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THE ORDERING OF CRYSTALLOGRAPHIC SHEAR PLANES: THEORY OF REGULAR ARRAYS

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Abstract—In certain non-stoichiometric transition metal oxides, crystallographic shear planes are found instead of isolated oxygen vacancies. These planes tend to form arrays with regular spacings. The interactions responsible for this ordering have not been understood in the past. We propose that the major interaction comes from elastic strain, with smaller electrostatic terms: the configuration of the planes is one which minimises the elastic strain energy. Quantitative results are given for a realistic model, and agree with the main features observed experimentally. Thus the regular array of planes is stable, and the equilibrium separation of planes in the array is about half that predicted for an isolated pair of planes. The interaction between isolated planes proves an oscillatory function of their separation. One can understand from its detailed form why the observed mean spacing gets smaller as the planes come together to form larger groups.

1. INTRODUCTION

ELECTRON microscopy has shown that in certain transition metal oxides (e.g. TiO_2, MoO_3, WO_3, etc.; see the recent reviews by Fender[1], Tilley[2] and Anderson[3]) partial reduction gives rise to crystallographic shear planes with few, if any, isolated oxygen vacancies. The metal ions in each shear plane retain their original octahedral coordination; the excess metal is incorporated by altering the linkage of the octahedra. In oxides based on the ReO_3 structure, there is a change from corner-sharing in the perfect crystal to edge-sharing in the shear plane. Likewise, in rutile, there is a change from edge-sharing to face-sharing. The features of shear planes of interest here are shown by the structural changes observed in rutile (TiO_{2-x}) with increasing oxygen deficiency, x. Shear planes are found even for very low deficiencies. They have {132} orientations, and tend to cluster in small groups. As x increases, the planes form regular arrays extending throughout the crystal, giving a homologous series of 'shear compounds'. Further reduction leads first to a regime in which regions of ordered {132} and {121} planes coexist, and then to a homologous series of compounds based on {121} planes.

We shall discuss the ordering of these shear planes, including their spacing in large arrays and the variation of the spacing across smaller groups of planes Experiment suggests a long-range interaction between planes (i.e. not just between adjacent planes) and that, as more and more planes are added to a particular group, the planes can move to minimise the total free energy. Plausible mechanisms of plane motion have been given by van Landuyt, Gevers and Amelinckx[4] and by Anderson and Wadsley[5]. Bursill and Hyde[6] have analysed spacings of planes in some detail. They show that spacings are largest near the outside of a given group of planes, and they derive a plausible plane–plane interaction consistent with this. Our calculations should give a very similar distribution of planes, but the interplanar interaction is very different in form.

The present work suggests the main interaction comes from elastic strain energy, with a

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smaller electrostatic contribution. We argue that the planes adopt a configuration which minimises the elastic strain energy. There is some indirect evidence that strain is important. Cowley[7] has observed that there is considerable distortion of the octahedra near the shear planes, so that elastic energies may be substantial. Elastic interactions also describe successfully another case of large-scale periodicity, the void lattice[8–11]. Further, it is hard to think of other interactions which lead naturally to the large spacings observed; in TiO_{2-x}, for example, the separations for isolated pairs of shear planes are about 87 Å, falling to 38 Å at the centre of large groups [6, 3]. Indeed, Anderson comments[3] that there appears to be no simple valid explanation based on electron delocalisation.

Previous explanations of the regular arrays of shear planes have been very tentative, drawing analogies with such diverse phenomena as spinodal decomposition and the electronic properties of metallic alloys. Clapp [12] has given a provocative discussion which includes some of the features of our model. He argues that the regularity is a result of a purely repulsive interaction between planes associated with lattice strain. Unfortunately, this is not consistent with observation; planes to order in groups, rather than staying as far apart as possible. One major difference in our approach is that we show the elastic terms (including both Clapp's 'phonon' and 'interatomic interaction' contributions) give an interaction which is not monotonic in separation, but gives a minimum energy at a finite separation. The internal energy proves to be the important part of the free energy; as in Clapp's analysis, we find the configurational entropy of the planes quite negligible. The existence of the minimum is a consequence of the periodic microscopic structure of the individual shear planes.

In the following sections we describe a model which retains the important features of real shear planes, but which is simple enough for detailed calculations. We assume that only one type of shear plane occurs, and we shall not discuss the reasons for this plane to be stable relative to isolated vacancies or other orientations. The energy per unit area of a shear plane in an infinite array is then calculated, and we also calculate the interaction of two isolated planes as a function of separation. We shall show that the elastic interaction energy between planes has minima for suitable configurations and that the predicted spacings for these minima are in good qualitative and satisfactory quantitative agreement with experimentally observed separations.

2. MODELS OF THE SHEAR PLANES

Our aim is to obtain reasonable estimates of elastic strain and electrostatic energies of real systems with shear planes and their dependence on interplanar spacing. We now describe a simple model which contains the important features. Further details for the model and its application to the void lattice are given in Ref. [10].

Estimates of the strain energy are most easily obtained in terms of 'defect forces'. The regions between the planes may be regarded as perfect crystal distorted by the presence of the shear planes. The defect forces are an array of forces which represent the effect of the shear planes, and which produce the same distortion in each region. We shall calculate the strain energy for suitable arrays of these defect forces in an anisotropic elastic continuum. Whilst some information about detailed atomic positions is lost in the continuum approximation, the model should give reasonable values for strain energies at the large interplanar spacings met in practice. We shall also use a continuum model in estimating the electrostatic energies, which can be calculated from the interactions of appropriate arrays of point charges in a dielectric continuum.

In our detailed calculations we assume that the continuum is an isotropic dielectric, but with cubically anisotropic elastic properties. Previous work on the void lattice[9, 10] suggested that elastic anisotropy was important and the present assumptions are the simplest which retain some degree of anisotropy. No effects of the shear planes themselves on the elastic properties are considered quantitatively, although experience with the void lattice[11] suggests that such corrections may affect the precise values of the spacings.

In principle, the defect forces could be obtained from a detailed study of the local strain near isolated planes. These results were not available to us. Instead, we have tried several plausible models for both the defect forces and the charge distribution associated with the planes, subject to two general conditions. First, we assume each plane electrically neutral overall. Secondly, we recognise the atomic structure within each plane by giving the defect forces a periodicity which corresponds to that of the crystal structure.

The specific model used in the later sections is an idealisation of a {100} plane in the ReO_3 structure. The perfect crystal can be regarded as alternating {100} planes ...*ABAB*..., where the *A* planes contain oxygen alone and the *B* planes are, on average, ReO_2. We consider shear in the {110} direction. Each shear plane may be constructed by removing an *A* plane, and by moving the crystal on one side through a nearest-neighbour Re–O spacing, $D/2$, parallel to one of the cube axes in the plane. The separation T of the two adjacent *B* planes will usually differ slightly from $D/2$. A small section of such a plane is shown in Fig. 1. Qualitatively, we expect four types of force. These are listed in detail in the Appendix. First, since the metal ions will be brought rather close, we put forces F_1 on them which repel them out of the plane. Secondly, we suspect that the oxygen ions will be pulled into the plane, although this is not critical. There are two inequivalent sets of oxygens, depending on whether the nearest metal ion in the plane is along or normal to the shear direction. Forces F_2 and F_3 are applied to the oxygens. All the forces F_1, F_2, F_3 are normal to the shear plane. Finally, we add forces F_4 parallel to the shear plane. These forces appear because the crystal near the shear plane would prefer to adopt a different lattice parameter from the perfect host crystal. Several sets have been tried, with very little effect on our results. The set used for the results given later is shown in Fig. 1, and has lower symmetry than the other features of our model. This additional complexity in forces F_4 compensates slightly for the oversimplifications in other aspects, notably that real shear planes have even lower symmetry than does our model. The in-plane forces F_4 need not act at nearest-neighbours of the shear plane only, and we have chosen a larger effective separation U.

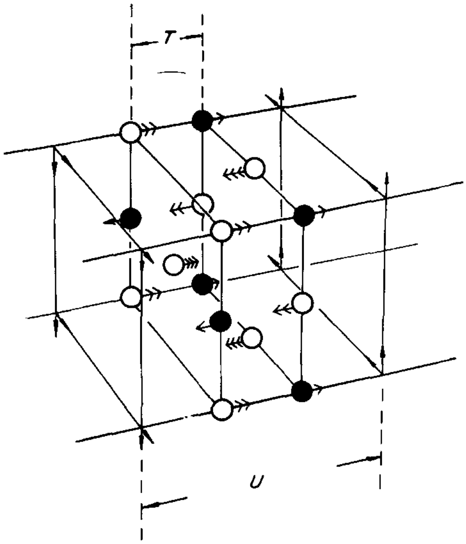

Fig. 1. Model of the forces associated with the shear plane. Only atoms adjacent to the plane are shown (metal atoms being full circles, oxygens open circles) and only one repeating unit given. The four types of force are $F_1(\rightarrow)$, $F_2(\twoheadrightarrow)$, $F_3(\rightarrow\!\!\!\twoheadrightarrow)$ and $F_4(\rightarrow)$.

The parameters chosen for the following calculations are these:

$$|F_1|:|F_2|:|F_3|:|F_4| = 3:1:2:1;$$
$$U/3 = T = \text{Nearest-neighbour Re–O separation.}$$

The ratios of elastic constants[13, 14] chosen are:

$$c_{11}:c_{12}:c_{44}=16:7:5.$$

Clearly there is a fair degree of arbitrariness in our model. We have tried many other sets of parameters, and shall comment on the effects of these variations. Here we merely observe that the absolute magnitudes of the F_i and c_{ij} do not affect the predicted spacings, although the absolute values of the energies are proportional to F_i^2/c_{kl}.

3. ENERGY OF AN ARRAY OF PLANES

3.1 *Calculation of elastic energies*

The energy of a distorted lattice containing no shear planes is quadratic in the displacements **x** of the atoms:

$$E_L(\mathbf{x})=E_L(0)+\tfrac{1}{2}\mathbf{x}\,.\,\mathbf{A}\,.\,\mathbf{x} \tag{3.1}$$

where **A** is the force-constant matrix. The effects of the shear planes are represented by defect forces **F**, which give an extra term in the energy:

$$E_D(\mathbf{x})=-\mathbf{F}\,.\,\mathbf{x}, \tag{3.2}$$

omitting a large term independent of x which represents the formation energy of the shear plane in an undistorted lattice. The equilibrium distortion is found by minimising (E_L+E_D), and it is readily shown that the relaxation energy is ΔE, where

$$\Delta E=-\tfrac{1}{2}\mathbf{F}\,.\,\mathbf{A}^{-1}\,.\,\mathbf{F}. \tag{3.3}$$

The matrix $\mathbf{A}^{-1}$ is the Green's function of the lattice, and can be written[13] in terms of the elastic constants for an elastic continuum.

We shall calculate ΔE, and hence the energy per shear plane in terms of Fourier-transformed forces $\tilde{\mathbf{F}}(\mathbf{q})$ and Green's function $\tilde{\mathbf{G}}(\mathbf{q})$. The two main advantages of working with the transforms are that the Green's function can be given exactly, rather than by a perturbation expansion in the anisotropy, and that we may exploit the geometric periodicity of the shear plane structures. The relaxation energy is written as a sum over the first Brillouin Zone of the lattice

$$\Delta E=-\frac{1}{2N}\sum_{\mathbf{q}}\tilde{\mathbf{F}}(\mathbf{q})\,.\,\tilde{\mathbf{G}}(\mathbf{q})\,.\,\tilde{\mathbf{F}}(-\mathbf{q}), \tag{3.4}$$

where N is the number of unit cells. $\mathbf{G}(\mathbf{q})$ is given in Ref. [13] for a cubic elastic continuum as:

$$c_{44}\tilde{G}_{ij}(q)=\frac{1}{q^2}\left[\Lambda_i\delta_{ij}-\Lambda_i\Lambda_j\frac{\gamma K_iK_j}{1+\gamma\sum\limits_{l=1,3}\Lambda_lK_l^2}\right] \tag{3.5}$$

where the K_i are the direction cosines (q_i/q) of **q** and

$$\Lambda_i(\mathbf{q})=(1+\delta K_i^2)^{-1}. \tag{3.6}$$

The dimensionless factors depend only on the elastic constants, c_{ij}:

$$\begin{aligned}\gamma&=(c_{12}+c_{44})/c_{44},\\ \delta&=(c_{11}-c_{12}-2c_{44})/c_{44}.\end{aligned} \tag{3.7}$$

The way in which energy minima can occur at finite separation can be seen from expressions like (3.3). If there are two defects, with forces $\mathbf{F}_1$ and $\mathbf{F}_2$, then (3.3) shows that the interaction energy between them can be written as the scalar product of the displacements $\mathbf{A}^{-1}\,.\,\mathbf{F}_1$ due to one with the forces $\mathbf{F}_2$ due to the other. Now the defects here are planes, each with their internal periodic structure. The displacement field is complicated, but is periodic in any plane parallel to the shear plane. As we bring the two planes closer and closer from a large initial separation, there will be spacings which optimise the relation between the forces $\mathbf{F}_2$ and displacements $\mathbf{A}^{-1}\,.\,\mathbf{F}_1$ to minimise ΔE. The minimum corresponds to an optimum phase relation of the forces of one plane with the displacements of the other. In Sections 3.2 and 3.3 we show this quantitatively by calculating the elastic strain energy as a function of the spacing.

3.2 *Elastic energy of an infinite periodic array of planes*

We now calculate the strain energy per unit area per plane in the array. If the planes are all normal to the x axis, then only certain discrete values of q_x will occur in (3.4). The periodicity in the x direction means that all transforms $F(\mathbf{q})$ of the forces vanish unless $\mathbf{q}$ reflects this periodicity. Thus, if the planes occur every L unit cells, finite $F(q)$ occur only at L equally-spaced planes in the Brillouin Zone. For the system discussed here, L can be regarded as the spacing of the planes in units of D, the period of the structure within any individual plane.

In the same way, simplification occurs because the forces associated with each shear plane have the translational symmetry of the plane itself. The forces repeat under translations D in the y or z directions. The consequence is that (3.4) need be summed over a finite number of points only in the Brillouin Zone. The exact number is proportional to the separation, L. Since $\tilde{G}(\mathbf{q})$ is known analytically, ΔE can be evaluated exactly for our model in a closed analytic form. We have used a computer to evaluate (3.4) because of the algebraic complexity of the terms; no approximation is involved.

The energy per unit area of a member of the infinite periodic array is shown in Fig. 2(a) as a function of interplanar spacing. The main feature is a minimum at a finite spacing $L = L_A$ of about 4 times the spacing of the forces within the plane. The energy increases rapidly away from the minimum. At very close spacings, when adjacent planes start to overlap, the energy begins to decrease again with spacing. This is a consequence of the details of the model and almost certainly lacks any physical significance. Similar unphysical behaviour at very small spacings was found for the void lattice. We return to this point later.

The value of L_A is insensitive to many of the parameters. The optimum spacing varies little with elastic anisotropy, nor does it depend significantly on the relative magnitudes of the four types of elastic forces (although the minimum disappears for the special case of elastic isotropy and $F_4 = 0$). The optimum spacing in units of the period within the plane changes appreciably only with one parameter: L_A increases with the plane 'thickness' U. We have tried several related models of the defect forces, and find very similar values of L_A.

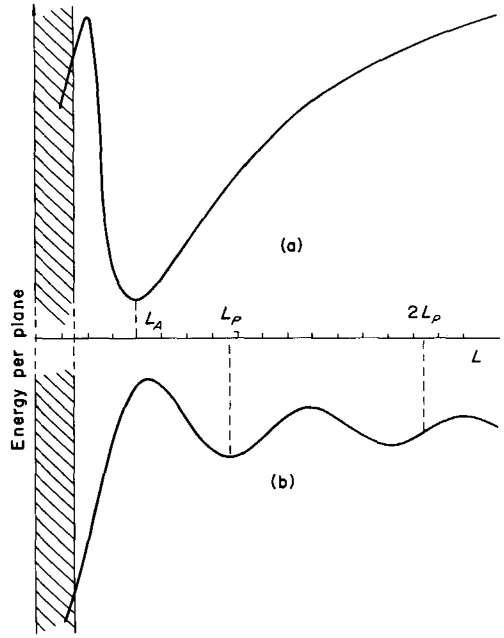

Fig. 2. Shear plane energies as a function of the spacing, L, measured in units of the period within each plane. Adjacent planes overlap in the shaded regions $L < 1{\cdot}5$. Elastic energies alone are given; electrostatic terms are repulsive and only appreciable below $L \sim 3$. (a) Energy per plane in an infinite array; (b) Energy for a pair of isolated interacting planes. The energy zeros are shifted for clarity; both tend to the isolated-plane limit at large L.

3.3 *Elastic energy of a pair of planes*

The interaction of a pair of planes as a function of spacing is more difficult, since the periodicity of an array cannot be exploited. However, we can still use (3.4). The difference is that, instead of a sum over discrete values of q_x, we now have a one-dimensional integral over q_x. The summations over q_y and q_z are not affected, since the structure of the individual planes is not altered. The dependence on spacing is most easily included in a different way than when dealing with the periodic array. For the periodic array the transformed forces $\tilde{\mathbf{F}}(\mathbf{q})$ for any one plane were independent of spacing, since the origin of coordinates was taken to be the plane itself. The dependence on L came through the specific values of q_x over which the sum was taken. For the pair of planes it is most convenient to choose the origin of coordinates to be midway between the planes. The transformed forces for the two planes together then depend on L, giving $\tilde{\mathbf{F}}(\mathbf{q},L)$. This approach has a number of technical advantages; the physical content is unaltered.

The energy as a function of separation is shown in Fig. 2(b). The striking feature is that the energy oscillates as a function of L. This is a general property, and not specific to the force model we have taken. The ultimate source of the oscillations is the dependence of the $\tilde{F}(\mathbf{q},L)$ on L. This dependence can be understood as follows. $\tilde{F}(\mathbf{q})$ is the Fourier transform of the forces associated with the two planes:

$$\mathbf{F}(\mathbf{q},L) = \sum_{p=1,2} \sum_{\mathbf{l}} \mathbf{F}_p(\mathbf{l}_p) \exp{(i\mathbf{q} \cdot \mathbf{l}_p)}, \tag{3.8}$$

where p labels the planes and $\mathbf{F}_p$ the defect forces acting at sites $\mathbf{l}_p$. Now the sets of defect forces $\mathbf{F}_1$ and $\mathbf{F}_2$ are identical apart from a relative displacement L along the x-axis, since the planes are equivalent. This can be exploited by writing the site coordinates, $\mathbf{l}_p$, as the sum of an internal coordinate, $\mathbf{l}$, measured from some standard origin within each plane, and the coordinate $(X_p,0,0)$ defining the origin. The only dependence on spacing L comes from X_p; in our case, X_1 is $L/2$ and X_2 is $-L/2$. Equation (3.8) becomes:

$$\begin{aligned}\tilde{\mathbf{F}}(\mathbf{q},L) &= \sum_{p=1,2} \sum_{\mathbf{l}} \mathbf{F}(\mathbf{l}) \exp{(i\mathbf{q} \cdot \mathbf{l} + iq_x X_p)} \\ &= \sum_{p=1,2} \exp{(iq_x X_p)} \left[\sum_{\mathbf{l}} \mathbf{F}(\mathbf{l}) \exp{(iq \cdot \mathbf{l})} \right] \\ &= 2 \cos{(Lq_x/2)} \left[\sum_{\mathbf{l}} \mathbf{F}(\mathbf{l}) \exp{(i\mathbf{q} \cdot \mathbf{l})} \right].\end{aligned}$$

The important factor is $\cos{(Lq_x/2)}$: there is an oscillatory dependence of $\mathbf{F}(\mathbf{q},L)$ on L. It is still possible to devise systems for which ΔE varies monotonically with L, but for all cases for which we find minima there are oscillations.

The oscillations in ΔE are not strictly periodic, for the minima get closer together at larger spacings. It is most unlikely that the apparent minimum at very small spacings is significant. At very small spacings a number of interactions become important which are omitted in our model, notably chemical effects and anharmonic corrections. Other omitted terms in Fig. 2 are the electrostatic contributions, which are repulsive, and which become particularly important below $L \sim 3$. Thus the first physically-significant minimum is at $L_P \sim 8$, about twice the optimum spacing $L \sim 4$ found for the array. Like L_A, L_P is insensitive to the elastic anisotropy and to most details of the defect forces.

3.4 *Electrostatic energies*

The type of electrostatic forces can best be illustrated by an example of cation ordering in a non-shear structure. Consider a system $Ti_nA_2BO_{2n+m}$ which orders with the cation sequence . . . Ti Ti A B A Ti Ti . . . . Then each of the layers A B A will have a different charge distribution from the sequence TiTiTi they may be assumed to replace. The difference corresponds to an array of electric quadrupoles. Quadrupolar terms should always be present, although dipole contributions may also appear in some structures.

The energy of the array can be found by methods exactly analogous to the strain energy treatments. For present purposes, however, qualitative arguments suffice. It is easily seen that the interaction is repulsive and that it falls off rapidly at large spacings, as does the field of an isolated quadrupole. This repulsion helps to counteract the decreases in elastic energies at very close spacings, and may shift the minima to slightly larger spacings.

A rough estimate of the separation L_Q at which the quadrupole and strain terms are equally important can be found by comparing the interaction energies of an isolated pair of the component quadrupoles with that of a pair of force dipoles. It is very hard to determine relative magnitudes of the defect forces without detailed microscopic information not available at present. The data we used assumed a force dipole such as to give a volume change of 10 Å^3, a value $1{\cdot}6 \,.\, 10^{12}$ dynes/cm^2 for c_{11}, a dielectric constant of 10 and a quadrupole of total length 8 Å. Whilst these may not be precise, our feeling is that L_Q is about 3, rather less than L_A; the strain terms dominate near the minimum. The magnitude also depends on the distribution of charge over the plane; in the special case of a uniform charge distribution, the quadrupole terms vanish identically.

We have also considered other electrostatic contributions, including the effects of small numbers of isolated vacancies and of ionisable defects between the planes. These contributions appear to be negligible.

4. DISCUSSION

Several predictions of our model can be compared with experiment. First, it predicts correctly that planes prefer to order into a regular array. The spacing depends on the structure within the individual planes and on the elastic properties of the crystal. Quantitatively, the model predicts a spacing L_A of about four times the width of the repeating unit within each plane. In the crystals of interest, the repeat units are probably in the range 6–10 Å, so spacings from 24 to 40 Å might be expected. Observed spacings are indeed in this general range, although we cannot claim any precise agreement because of the simplicity of the model.

The second prediction is that the separation of planes in pairs, L_P, should be about twice that for planes in large arrays. This is fully in line with observations of Bursill and Hyde[6] (see also Ref. [3], p. 25) on reduced rutile. There pairs of crystallographic shear planes are separated by about 87 Å in $TiO_{1{\cdot}988}$, whereas the spacing at the centre of large groups in $TiO_{1{\cdot}973}$ was about 38 Å, a ratio of 2·29. Again, agreement is as good as one might hope for such a simple model. One obvious omission is the effect of the shear planes on the elastic constants, an effect which is important in the void lattice[11]. Here one effect would be a composition dependence of the elastic constants and hence of L_A and L_P. The rather good agreement of the observed ratio with experiment suggests this effect is not very large. We also note that if the shear planes affect the elastic constants, one can no longer talk of a purely pairwise interaction between planes; the interaction between any two planes will be modified by the presence of a third.

The third prediction is that the interaction between pairs of planes is oscillatory. This is very different from the simple $(AL^{-n}-BL^{-m})$ potential with which Bursill and Hyde attempted to fit their data. So far as the variation of spacings over groups of planes is concerned, both forms will give the same general features, namely closer spacings near the centre of groups. This can be understood from Fig. 2(b). Two planes A and B together tend to lie at a spacing L_P given by the first minimum. A third plane C can be placed at the same distance from B. But the interaction of A and C favours a separation smaller than $2L_P$ (about 10 per cent smaller for this model). The separation finally achieved will be a compromise, rather smaller than the pair separation. The picture becomes more complicated as more planes are added, but in the end the correct spacing L_A for the array must be reached. The oscillatory interaction does, however, have the interesting consequence that pairs of planes may occur at a number of different discrete separations, corresponding to the different minima of Fig. 2(b).

Finally, the dependence of strain energy on array spacing helps to clarify the change from one type of shear plane to another when the oxygen deficiency is sufficiently great. An example was mentioned in Section 1, namely the observed change from {132} to {121} shear planes as x, the oxygen deficiency, is increased. The interactions between the shear planes play a role which is illustrated in Fig. 3. The figure shows schematically as functions of x the free energies per vacancy assimilated for a system which may contain shear planes of two possible types I and II. The abscissa is the reciprocal of the number of vacancies assimilated per unit volume, and is proportional to $1/x$; for a given type of plane, this is a measure of the mean separation of adjacent planes.

The differences between the energy curves for the two types of plane occur because of three factors, all of which are associated with differences in the defect forces. These are first, the differences in energy of isolated planes of type I and II from Madelung energies, covalency and similar contributions, second, the different number of vacancies which can be assimilated per unit area because of the different geometries, and third, the different values of spacing L which minimise the interaction energies between the planes. At low deficiencies, the energy of the isolated planes is the dominant factor. But as the deficiency is increased, the strain energy becomes more important. A change from Type I to Type II planes is expected if there is a crossover in the energy curves, as shown in Fig. 3. In other systems, with different parameters and geometry, it is possible that a single type of plane may be favoured at all accessible deficiencies. In such cases crossovers are not expected.

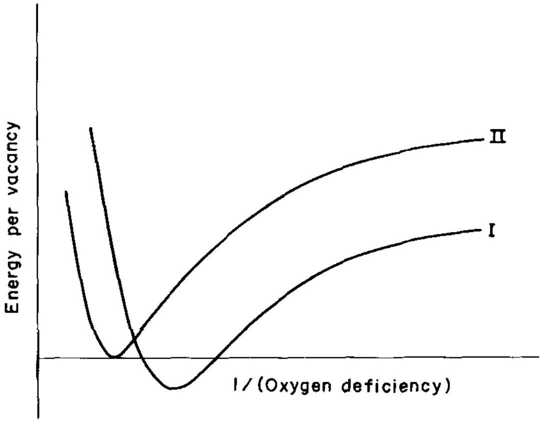

Fig. 3. Schematic diagram of energies per vacancy assimilated for two alternative shear plane arrays which take up different numbers of vacancies per unit area. The oxygen deficiencies correspond in the two cases. The differences in energy come partly from the energies of the isolated planes and partly from the different interactions.

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APPENDIX

Defect forces for shear planes

If there is a single shear plane normal to the x axis in an infinite crystal, then the defect forces and the sites at which they operate are as follows:

Force	Site
$F_1(-1,0,0)$	$\frac{1}{2}(-T,O,D)$
$F_1(1,0,0)$	$\frac{1}{2}(T,O,D)$
$F_2(1,0,0)$	$\frac{1}{2}(-T,O,O)$
$F_2(-1,0,0)$	$\frac{1}{2}(T,O,D)$
$F_3(1,0,0)$	$\frac{1}{2}(-T,D,D)$
$F_3(-1,0,0)$	$\frac{1}{2}(T,D,O)$
$F_4(0,1,0)$ $F_4(0,0,1)$	$\frac{1}{2}(-U,O,O)$
$F_4(0,-1,0)$ $F_4(0,0,-1)$	$\frac{1}{2}(U,O,O)$

Because of the periodic structure within the plane, equivalent forces occur at sites related by translations D in the y or z directions. In consequence, the Fourier transforms of the set of defect forces are only finite for values of q_y and q_z which are multiples of $2\pi/D$. The transforms for individual planes are trivial to obtain, and we shall not quote them.

If we now consider two shear planes separated by L in the x direction, then it is straightforward to write down the positions and magnitudes of the defect forces. With the ratios of forces given in Section 2, the Fourier transforms can be written, for wavevector $(q_x, 2\pi M/D, 2\pi N/D)$ as:

$$\mathbf{F}(\mathbf{q},L) = F\cos(q_xL/2)\,(4i\sin(q_xT/2)\delta_{M1}\delta_{N0} + 2\cos(q_xT/2)[\delta_{M0}\delta_{N1} + 3\delta_{M1}\delta_{N1}], 4\sin(q_xU/2), 4\sin(q_xU/2)).$$

When we consider an infinite array of planes, the only values of q_x which give finite values of $F(\mathbf{q})$ are integral multiples of $2\pi/L$.