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In plane translations at crystalline interfaces(*)

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THE RESULTS of computer simulation studies, based on empirical interatomic potentials, of the structures of twin boundaries in α-iron and a particular twist boundary in copper are presented. In both cases the calculations suggest that the structures with the lowest energy may be displaced from the normally accepted models by rigid body translations parallel to the interfaces. However, the resulting structures still have a high degree of symmetry. Quantitative values for the volume increase associated with the interfaces are also deduced. The results suggest that interfacial dislocations associated with these boundaries will have different Burgers vectors from those assumed previously. Similar results are obtained for other interfaces and the results are considered to have general significance.

Przedstawione są wyniki symulacji komputerowej struktury granic bliźniaków w żelazie α oraz pewnych skręconych granic ziaren w miedzi, oparte na empirycznych potencjałach międzyatomowych. W obu przypadkach wyniki obliczeń sugerują, że struktury o najniższej energii można przemieścić z normalnie przyjmowanych modeli za pomocą sztywnego przesunięcia równoległego do płaszczyzn międzykrystalicznych. Jednakże powstałe struktury zachowują w dalszym ciągu wysoki stopień symetrii. Wyprowadzono ilościowe zależności, dotyczące wzrostu objętości, związane z tymi powierzchniami. Otrzymane wyniki wskazują na to, że odpowiednie przemieszczenie wzdłuż płaszczyzn międzykrystalicznych mieć będzie wektory Burgersa inne od przyjętych początkowo. Podobne wyniki otrzymano dla innych płaszczyzn międzykrystalicznych, posiadają one zatem bardziej ogólne znaczenie.

Представлены результаты численного моделирования на основе экспериментальных межатомных потенциалов структуры границ двойникования в α-железе и частного вида границ вращения в меди. В обоих случаях результаты вычислений указывают на возможность того, что структуры с наименьшей энергией могут быть перемещены из обычно принятых моделей путем жесткого переноса в плоскости параллельной границы. Несмотря на то полученные структуры все еще обладают высокой степенью симметрии. Найдены также численные знфчения приращения объема связанного с появлением границ раздела. Результаты указывают, что дислокации связанные с этими границами имеют, по-видимому, отличные от ранее проедполагаемых векторы Бюргерса. Аналогичные результаты получены и для других типов границ и следует их рассматривать как весьма общие.

1. Introduction

THE PROPERTIES of polycrystalline materials are to a large extent controlled by grain boundaries and their interactions with other defects. It is therefore important to have satisfactory models of the structure of these interfaces. However, experiments and traditional theoretical treatments can provide little direct information on the atomic configurations which arise at boundaries. In recent years therefore real space computer simulation studies, based on empirical interatomic potentials, have been used to investigate these defects. The present paper describes some results that have been obtained in this way for two

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special cases, twin boundaries in body-centred cubic (bcc) metals and twist boundaries in face-centred cubic (fcc) metals. In both cases the structures determined involve a rigid body displacement of one of the grains parallel to the boundary and the importance of these in-plane translations is examined.

The procedure which was used to obtain the results involved constructing a computer model of a perfect crystallite containing up to 10^4 discrete atomic sites [1]. A first approximation of the interface being studied, based on simple geometrical ideas, was then introduced across the centre of the model and the atoms where allowed to relax to their minimum energy positions using lattice-handling techniques known as DEVIL developed at A.E.R.E., Harwell [1]. This programme utilizes a modified steepest descent minimization procedure called the method of conjugate gradients [2]. During a given relaxation process the two outer boundaries parallel to the interface were kept rigid and cyclic boundary conditions were imposed on the other four faces. Elastic regions of thickness greater than the range of the potentials being used were attached to the outside of the rigid boundaries. In this way the models studied were effectively infinite in extent [1].

The results to be described were obtained using the pair-potentials representing α-iron (bcc) and copper (fcc) illustrated in Fig. 1. The former is due to JOHNSON [3] and consists

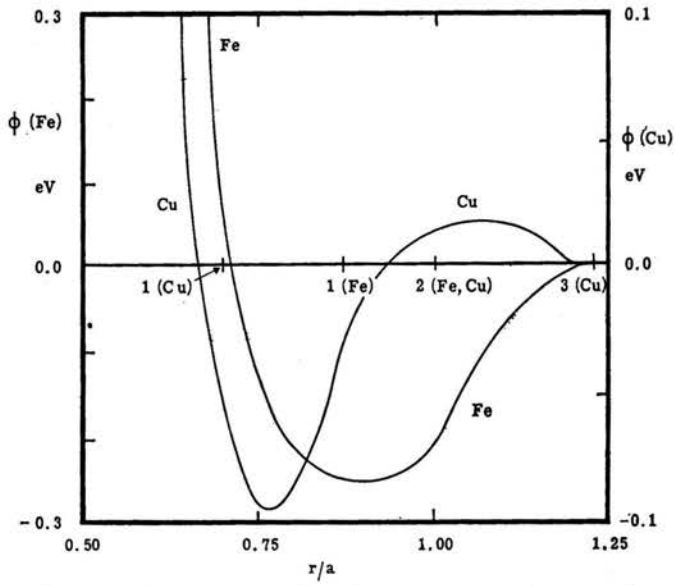

FIG. 1. The interatomic potentials $\phi(r)$ for iron due to JOHNSON [3] and for copper due to DONEGHAN [4] used in the calculations. The different energy scales for iron and copper are marked at the left and right, respectively. Nearest neighbour distances are indicated on the r/a axis, the lattice parameter a corresponding to the second nearest neighbour distance in each case.

simply of three linked cubic splines. It holds models in equilibrium at the correct lattice parameter and also matches satisfactorily the elastic constants, the phonon dispersion data and the vacancy formation energy. The copper potential is due to DONEGHAN [4] and consists of nine cubic splines fitted to available experimental data, including the stacking fault energy. It is a non-equilibrium potential, the correct lattice parameter being

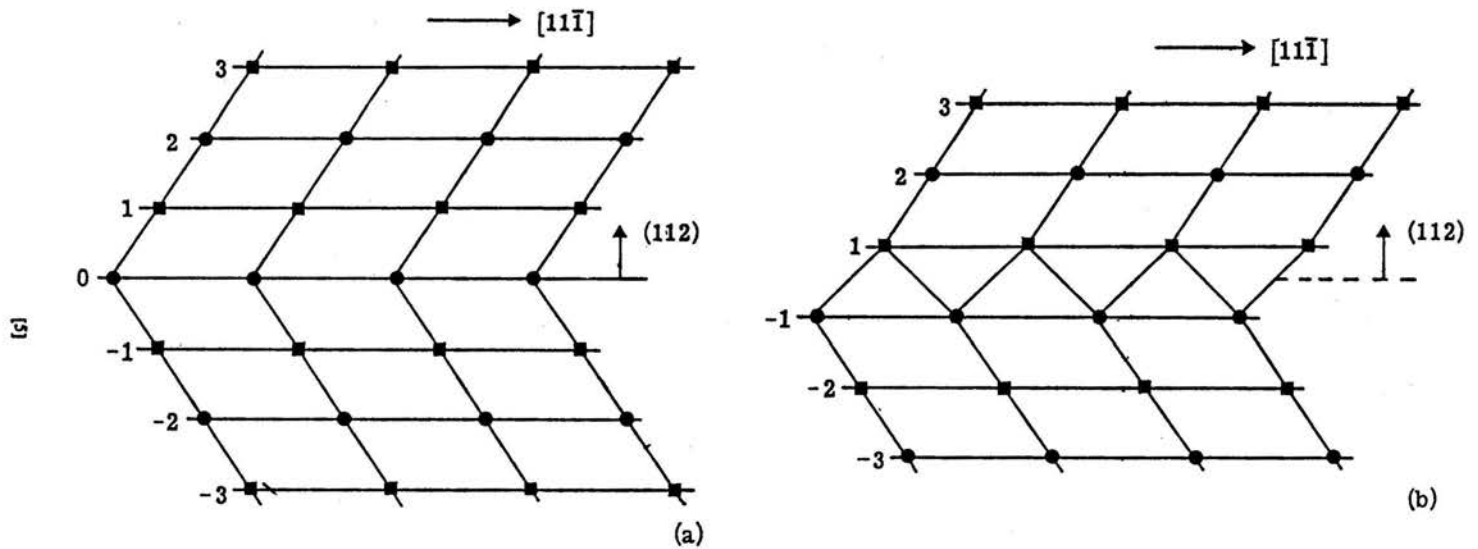

FIG. 2. Two possible schematic structures for a (112) twin boundary in bcc crystals shown projected on to the (1$\bar{1}$0) plane. Atoms represented by circles and squares lie on adjacent (1$\bar{1}$0) planes. The conventional reflection twin is shown at (a) and the alternative isosceles structure at (b).

obtained through the use of an external pressure which was imposed by means of the boundary conditions. This pressure may be considered to represent the cohesive effects of the free electron gas.

2. Twin boundaries in body centred cubic metals

It is normally assumed that both at a macroscopic and at an atomic level twin boundaries in body centered cubic metals satisfy the classical orientation relation [5] of reflection in the interface. In this case the boundary, which is parallel to the (112) plane, has the structure shown schematically in Fig. 2(a). However, some earlier computer simulation studies [6, 7] suggested that the alternative schematic structure illustrated in Fig. 2(b) might be preferred. This involves an additional translation at the interface to produce a structure which projects as a layer of interlocking isosceles triangles. The structures and energies of these two boundaries have been examined in detail by BRISTOWE and CROCKER [1] using potentials representing several bcc metals. The results for iron to be discussed here are particularly interesting as the two structures have similar energies.

Models with initial atomic configurations based on the structures shown in Fig. 2 were constructed in the computer and allowed to relax using the iron potential. Both structures were found to be stable or metastable, the interfacial energies being 270 mJm^{-2} and 267 mJm^{-2} for the reflection and isosceles types respectively. In both cases there was a volume increase at the twin boundary so that the outer parts of the models were in

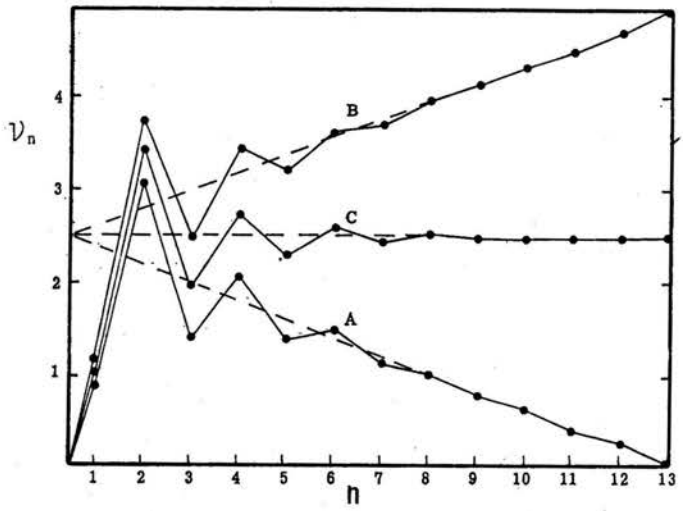

FIG. 3. Displacements ν_n (in units of 10^{-2} (112) interplanar spacings) of planes $\pm n = 1, 2, 3, \ldots 12$, perpendicular to the isosceles bcc twin boundary relaxed using the iron potential. Curve A is for zero volume change corresponding to a compressive long range strain. Curves B and C are associated with tensile and zero long range strains, respectively. The broken lines demonstrate that the equilibrium volume increase corresponding to the horizontal section of C can be deduced by extrapolating the linear sections of A or B back to the interface at $n = \frac{1}{2}$.

compression. This is illustrated by curve *A* of Fig. 3, which gives the displacements perpendicular to the isosceles boundary for the twelve (112) planes on one side of the interface. Equal and opposite displacements were obtained for planes on the other side of the interface and a similar curve was found for the reflection boundary [1]. A series of computer simulations was then carried out in which the outer rigid boundaries of the models were moved outwards until the long range compressive strains were eliminated. Thus curve *B* of Fig. 3 shows a case in which too large a correction was applied and curve *C* represents the final solution with zero long-range strains. The broken lines in Fig. 3 demonstrate that an accurate estimate of the equilibrium volume increase can be determined by simply extrapolating the near-linear sections of curves *A* and *B* back to the location of the interface. These volume increases are equivalent to 11% and 5% of the (112) interplanar spacing for the reflection and isosceles boundaries, respectively. The corresponding expansions required by hard sphere models of these boundaries are calculated to be 12% and 9%. Small reductions in the interfacial energies accompanied these volume changes, the final values being 264 mJm^{-2} and 266 mJm^{-2}, respectively, for the reflection and isosceles twins [1].

In addition to relaxations perpendicular to the twin boundaries, additional displacements occurred parallel to the interfaces. The largest of these were for the atoms in the reflection twin boundary which relaxed about 7% of 1/2 $[\bar{1}\bar{1}1]$, the nearest neighbour distance, to give a sharper profile to the boundary without destroying the reflection orientation relation. In the case of the isosceles boundary, equal displacements occurred on the two sides of the interface so that the isosceles structure was retained but displaced about 2% of 1/2 $[\bar{1}\bar{1}1]$ to give a slightly blunter profile. The most significant features of the results, however, are that quantitative values are obtained for the volume changes and that the isosceles interface involving an in-plane translation from the expected reflection structure may be preferred. It is also striking that this alternative isosceles-type boundary is itself highly symmetric, having a 2-fold screw-axis parallel to $[\bar{1}\bar{1}1]$, the shear direction, rather than a simple 2-fold axis in this direction, which is equivalent to the mirror reflection which describes the usual twin orientation relation [5].

3. Twist boundaries in face centered cubic metals

Twist boundaries may be formally produced by rotating two adjacent parts of a crystal with respect to each other about the normal to a common planar interface [8]. For boundaries of this kind on high symmetry crystallographic planes particular misorientations arise at which a fraction of the atomic sites of the two grains would coincide if their lattices interpenetrated [8]. A simple example of this type of twist boundary occurs on the (001) plane of fcc crystals when the misorientation is 36.9°. One-fifth of the lattice points then coincide and the interface is known as a $\Sigma = 5$ coincidence site lattice (CSL) boundary [8]. This interface which will be considered in detail in this section is illustrated schematically in Fig. 4, where (a) and (b) represent the structures of the separate grains and (c) shows the structure obtained when (a) and (b) are superimposed. Atoms at the corners and at the centre of the unit cell shown in (c) are in coincidence positions but the remaining atoms are not. When due allowance is made for the fact that the corner atoms are shared

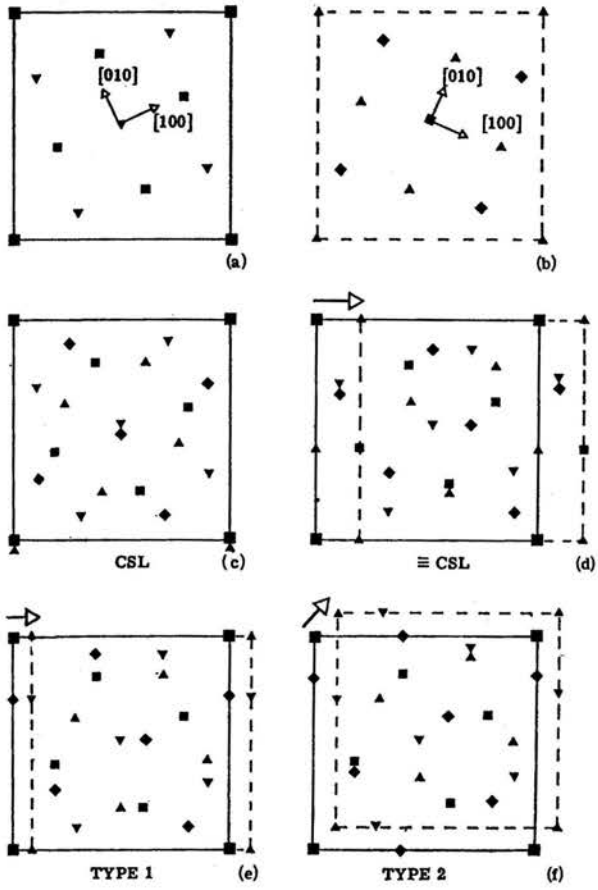

FIG. 4. Schematic structures of $\Sigma = 5$ (001) fcc twist boundaries. The two grains represented by cells shown by continuous and broken lines in (a) and (b) are superimposed to give the CSL structure (c). In-plane translations $\mathbf{d}_1$, $\mathbf{d}_1/2$ and $(\mathbf{d}_1+\mathbf{d}_2)/2$ given by the bold arrows in (d), (e) and (f) result in an equivalent CSL structure, the Type 1 structure and the Type 2 structure, respectively. Triangular and square symbols represent atoms in odd and even planes as counted from the interface. In (c), (d) and (f) double symbols represent superimposed sites.

between four adjacent unit cells, Fig. 4(c) confirms that in this case 1/5th of the atoms are at coincidence positions. Other CSL twist boundaries all with characteristic angular misorientations, arise on this same plane with for example $\Sigma = 13$, 17 and 25. It is generally considered that these particular boundaries have lower energies than those with arbitrary misorientations [8].

If the two grains of Fig. 4(c) are displaced with respect to each other by $\mathbf{d}_1 = \frac{1}{10}[3\bar{1}0]$, which is 1/5 th of the edge of the CSL unit cell, an equivalent CSL structure is produced. As illustrated in Fig. 4(d) the coincident atomic sites in the new arrangement occur at interior points of the unit cell but the configuration of atoms is the same. Similarly, an orthogonal displacement of $\mathbf{d}_2 = \frac{1}{10}[130]$ produces an alternative but equivalent CSL

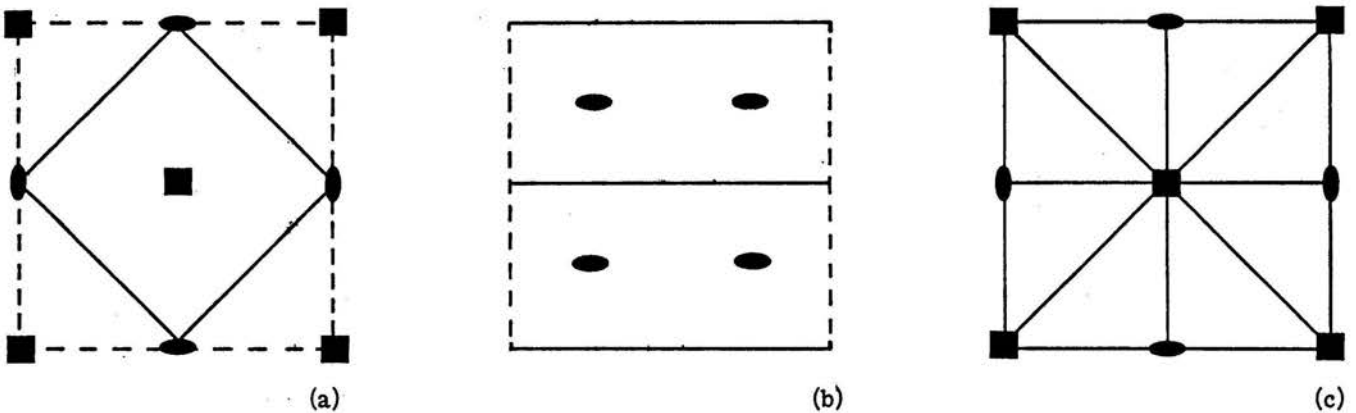

FIG. 5. Symmetry properties of (a) CSL, (b) Type 1 and (c) Type 2, $\Sigma = 5$ (001) fcc twist boundaries. Lenticular and square symbols represent the location of 2- and 4-fold axes perpendicular to the boundaries and continuous lines 2-fold axes in the plane of the boundaries. The cells shown correspond to the structural unit cells of Figs. 4 (c), (e) and (f) but different origins are used for (b) and for (c).

structure. Smaller translations give rise to different boundary structures but two special cases corresponding to displacements of $\mathbf{d}_1/2$, or the crystallographically equivalent $\mathbf{d}_2/2$, and of $(\mathbf{d}_1+\mathbf{d}_2)/2$ are of particular interest. These displacements are illustrated in Figs. 4(e) and (f) and will be referred to as Type 1 and Type 2, respectively. Although at first these structures appear to have low symmetry they are in fact highly symmetric. This is demonstrated in Fig. 5 where the symmetry elements of the CSL and Types 1 and 2 displaced boundaries are shown schematically. In particular, it is seen that the Type 2 boundary is more symmetric than the original CSL structure. These are the only in-plane translations of this interface which produce symmetric structures.

Models of the CSL and Types 1 and 2 displaced $\Sigma = 5$ (001) fcc twist boundaries were constructed in the computer and allowed to relax using the copper potential shown in Fig. 1. The boundary conditions used were the same as those adopted for the simulation of twin boundaries in α-iron, which are described in Sect. 2. All three twist boundaries relaxed to equilibrium structures with the same symmetry as their initial configurations. All three structures are therefore either stable or metastable. The equilibrium interfacial energies were 1.21, 1.16 and 1.20 Jm^{-2} for the CSL, Type 1 and Type 2 arrangements, respectively. Alternative initial translations from the basic CSL structure were also simulated but these always relaxed to one of the three symmetric types. Thus the most stable $\Sigma = 5$ (001) copper twist boundary was found to be of Type 1.

Hard sphere models of the $\Sigma = 5$ CSL, Type 1 and Type 2 (001) fcc twist boundaries are calculated to involve volume increases at the interface corresponding to displacements of 34%, 38% and 41%, respectively, of the (001) interplanar spacing. In all three of the relaxed models these displacements which are normal to the interface were about 16% of this spacing. These values were deduced from models in which no overall volume increases were allowed, by extrapolating the linear portions of displacement curves back to the interfaces as explained in Fig. 3. However, in the case of twist boundaries the relevant curve is that representing the weighted average displacement of atoms from the interface. This is illustrated in Fig. 6 for the simple case of the equilibrium CSL structure. Six planes were allowed to relax on each side of the interface and as shown in Fig. 4(c) each of these planes contained four atoms in equivalent non-coincidence positions for every CSL atom. Figure 6 shows the normal displacements for the two types of atoms and the resulting average curve. The Type 1 and Type 2 boundaries produce similar curves except that the former has three kinds of atoms rather than two. The relaxations parallel to the interface were all consistent with the symmetry elements of Fig. 5. The maximum displacements were approximately 5% of the nearest neighbour distance and occurred in the planes of atoms adjacent to the boundary. Thus, as in the case of the bcc twin boundaries, computer simulation studies have provided quantitative values of volume increases associated with these twist boundaries and have demonstrated that in-plane translations away from the generally accepted structure may arise in practice.

4. Discussion

There is ample evidence in the results of this investigation that the computer programs used are working satisfactorily. In particular, all the relaxations are consistent with the

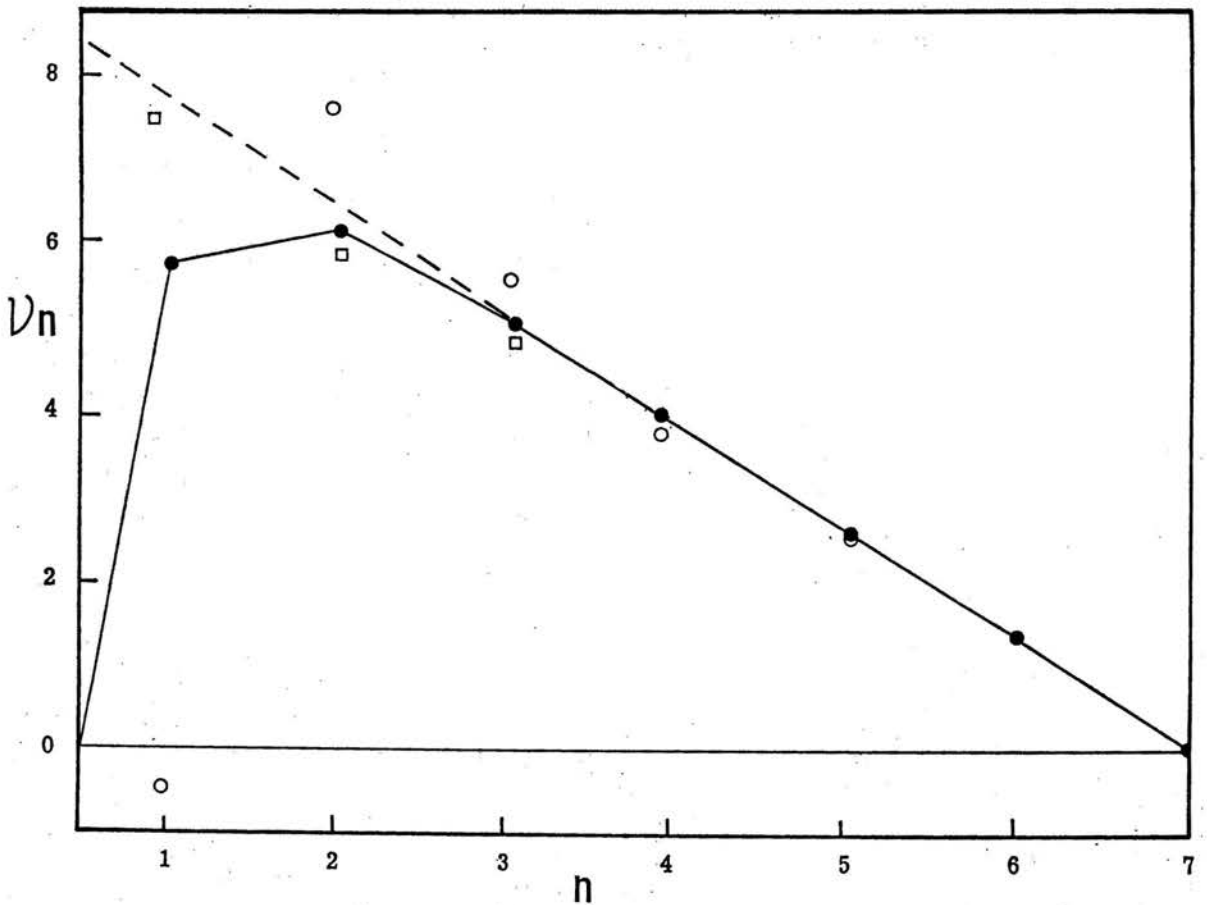

FIG. 6. Displacements ν_η^- (in units of 10^{-2} (001) interplanar spacings) of planes $\pm n = 1, 2, \ldots 6$, perpendicular to the CSL $\Sigma = 5$ (001) fcc twist boundary relaxed using the copper potential. Open circles and squares represent displacements for coincidence and non-coincidence site atoms, respectively, and closed circles which lie on the curve the weighted averages of these values. The broken line extrapolates the linear portion of the curve back to the interface to predict an equilibrium volume increase corresponding to $\nu_n = 8.3$.

basic symmetry properties of the interfaces examined. Also, although the in-plane translations discovered were not anticipated, they give rise to very plausible structurally symmetric configurations. The potentials used may not of course represent accurately the interactions of atoms in iron and copper. However, computer experiments on bcc twin boundaries using other potentials including some matched to molybdenum and tungsten [1, 9] and on fcc twist boundaries using a nickel potential [10] give compatible results. The main differences are that for the other bcc potentials either the reflection or the isosceles twin boundary is preferred rather than both having essentially the same energy, and that for nickel the Type 2 $\Sigma = 5$ (001) twist boundary has marginally the lowest energy. It therefore appears that the structures described here are typical of bcc and fcc crystals. Preliminary results on $\Sigma = 13$, 17 and 25 (001) twist boundaries in copper and nickel have also been obtained [10]. In all cases the CSL, Type 1 and Type 2 interfaces are stable or metastable with similar energies. Examples arise in which each of the three types has the lowest energy and is therefore expected to occur in practice. Although the structures and hence the displacement vectors of these boundaries are very different from the $\Sigma = 5$ case the symmetry properties illustrated in Fig. 5 are the same. These diagrams are also relevant when discussing related twist boundaries in simple cubic and bcc crystals. Similar computer simulation studies have also been carried out [11] for symmetrical high angle fcc tilt boundaries using an aluminium pseudopotential. It was again found that displaced boundaries were favoured and it therefore seems likely that the effect is of general occurrence.

The fact that in-plane translations are possible at crystalline interfaces has important implications for studies of grain boundary dislocations. For example, steps in twin boundaries have the same long range strain fields as dislocations [1, 9]. In the past it has been assumed that these twinning dislocations in bcc crystals must link adjacent regions of the reflection-type boundary. If, however, the reflection and isosceles boundaries have similar energies, as found for the iron potential in Sect. 2, steps of half the normal height linking regions of different character are possible [1, 9]. These fractional steps correspond to partial twinning dislocations with Burgers vectors one-half as large as those usually expected and hence with energies reduced by a factor of four. Similar consequences arise for the twist boundaries. If a $\Sigma = 5$ CSL (001) fcc twist boundary is rotated a small amount about [001] away from its exact $\Sigma = 5$ misorientation, adjacent regions of the interface will suffer relative displacements of the vector $\mathbf{d}_1$ shown in Fig. 4(d) or the crystallographically equivalent vector $\mathbf{d}_2$. These regions will then be separated from each other by a cross grid of screw dislocations of Burgers vectors $\mathbf{d}_1$ and $\mathbf{d}_2$ [8]. As the misorientation increases the spacing of the dislocations decreases, as in the case of low angle twist boundaries [8]. For a $\Sigma = 5$ Type 1 twist boundary, adjacent regions may be displaced, for example, by $\mathbf{d}_1/2$ and $\mathbf{d}_2/2$. The resulting screw dislocations will then have Burgers vectors of type $(\mathbf{d}_1 - \mathbf{d}_2)/2$ and be oriented at 45° to the anticipated CSL grid. For Type 2 boundaries adjacent displacements may, for example, be $(\mathbf{d}_1 + \mathbf{d}_2)/2$ and $(-\mathbf{d}_1 + \mathbf{d}_2)/2$ so that the associated dislocation has Burgers vector $\mathbf{d}_1$ as in the case of the CSL boundary. However, the calculations of the present paper suggest that all three twist boundaries, CSL Type 1 and Type 2, have similar energies and more complicated networks of dislocations may then arise. Similar arguments hold for the $\Sigma = 13$, 17 and 25 boundaries.

The importance of these deductions about the types of dislocation which can exist in twist boundaries rests in the fact the dislocations of these types can be observed directly using transmission electron microscopy (TEM) of thin film bicrystals [12]. Attempts are also currently being made using TEM to observe the predicted in-plane translations in bcc twin boundaries [13]. Good agreement between predicted and experimentally measured translations has also been obtained recently for tilt boundaries in aluminium [14]. The quantitative values of volume increases at interfaces provided by the present studies are also valuable as they enable the atomic structure of boundaries to be deduced from *X*-ray diffraction data [15]. It thus appears that future links between computer simulation and experimental investigations should provide a wealth of detailed information. However because the size of the crystals which can be studied using the computer simulation technique is very small, this information will be largely restricted to isolated interfaces and their interactions with other individual defects. The properties of real materials on the other hand are controlled by the interactions of very large numbers of defects and a continuum approach incorporating the results of discrete calculations is therefore often needed to predict the observed macroscopic behaviour. The nonlocal theories of elasticity currently being developed and applied [16] are attempting to meet this need and it will be interesting to see whether they can accommodate the in-plane translations at interfaces described in the present paper.

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References

1. P. D. BRISTOWE and A. G. CROCKER, *A computer simulation study of the structures of twin boundaries in body-centred cubic crystals*, Phil. Mag., **31**, 3, 503–517, 1975.
2. R. FLETCHER and C. M. REEVES, *Function minimization by conjugate gradients*, Comp. J., **7**, 149–154, 1964.
3. R. A. JOHNSON, *Interstitials and vacancies in α-iron*, Phys. Rev., **134A**, 1329–1336, 1964.
4. M. DONEGHAN, *The computer simulation of the structure of point defects in copper*, Ph. D. Thesis, University of Surrey, Guildford 1976.
5. B. A. BILBY and A. G. CROCKER, *The theory of the crystallography of deformation twinning*, Proc. Roy. Soc., **A288**, 240–255, 1965.
6. V. VITEK, *Multilayer stacking faults and twins on* (211) *planes in* b.c.c. *metals*, Scripta Met., **4**, 9, 725–732, 1970.
7. P. D. BRISTOWE, A. G. CROCKER and M. J. NORGETT, *The structure of twin boundaries in body-centred cubic metals*, J. Phys. F., **4**, 1850–1864, 1974.
8. W. BOLLMANN, *Crystal defects and crystalline interfaces*, Springer-Verlag, Berlin 1970.
9. P. D. BRISTOWE and A. G. CROCKER, *A computer simulation study of the structure of twinning dislocation in body-centred cubic metals*, Acta Met., **25**, 1363–1371, 1977.
10. P. D. BRISTOWE and A. G. CROCKER, Phil. Mag. [in press].

11. D. A. SMITH, V. VITEK and R. C. POND, *Computer simulation of symmetrical high angle boundaries in aluminium*, Acta Met., **25**, 5, 475–483, 1977.
12. R. W. BALLUFFI, Y. KOMEM and T. SCHOBER, *Electron microscope studies of grain boundary dislocation behaviour*, Surface Science, **31**, 68–103, 1972.
13. K. MARUKAWA *Electron microscope study of the atomic structure of twin boundaries in body-centred cubic crystals*, Phil. Mag., **36**, 6, 1375–1383, 1977.
14. R. C. POND and V. VITEK, *Periodic grain boundary structures in aluminium*, Proc. Roy. Soc., A **357**, 453–483, 1977.
15. W. GAUDIG, D. Y. GUAN and S. L. SASS, *X-ray diffraction of large angle twist boundaries*, Phil. Mag., **34**, 5, 923–928, 1976.
16. D. ROGULA [ed.], *Non-local theories of material systems*, Polish Academy of Sciences, Institute of Fundamental Technological Research, Warsaw 1976.

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