear plane h_i is perpendicular to an n -fold axis. The vectors r_α^i then occur in groups of n with

$(r_\alpha^i h_i)$ constant, as shown for the case of $n=3$ in Fig. 2(a). Thus equation (1) reduces to

$$\sum_{\alpha=1}^n (r_\alpha^i u^j c_{ij}) = 0$$

which is equivalent to the identity

$$\sum_{\alpha=1}^n \cos \left(\theta + \frac{2(\alpha-1)\pi}{n} \right) = 0$$

where, as shown in Fig. 2(b), θ is the angle between u^i and the projection of r_1^i on to the plane h_i . Thus equation (1) is satisfied by each group of n vectors and hence by all vectors r^i crossing the fault plane. Similarly the second group of solutions arises when the shear direction u^i is parallel to an n -fold axis. The term $(r_\alpha^i u^j c_{ij})$ is then constant so that equation (1) reduces to $\sum_{\alpha=1}^n (r_\alpha^i h_i) = 0$, which is equivalent to the above identity if θ is now the angle between h_i and the projection of r_1^i on to the plane normal to u^i . Note that in these two solutions the second shear elements, u^i and h_i respectively, are unrestricted, as is the number of crystallographically distinct bonds r^i . However, for crystals, n is restricted to 2, 3, 4 and 6. For $n=2$ and 4, when the shear plane is a mirror plane or the shear direction is perpendicular to a mirror plane, these solutions are trivial as the structures of the pairs of faults are identical, although oriented differently. However for $n=3$ and 6 positive and negative shears produce distinct structures for the faults, so that the fact that identical sets of distorted bond lengths occur in the two cases is most unexpected.

Returning to the $(112) [11\bar{1}]$ faults in b.c.c. crystals which prompted this study, it is now seen that they produce symmetric variations in fault energies because the shear direction is a threefold axis. The same result would also have been obtained for any shear plane $(h_1, h_2, h_1 + h_2)$ containing this axis and for any pair potential extending to any number of neighbours. Also the crystal structure need not have been b.c.c. as long as the shear direction remained a threefold axis. Finally in the b.c.c. structure symmetric unrelaxed fault energies must also arise for shears in any direction on the $\{110\}$ and $\{111\}$ planes and for shears on any plane in the $\langle 110 \rangle$ direction.

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Reference

- BRISTOWE, P. D., CROCKER, A. G. & NORGETT, M. J. (1974). *J. Phys. F*, In the press.