A thesis entitled

The Structural Characteristics of Twin Boundaries in Body Centred Cubic Metals

by

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Abstract

The structure and energy of \{112\} twin boundaries and twinning dislocations in α-iron, molybdenum and tungsten have been studied using a real space discrete lattice model. This method of calculation, otherwise known as the computer simulation or atomistic technique, involves the iterative minimisation of the potential energy of the atomic configuration. It has revealed that two distinct twin boundary structures can be stable in those body centred cubic metals. These are the conventional twin boundary defined by a reflection orientation relation and a twin in which the boundary consists of a layer of cells which project on the \{110\} plane as isosceles triangles. In the case of iron the two boundaries, when fully relaxed, are found to have almost identical energies but for molybdenum and tungsten the reflection boundary is preferred. The twin boundary energies for these two metals are three or four times as large as those for iron. The results suggest that in some bcc metals both types of boundary may arise in which case each perfect twinning dislocation is likely to be dissociated into two partials each with Burgers vector \(\frac{1}{12} \langle 1\overline{1}1\rangle\).

The core structures of bcc edge twinning dislocations with Burgers vectors \(\frac{1}{12} \langle 1\overline{1}1\rangle\) and \(\frac{1}{6} \langle 1\overline{1}1\rangle\) have been examined with the aid of differential displacement mapping procedures. In molybdenum and tungsten the perfect twinning dislocation of Burgers vector \(\frac{1}{6} [11\overline{1}]\) was found to be stable and well localised. However, in iron the perfect twinning dislocation always dissociated into two separate partials each of Burgers vector \(\frac{1}{12} [11\overline{1}]\) so that ribbons of isosceles and reflection twin were obtained. The separation of these partials was found to be large and the steps diffuse corresponding to negligible lattice resistance to nucleation and growth of a new layer.
In addition the interaction of vacancies and divacancies with twin boundaries and twinning dislocations has been investigated. These calculations have located the regions of maximum binding energy so that the ability of the boundaries and dislocations to act as vacancy sources or sinks can be evaluated.

Finally the results are discussed in relation to the theory of coincidence site lattices. Also the overall reliability of the computer simulation method for investigating the structure of crystalline interfaces is assessed.

The research described in this thesis was performed at the University of Surrey between October 1972 and October 1975. Parts of the work have been or will be discussed in the following publications.


Bristowe P.D. and Crocker A.G. (1975) Phil. Mag. 31, 503 (Chapter 5)

To my father and

my late mother
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CHAPTER 1 Basic Concepts

1.1. Introduction

Despite overwhelming evidence indicating clearly that crystalline interfaces govern many technologically important metallurgical processes, astonishingly little is known about the basic mechanisms and quantities involved. For instance, it is known that a grain boundary can impede the motion of a dislocation and thereby effectively increase the strength of a polycrystalline material. On the other hand, a grain boundary is a considerable source and sink for vacancies so that under applied stress and at elevated temperatures the diffusion of vacancies from one boundary to the next will result in a weakening of the material. Nevertheless neither the process of work-hardening or the phenomenon of diffusional creep is properly understood especially at a microscopic level. New experimental techniques have recently been used to resolve the detailed geometry of some special crystalline interfaces but it is difficult experimentally to predict other important parameters such as their interaction and surface energies. A theoretical technique, the discrete lattice calculation or computer simulation method, is available and capable of determining these parameters as well as the details of the atomic configuration.

As part of a programme of theoretical research at the University of Surrey on the structure and energy of crystalline interfaces using the discrete lattice calculation this thesis reports a study of \{112\} twin boundaries and twinning dislocations in body centred cubic crystals and their interaction with vacancies. Although the unique symmetry of a twin boundary makes it a rather exceptional kind of interface it is clearly a particularly appropriate starting point.
especially since the role twin boundaries play in deformation processes is not obvious and certainly cannot be overlooked. Indeed some of the unusual and unexpected results reported in the present calculations mean that future work on more general interfaces such as grain and martensitic boundaries will require careful interpretation. Further work will also not be limited to the study of interfaces in bcc metals. The reason for choosing these metals in the present work was two-fold: firstly it is clear that they are representative of many technologically significant materials and secondly various empirical interatomic potentials which give a stable bcc structure are available.

The computational methods used in this new work are described in Chapter 3. Chapters 4 and 5 give the results on faults and coherent twins in some bcc metals where it is shown in particular that the orientation relationships usually used to define twin boundaries need not always occur in practice. The structures of a number of twinning dislocations are computed and described in Chapter 6 and the results related to various nucleation and growth mechanisms. Chapter 7 examines the interaction of vacancies with coherent and incoherent twin boundaries and the possibility of these boundaries acting as vacancy sources and sinks. In the remainder of the present chapter the relevant theoretical and experimental background to deformation twinning is presented.

1.2. Twinning Crystallography

Ever since the theory of the crystallography of deformation twinning was placed on a formal basis over half a century ago (Friedel 1926) a considerable number of original papers, reviews and texts on
twinning have appeared in the literature. It is not the purpose of
the present work to develop any new experimental or theoretical
analysis of twinning. Neither is it considered suitable to reproduce
in full the vast amount of information that already exists and has
in any case been completely catalogued by several other authors (Cahn
1964, Bilby and Crocker 1965, Christian 1965, Mahajan and Williams
1973). However, it is considered necessary and appropriate to
summarise in the present and following section the basic concepts of
the theory and experimental techniques as they apply to highly
symmetric lattice structures. Detailed accounts of how the theory has
been applied to more complex structures may be found in Guyoncourt
and Crocker (1968) or Crocker and Bevis (1970).

In simple terms a twinned crystal is composed of two parts,
the parent and product, which although they have the same crystal
structure and are in contact along a common crystallographic plane,
are misorientated in some well defined way. The easiest orientation
relationship to visualize is where the product crystal is the mirror
image in the interface of the parent. The deformation necessary to
produce such a compound crystal which does not change in volume is
observed to be a simple shear of the lattice. Within the classical
theory it is conventional to denote the direction of shear by \( \eta_1 \) while
the plane containing \( \eta_1 \), which remains both undistorted and unrotated
under the deformation, is denoted by \( K_1 \) and called the composition
or twinning plane. There is however another plane which remains
undistorted (but not unrotated) by the simple shear and this is
labelled \( K_2 \). If the angle between \( K_1 \) and \( K_2 \) is \( \theta \) then the angle of
rotation of \( K_2 \) is \( \pi - 2\theta \). The plane perpendicular to \( K_1 \) and \( K_2 \) is
called the plane of shear, and the direction along which this plane
intersects $K_2$ is called $n_2$. The complete set $K_1, K_2, n_1, n_2$ are
collectively called the twinning elements although just two ($K_1$ and $n_2$
or $K_2$ and $n_1$) are sufficient to describe uniquely a particular twinning
mode. Their interrelationship is illustrated in fig. (1.1). It is
possible to interchange the twinning elements in such a way as to
retain the same magnitude of shear and obtain a conjugate (or reciprocal)
twinning mode, thus: $K'_1 = K_2, K'_2 = K_1, n'_1 = n_2, n'_2 = n_1$. The primed
characters are known as the conjugate twinning elements.

One orientation relationship which leaves the composition plane
invariant has already been mentioned: reflection in $K_1$. It is clear
from fig. (1.1) that there exist at least three others: rotation of
$\pi$ about the normal to $K_1$, reflection in the plane normal to $n_1$ and
rotation of $\pi$ about $n_1$. Further classification of twinning into two
types has been made based on these relationships and the rationality
of the twinning elements. For type I twins $K_1$ and $n_2$ possess rational
indices and the first pair of relationships above are operative. For
type II twins $K_2$ and $n_1$ are rational and the second pair of relation­
ships operate. In highly symmetric lattice structures, for instance
bcc, the reflection and rotation operations are equivalent so that the
twinning mode is degenerate and all the elements are rational. In
some multiple lattices it is usually geometrically impossible to
produce a twinned crystal by a simple shear alone and therefore a re­
shuffling of some of the atoms is necessary. Crocker (1962) has
discussed the possibility of other orientation relationships which
involve atomic shuffles and Bevis and Crocker (1968, 1969) have
widened the classical theory to include twinning modes which have
four irrational elements. These theories are not dealt with here.
but it appears that the geometrical rules governing the operation of observed deformation twinning modes are always the same, namely that the shuffles (if any) and the magnitude of the shear should both be as small as possible.

Throughout this thesis the symmetry rule relating parent lattice to product lattice in a bcc crystal will be the classical orientation relationship of reflection across the twinning plane. The resulting interface is then said to be fully coherent. However the possibility of a quasi-coherent interface in a bcc crystal will also be considered here although previous theories have tended to neglect such a possibility. A quasi-coherent interface may be constructed by a series of special atomic displacements which are applied to all the atoms in the product crystal and which have the same magnitude and direction. This has the effect of translating the product crystal relative to the parent by a vector \( t \) which may, of course, have components both parallel and perpendicular to the composition plane. In terms of the simple shear \( S_{j} \) this translation is given by

\[
t_{i} = v_{i} - S_{j} u_{j} \tag{1.1}
\]

where \( v_{i} \) and \( u_{j} \) specify lattice points in the product and parent structures respectively. Recent experimental work (Pond and Smith 1974) has suggested that a translation of this kind can exist at least in some highly symmetric structures and it is one of the purposes of the present work to identify its magnitude and direction for twinning in the bcc structure. Finally, the existence of the incoherent or stepped interface cannot be overlooked but this will not be treated in detail until Chapter 6.
1.3. Twinning in BCC Metals

In this section some of the experimental techniques that have been used to determine the twinning elements and boundary energies in bcc metals are reviewed. In particular, reference will be made to measurements performed on α-iron, molybdenum and tungsten since these metals are of special interest in the present work.

The basic procedures used to determine the twinning elements have usually relied on optical microscopy and the use of X-rays and goniometry (Barrett 1952). After deformation the surface traces delineating the twin system are readily visible although it is sometimes convenient to use standard polishing and etching methods to distinguish them from the slip lines. The Laue back-reflection X-ray technique is used to determine the orientation of the crystal axis, and by rotating the crystal about this axis the angle over which the trace is visible is determined. By plotting the results on a stereographic projection for a number of traces the twinning plane can be identified. The direction of shear may also be determined in a similar manner by measuring angular rotations but rarely can all the twinning elements be found from a single experiment. Paxton (1953) was the first to determine the twinning elements in α-iron using surface trace analysis. As predicted by Kelly (1953) they were found to be

\[(112) \quad (\overline{1}1\overline{2}) \quad [\overline{1}\overline{1}1] \quad [111]\]

with a twinning shear of 0.707. Using similar techniques the same twinning system has been found to operate in molybdenum and molybdenum-rhenium alloys at the temperature of liquid oxygen and at room temperature (Cahn 1955, Feng 1960, Schadler and Lawley 1961). Twins have also been extensively examined in tungsten using surface analysis
combined with X-ray determinations in an effort to determine the
twinning system. In particular Schadler (1960), Wolff (1962) and
Schnitzel and Keith (1962) all confirm the same twinning mode as
found in α-iron and again over a wide temperature range. More recently
techniques have been developed to determine the twinning elements
using transmission electron microscopy and electron diffraction (Hirsh
et al 1965). These procedures have been used in conjunction with
surface trace analysis (Mahajan 1971) in order to evaluate $K_1$ and $n_1$
in a cobalt-iron alloy (Mahajan and Williams 1973) and a molybdenum
rhenium alloy (Mahajan 1972). The usual (112) [111] twinning system was
once more confirmed.

The determination of the free energy associated with a \{112\}
twin boundary in a bcc metal has proved more difficult than establi­
shing the twinning elements. The intrinsic stacking fault energy on
\{112\} planes is so high that faults on these planes have never been
observed. Indirect estimations of the twin boundary energy from the
stacking fault energy have therefore been unsuccessful. A method not
unlike that of Barrett (1952) relying on surface morphology measurements
has been applied to determine the twin boundary energy in several fcc
metals (Groves and Kelly 1970) but only occasionally to bcc metals.
The technique uses equations originally derived by Herring (1951) which
relate the forces acting on a grain boundary groove to the surface
tension. At high temperatures when a grain boundary meets a surface,
grooving always occurs in order to balance these forces. Thermal
grooving will also occur when a twin boundary intersects a surface and
Mykura (1957, 1961) has shown that in this case Herring's equation
can be simplified. The twin boundary energy can be determined from
a knowledge of the surface energy and by measuring the angles of the
grooves relative to the surface. Such measurements have been performed on α-iron by Blakely and Mykura (1963) and Nilles and Olson (1970) who found the (112) twin boundary energy to be 240 mJm$^{-2}$ and 160 mJm$^{-2}$ respectively. A similar investigation on silicon iron by Dunn et al. (1950) discovered an interfacial energy of 186 mJm$^{-2}$. Apparently no measurements have been made to date on twins in molybdenum and tungsten.
2.1. Introduction

It is nearly two decades since a computer was first used to study the properties of defects in the condensed state. Although originally only point defects in metals were studied the calculations have now been extended to line, planar and volume defects in rare gas solids and alkali halides as well as pure metals. The rapid advance of computer technology has meant that with the larger and faster machines it is possible at the present time to determine, at least in principle, the properties of any defect or combination of defects in any class of material. As always, however, the results of such calculations would require careful interpretation and the validity and reliability of the interatomic potentials, boundary conditions and minimisation procedures critically assessed. In view of the vast amount of work published to date in the whole field of computer simulation it is considered appropriate to restrict this review to a selective chronology on calculations of planar defects in metals. The survey presented here must not be taken as exhaustive but rather as a collection of references which have been considered to be representative of either a particular form of planar defect, e.g. a tilt boundary, or of a particular computational procedure, or perhaps of both. For extensive reviews of other types of defects the reader is referred to the Report on the Battelle Colloquium (1972), Johnson (1973), or Vitek (1974).
2.2. Planar Defect Calculations

2.2.1. Faults and Twin Boundaries

The first significant contribution to the understanding of stacking faults in bcc and fcc metals using a computer simulation method came from Vitek (1968). Using the now well-established technique (see Chapter 4) of rigidly translating one half of the model crystal with respect to other by a variable fault vector he could obtain a relaxed energy contour for a chosen crystallographic plane (a so-called γ-surface). By studying the shape of these contours Vitek was able to conclude that there was a stable stacking fault equal to \( \frac{1}{6} [112] \) on a \{111\} plane in a fcc crystal as predicted by the hard sphere model. However he was unable to find any stable faults on either \{110\} or \{112\} planes in a bcc crystal. Fourteen different potentials (both semi-empirical and truncated pseudo) were used in the calculations and although they each give a different magnitude for the fault energy, the approximate shape of each γ-surface (for a particular crystallographic plane) was the same. It was concluded therefore that the results were general for all crystals with the bcc structure. The calculations which are convincing would have been even more so if relaxation had been allowed in all directions (not just perpendicular to the fault plane), the actual relaxation algorithm stated, a larger crystallite used and the boundary conditions specified. These comments also apply to two other calculations by Vitek (1970) and Bevis and Vitek (1970) on multi-layer stacking faults and twins in bcc metals. However in these references the computational procedure is quite clear. Atoms at infinity on one side of the boundary are fixed and then the relaxation carried out plane by plane so that any components of displacement common to all atoms in a plane
are immediately applied to all succeeding planes. The translation at infinity can then be found by summing the individual translations near the boundary. Using this method Vitek (1970) found that although a three-layer fault was metastable successive displacements of the layers were not the expected $\frac{1}{6} [\overline{1}11]$. Instead they were approximately $\frac{1}{12} [\overline{1}11]$, $\frac{1}{6} [\overline{1}11]$ and $\frac{1}{12} [\overline{1}11]$. Moreover, calculations on wider faults lead Vitek to conclude that an infinite twin is not "sharp" but that the twinned half of the lattice is shifted by $\frac{1}{12} [\overline{1}11]$ along the boundary. It should be noted that fig. (3b) of that paper is drawn incorrectly (see Chapter 4). Bevis and Vitek (1970) in their paper compared the energies of various twinning modes in bcc metals when the twin was in both the sharp and displaced configurations. They deduced from their calculations that, using several different interatomic potentials, not only was the $(112) [\overline{1}11]$ mode the most energetically preferred but the displaced configuration always had a lower energy than the sharp configuration.

Atomistic calculations on stacking faults in other crystal structures have also been made. Schwartzkopff (1969) has considered metastable stacking sequences in an hcp structure representing magnesium. Using a Morse function he was able to obtain unrelaxed energy contours for a number of known slip planes. By locating the minima in these contours definite stacking faults could be predicted and also the direction of motion of their associated partial dislocations. However, because no relaxation process was involved in the calculations, the results must only be considered indicative of what actually occurs in practice and certainly no importance can be attached to the actual magnitudes of the energies obtained. Harrison (1973) has calculated relaxed lattice displacements in the vicinity
of stacking faults and twins on close-packed planes in a fcc structure that represented aluminium. Relaxation was allowed perpendicular to the fault in a model containing 21 close-packed layers in a crystal that was held at constant volume (rigid boundary conditions). The atoms, which interacted via a truncated pseudo-potential, were relaxed using a method based on inverse linear interpolation of the energy sum gradient. By plotting the lattice distortion perpendicular to the fault plane Harrison could identify regions of contraction and expansion and hence consider whether solute atoms could be accommodated near the fault. He also found that the relaxation energies were up to 10% of the unrelaxed fault energies. More recently Vitek (1975) has reported a calculation on stacking faults on {111} and {110} planes again in a model representing aluminium where the interatomic potential used was constructed on the basis of pseudo-potential theory. The method of calculation was basically the same as that used by Vitek (1968) so that by faulting the model crystal cross-sections of the γ-surfaces could be obtained on both the (111) and (110) plane. The cross-section of the γ-surface in the [112] direction for the (111) plane revealed a minima at $\frac{1}{6} [\bar{1} \bar{1} 2]$ (not $[\bar{1} \bar{1} 2]$ as misprinted in the paper) corresponding to the usual stable stacking fault. In the case of the (110) plane the shape of the [110] cross-section depended on the size of the model used. Allowing relaxation perpendicular to the fault in a model containing three (110) planes no local minima were found. However when a volume increase of 4% was allowed and also when the model size was increased to seven (110) planes a minimum was obtained at $\frac{1}{4} [1 \bar{1} 0]$. It was hence postulated that this could be a stable stacking fault which may also occur in other fcc materials with high stacking fault energies. The same kind of calculation has also been performed by the present author using a
semi-empirical potential for copper constructed by Englert et al. (1970). The cross-section of the \( \gamma \)-surface on the (111) plane confirms the work of Vitek (1968, 1975) in so much as a local minimum was found at \( \frac{1}{6} [\overline{1}12] \). However it was difficult to agree with the result of the calculation for the (110) plane. Even in a model containing 75 (110) planes and only allowing relaxation perpendicular to the fault no local minima were found. When relaxation was allowed in all directions, however, a plateau in the \( \gamma \)-surface was revealed around \( \frac{1}{4} [1\overline{1}0] \). The structure of the fault was not as expected though. Instead of being confined to one (110) plane it was spread over four planes. The discrepancy between these and Vitek's results may be due to the latter's computational procedures. It is difficult to justify using a long range pseudo-potential in a small model crystal and also not allowing relaxation parallel to the fault vector.

2.2.2. Grain Boundaries

The atomistic nature of a more general kind of interface, the grain boundary, has received considerable attention in recent years not only in an effort to understand several important metallurgical processes but also to determine the validity of purely geometrical concepts such as lattice coincidence and atom sharing. Weins and his co-workers have reported a number of computer calculations on the structure and energy of high angle grain boundaries (Weins et al. 1969, Weins et al. 1970, Weins et al. 1971, Weins 1971) most of which have been summarised by Weins (1972). Their computational procedures are quite clear. Initially they constructed an exact coincidence boundary in which several of the atomic sites in the model formed a superlattice common to both crystals on each side of the boundary. One crystal was
then rigidly translated with respect to the other until the initial energy of the configuration was a minimum. This initial energy was calculated by summing pairwise interactions given by a Morse function that represented either gold or aluminium. The lowest energy configuration is then found by relaxing the atoms, so that they effectively experience no net force, using an iterative procedure called conjugate gradients (see Chapter 3). A relatively small size model was used but with periodic boundary conditions in the direction of translation. An interesting problem with all grain boundary simulations is knowing how many atoms should surround the actual boundary region. Weins (1972) used the criterion that if, after the crystals had been rigidly translated, there existed voids greater than 90% of the lattice parameter in diameter then additional atoms were inserted. His calculations, which were on several symmetric tilt boundaries and twist boundaries, each gave a lowest energy configuration which destroyed boundary coincidence and therefore he concluded that relaxed boundaries in general contained no coincidence sites. This result is significant in that earlier theories (Brandon et al. 1964, Bishop and Chalmers 1968) had ascertained that grain boundary structure will always contain coincidence sites or shared atoms.

Another series of atomistic calculations (Hasson et al. 1970, Hasson and Goux 1971, Hasson et al. 1972) on the structure and energy of several symmetric and asymmetric tilt boundaries in crystallites representing copper and aluminium have independently found the same result. However their computational procedures are not quite so clear. Unlike Weins (1972) they apparently consider the translation away from exact coincidence separately from the atomic relaxation. Also they determine the number of atoms around the boundary by starting the simulation with a model that contains deliberately far too many atoms.
Upon relaxation they remove the atom with the highest energy and iterate the procedure until the removal of an atom causes the energy of the crystallite to rise. Again, however, although cyclic boundary conditions were imposed the effective size of the model was still small since it was limited to the size of the elementary cell defined by the periodicity of the crystal structure. Clearly the results would have appeared more convincing if a multiple cell had been used. Additionally the relaxation algorithm is not specified completely but can at least be assumed to be of quasi-dynamic type. Hasson et al. (1972) illustrate the variation of energy with misorientation angle for symmetrical tilt boundaries about [100] and [011] in a simulated fcc crystallite. Cusps occurred in the curve significantly at coincidence (or near coincidence) site misorientations such as that of a (111) twin boundary.

Dahl and his co-workers have also considered the computer simulation of extended defects in metals (Dahl 1970, Dahl et al. 1971, Dahl et al. 1972). Using both the dynamic and quasi-dynamic relaxation techniques they are able to calculate the structure and energy of both high and low angle grain boundaries in a fcc structure representing γ-iron. The influence of grain boundaries on the formation and migration energies of vacancies was also determined (see Chapter 7). The size of their model crystal was stated to be large enough so that the imposed rigid boundary conditions did not effect the relaxation of the grain boundary. Only asymmetric tilt boundaries were studied that lay in the (010) plane and had an axis of rotation <100>. The structure and energy of the boundaries were obtained for various angles of misorientation between 5 and 85 degrees. The structures were said to contain regions of "good and bad fit", and
the stresses around the boundary were short-ranged as predicted by Hirth and Lothe (1968). When the variation of the energy of the tilt boundary as a function of angle was plotted it was seen that narrow cusps occurred at some coincident site boundaries. Other cusps, however, were more shallow indicating that low-energy configurations can not only occur at special grain boundary angles but also at small perturbations around these angles.

Most of the calculations reported by the Weins, Hasson and Dahl groups actively engaged in the simulation of grain boundaries have confirmed the dislocation models of low angle boundaries (Read and Shockley 1950) and the importance in high angle boundaries of periodic configurations. In addition they have apparently found that the energy of a coincidence high-angle boundary may be reduced by a relative translation away from the coincidence site position. However, an extensive investigation performed recently by Bruggemann and Bishop (1973) has revealed that these rigid translations do not destroy the pattern of coincidence sites. According to them analysis of the magnitudes of the translations given, for instance, by Weins et al. (1971) shows that they are virtually equal to the magnitudes of the vectors defining the "complete pattern shift lattice" or DSC lattice as given by Bollmann (1970). These special vectors shift, but do not destroy, the pattern of coincidence sites and therefore do not destroy coincidence. Bruggemann and Bishop (1973) hence concluded that the results of computer simulations of grain boundaries to date give little cause for rejecting the concept of atom sharing. Nevertheless they also point out that short wavelength periodicity and not atom sharing is probably the dominant structural feature of a grain boundary that results in, for example, energy cusps. This periodicity clearly remains even when the boundary is in near coincidence.
All the references cited so far in this chapter have described simulations which fall within a broad class of calculations called molecular statics (see Chapter 3). In these calculations interest is focussed solely on the final static or lowest energy configuration that is generated at the end of the simulation. This configuration is clearly artificial inasmuch as the temperature to which it corresponds is absolute zero. Obviously it is of some importance to determine how the properties of defects in metals are influenced by such thermodynamic quantities as temperature and pressure. It would be inappropriate to exclude from this review another class of atomistic calculation capable of such determinations: molecular dynamics (Alder and Wainwright 1959, Gibson et al. 1960). Basically in this technique the velocity and position of the atoms can be adjusted so as to simulate any desired temperature (which is proportional to the square of the velocity) or pressure (proportional to the atomic density). The method has had some success in dealing with point defects (Cotterill and Pedersen 1972) and has recently been applied to problems of grain boundary structure and migration (Cotterill et al. 1974). In the latter calculation a two-dimensional 'liquid' of 400 atoms interacting via a Lennard-Jones potential is introduced between 2 two-dimensional close-packed crystallites at a fixed misorientation of 21.8°. A pressure could be simulated by varying the distance between the crystallites and in practice was typically in the range 10-100 atmospheres. A potential barrier prevented atoms from being squeezed out of the model between the crystallites. The temperature of the liquid could then be lowered until solidification (densification) occurred so that the model could relax at a temperature above absolute zero. In this way it was possible to simulate a grain boundary structure at a given temperature under various pressures.
and vice-versa. Cotterill et al. (1974) found that the effect of decreasing the temperature (from 50 K) under constant pressure was to make the grain boundary less diffuse and more defined. At absolute zero the boundary was seen to be straight and localised as is found in molecular statics calculations. The application of pressure at absolute zero had little effect on the boundary but at ~40 K an increase in pressure caused the boundary to become more dense. All of the relaxed structures obtained lacked any form of periodicity even at 0 K which is not in agreement with the molecular statics calculations. However it is difficult to make a true comparison in this respect because the boundary conditions which can strongly influence the results were different in both calculations. Even though the model described by Cotterill is essentially quite crude in that it was only two-dimensional it is clear that the molecular dynamic technique is very powerful and will in future provide important information on how thermodynamic quantities affect defect structures.
CHAPTER 3 The Computational Model, Numerical Procedure and Pair-Potentials

3.1. Previous Methods

Probably the most significant step forward in the construction of a lattice model amenable to numerical treatment with the help of a computer was made by Gibson et al. (1960). Their general formulation of the problem of determining the atomistic structure of defects in crystals has not changed, although the details of the numerical procedures have now become more sophisticated. Indeed this is evident from the work of the many authors already mentioned in the previous chapter.

Therefore the general principles behind each such atomistic calculation may be defined as follows. Initially a perfect model crystal is built mathematically with the correct lattice structure of the material to be simulated and an orientation and size most suitable to the chosen defect. Conventionally the resulting crystallite is divided into two regions. Region I, the so-called computational cell, contains the atoms whose behaviour is to be studied and which are free to move to their equilibrium configuration. Region II, the outer mantle, contains atoms which may or may not be free to move depending on the type of boundary condition imposed. Essentially the purpose of the outer mantle is to simulate an infinite crystal or at least to ensure that every atom in the computational cell has a complete set of neighbouring atoms lying within the range of the interatomic potential. Since the work of Gibson et al. (1960), who used compliant boundary conditions, where atoms on the outer faces of the computational cell are given extra forces simulating the reaction of atoms outside, basically three other boundary conditions
have been used. These are (i) rigid (ii) periodic and (iii) elastic. The present work employs all three of these conditions, which are described in more detail in §3.2.2.

After the introduction of the defect, which may be nothing more than a guess at the relaxed structure but is more often based on elasticity theory, the total potential energy of the atoms in the computational cell is minimised. The minimisation process, which produces the required relaxation of the lattice, is computationally the most important procedure since it determines the overall computer processing time of the simulation. Until 1972 the best known and most widely used way of minimising the potential energy function was the quenched dynamical method of Gibson et al. (1960). Several authors, notably Johnson (1964), Bullough and Perrin (1968) and Dehl et al. (1971) have used the method on different defect problems with considerable success. Briefly, in this procedure the classical equations of motion for the atoms are numerically integrated simultaneously using a central difference approximation. The kinetic energy of the assembly is monitored and when it reaches a relative maximum all the velocity components of the atoms are set to zero. This quenching process is iterated until equilibrium is attained. Its simplicity and ability to avoid metastable configurations has meant that the method has been advantageous to use. However simulations of defects which require large crystal models can be time consuming.

In the present work a routine that minimises the potential energy function directly knowing its first derivative or gradient has been adopted. The procedure is a modified method of steepest descents called conjugate gradients and is due to Fletcher and Reeves (1964). The details are discussed in §3.2.3. Several authors, for instance,
Weins (1972) and Norgett et al. (1972) have shown that the method is very fast in convergence. It is particularly suitable for the minimisation of a function of a large number of variables and also where the interatomic potential is fairly simple, as is the case for cubic metals. Another method based on the determination of the matrix of second derivatives is even more efficient but requires a large computer store and has only so far been applied to simulations in ionic solids where the interatomic potential is more complicated (Lidiard and Norgett 1972).

The success of the computational models and numerical procedures that have been summarised in this section relies crucially, of course, on the accuracy of the assumed interatomic interaction. No attempt has been made in the present work to construct such an interaction. Instead, potentials have been taken from the literature that, primarily satisfy the important stability conditions of the lattice (see e.g. Born and Huang 1954 or Vitek 1968) but also have consistently produced results similar to those obtained using other types of interaction, e.g. pseudopotentials (see Vitek 1970). A description of these potentials, their construction and the metals they represent may be found in §3.3. For an up-to-date review of empirical potentials used in simulation studies see Johnson (1973) or Torrens (1972).

Finally it is important to mention that the general methods described in this section, and indeed the methods used in the present work, may be termed molecular statics calculations, i.e. the simulation is effectively performed at absolute zero. Molecular dynamic calculations where the simulation is performed at a known finite temperature have also been attempted by several workers. For a recent calculation of this type on grain boundary structure see Cotterill et al. (1974).
3.2. Present Method: The DEVIL Package

All of the results described in this thesis were obtained using a standard lattice defect package called DEVIL (Defect Evaluation In Lattices), the bulk of which was developed at A.E.R.E., Harwell. The program itself may now be considered as a prototype since it has been rewritten to introduce a number of refinements. However, besides the present work the original has been used successfully by several other authors, e.g. Norgett et al. (1972), Perrin and Savino (1973) and Savino and Perrin (1974) to predict the energetic and structural characteristics of various types of defect. The following sections in this chapter describe in detail the basic stages in the simulation process that are contained in DEVIL, i.e. the construction of the model crystal with appropriate boundary conditions, the creation of the defect, and the relaxation procedure. Also a routine is described that enables the initial and relaxed configurations to be plotted and finally a simple flow diagram of the whole package is presented.

The program is currently held on disk at the Rutherford Laboratory and is run via the ELECTRIC remote job entry facility on the IBM 370/195. The display procedures are accessed on a Tektronix 4010 V.D.U.

3.2.1. The Lattice Handling Techniques

In general the model crystal is created in the form of a rectangular block of atoms having the desired lattice structure and orientation. In principle any Bravais structure and any orientation may be specified. In the present work where the defect studied is \{112\} <\overline{1}11> twinning in bcc crystals, the block edge vectors are read in so as to make the faces of the crystallite (1\overline{1}0), (1\overline{1}1) and (112). Obviously the lattice basis vectors of the bcc structure are
also input along with the number of basis atoms, which is one. In subroutine LATTIS (see Flow Diagram) several crystallographic parameters are calculated which are used throughout the program. Along with the set of reciprocal lattice vectors they include the volume of the unit cell, the spacing between planes along the block edge directions and the packing factor or number of cubic mesh sites per unit cell (the cubic mesh is formed when the lattice vectors are rotated onto the block edge vectors).

After the size and shape of the computational cell (which is governed by the dimensional nature of the defect) has been read in, subroutine REGION calculates the overall dimensions of the crystallite (region I and region II) from the range of the given interatomic interaction. As stated previously this is done on the criterion that every atom in region I must have a complete list of neighbours. The actual size of region II will also depend on the imposed boundary condition. This will become clear from §3.2.2. Subroutine REGION also indexes or numbers the atoms. In order to avoid having a neighbour list for every atom in the computational cell the indexing is performed such that the change in index from one atom to another is dependent only on their relative position. Thus the indices of the neighbours of a particular atom are found simply by adding constant values to the index of that atom. Therefore the storage is reduced by having only one neighbour list for each sublattice. The introduction of a defect into the perfect lattice may of course upset the indexing scheme. This would happen, for example, if large translations of the lattice have occurred or if vacancies or interstitials have been introduced. Subroutine LOOKUP ensures that the correct modification of the neighbour lists is made in such cases. The actual insertion
of the defect may or may not be complicated depending not only on
the type of defect but on how accurate a first approximation to the
relaxed configuration is desired. For twins in single lattice
structures, for instance, only a shuffling of atomic planes is
required however for edge dislocations in anisotropic elastic media
the standard partial differential equations for the atomic displace­
ments have to be solved. The solution is complex even for special
cases of high symmetry (Hirth and Lothe 1968).

3.2.2. The Boundary Conditions

There are three types of boundary condition that have been
used in the present work, rigid, periodic and elastic. However it
is only necessary to describe in detail here the first two since the
elastic boundary condition is derived from the rigid by simply displacing
atoms by a prescribed amount according to the elastic solution of
the appropriate defect. The atoms in the elastic region still remain
rigid although no longer, of course, in their perfect lattice
configuration.

When rigid boundary conditions are applied in a given direction
atoms in region II of that direction are fixed and remain so through­
out the simulation. When periodic boundary conditions are applied in
a given direction the computational cell is extended in that direction
in a cyclic fashion so as to form an array of supercells. Atoms in
the periodic regions move as if rigidly attached to their parents
in the computational cell. The application of periodic boundary
conditions in a certain direction is obviously advantageous when it
is required to have a repetition of the defect in that direction, for
example along the line of an edge dislocation. However care must be
taken to choose the correct boundary condition for a defect, since in certain circumstances the behaviour of atoms along the boundary can prejudice the relaxation in the computational cell.

3.2.3. The Relaxation Procedure

The conjugate gradient minimisation procedure is contained in subroutine RELAX. In order to use this procedure the total potential energy of the atoms in the computational cell and the forces on them must be determined. This is performed in subroutine FUNC which simply sums all the pairwise interactions between atoms from the assumed interatomic potential defined in POTN.

The actual conjugate gradient method, which was originally conceived by Hestenes and Stiefel (1952), modified by Fletcher and Reeves (1964) and bought into its present FORTRAN form by Fletcher (1972), may be summarised as follows. The n-dimensional function $E(x)$ representing the potential energy of the assembly of $n/3$ atoms having a configuration $x_k$ on the kth iteration is minimised along certain search directions $D_k$ proportional to $x_{k+1} - x_k$ where $x_{k+1}$ is an improved configuration. To ensure quadratic termination these directions are chosen such that they are mutually conjugate with the matrix $H$ of the second derivatives of $E$, or

$$D_i^T H D_j = 0 \quad i \neq j$$

Fletcher and Reeves (1964) showed that one way this condition may be satisfied is if the initial direction $D_0$ has the steepest descent, and if successive search directions are related linearly to the previous ones by
\[ D_i = -\frac{f_i}{\|f_i\|} + \frac{\frac{f_i^T f_i}{\|f_i\|} - \frac{f_{i-1}^T f_{i-1}}{\|f_{i-1}\|}}{\|f_{i-1}\|} D_{i-1} \]

where \( f_i \) is the gradient vector \((= \partial E/\partial x_i)\) and is known. Fletcher (1972) showed that alternative but similar expressions for \( D_i \) may be chosen without significant change in the minimisation. He also points out that the minimisation of a function of \( \approx 10^3 \) variables is found to occur within about 50 iterations which is in accord with the present work.

3.2.4. The Display Procedure

Subroutine DISPLAY writes out and plots the positions of atoms in the perfect and/or relaxed configurations. The plotting at present involves use of the SCFOR routines available from the Atlas Laboratory SC 4020 package. However, with the introduction in mid-1975 of a new FR80 visual display unit and associated software these routines will soon require modification and may in the long term need to be completely changed. Only two-dimensional plots have so far been attempted by taking relevant cross-sections across the computational cell and representing the atoms by points and crosses. Examples of the hard copy output obtained from the Tektronix are shown in figs. (6.10) and (6.11).
3.2.5. The Flow Diagram

The preceding sections describing DEVIL may be summarised in a simple schematic flow diagram. The routines follow each other sequentially and are self explanatory.

Start

Read

LATTIS

Write

Read

REGION

Write

FUNC (EP)  POTN

Output

Yes

DISPLAY

No

1

Read input data specifying lattice of model crystal.

Generate reciprocal lattice vectors and other parameters for subroutine REGION.

Write input data and parameters determined in LATTIS. Read data specifying boundary conditions and computational cell size.

Create perfect crystal. Apply fixed and/or cyclic boundary conditions.

Write input data and size of boundary mantle.

Calculate energy of perfect crystal EP

Write perfect crystal energy. Write and/or display atomic sites of perfect crystal.
Read defect data.

Create defect in perfect crystal.

Generate list of neighbours.

Calculate initial energy of crystal with defect.

Relax to minimum of energy using method of conjugate gradients.

Write energy of relaxed defect crystal. Write and/or display atomic sites of relaxed defect crystals.
3.3. The Pair-Potentials

Three empirical interatomic potentials $\phi(r)$ were used in the calculations described in this thesis. They are the Johnson $J_0$ potential for iron (Johnson 1964), a molybdenum potential developed by Kenny and Heald (1974) and a potential for tungsten due to Stabell and Townsend (1974). All three of these empirical potentials which are shown in fig. (3.1) terminate between second and third nearest neighbours. They consist of linked, cubic splines, three in the case of iron and tungsten, and two for molybdenum. The vacancy formation energies for iron, molybdenum and tungsten which they predict are 1.4, 2.2 and 3.9 eV, respectively, which reflects the depths of their potential wells. The iron potential differs significantly from the other two in that it holds the crystal model in equilibrium without the use of a second term to simulate the cohesive energy of the free electron gas. In practice this additional volume-dependent potential for molybdenum and tungsten is imposed by means of the boundary conditions.

As mentioned previously in this chapter it is crucial that the potential used in a computer simulation is an accurate representation of the material and its structure, otherwise the calculation becomes meaningless. On the other hand in a discrete lattice calculation of this type the potential must not become too complex or long range since the computing time then becomes excessive. It is believed that the potentials used here are at least accurate enough to predict consistent structural characteristics of defects in the crystals. They also have the advantage of being exceedingly simple in form.

For a good critical review and philosophy of potentials in computer simulation see the Report of the Battelle Colloquium (1972).
4.1. The Generalised \{112\} Stacking Fault.

In view of the fact that deformation twins may be regarded as ordered stacks of faults on \(K_1\) planes it is clear that it would not be inappropriate to precede a study of the structure of twin boundaries with that of the generalised stacking fault. In this chapter some detailed results are presented from a computer simulation study of generalised \{112\} stacking faults in a body centred cubic structure representing \(\alpha\)-iron. The method adopted is similar to that used by Vitek (1968, 1970) and the results, apart from a crucial plot of a stable fault found to be the nucleus of a twin boundary, are in complete agreement.

A generalised fault was created in a \((112)\) plane in a b.c.c. structure, as shown schematically in figure (4.1.a) by formally translating one part of the crystal by \(\frac{1}{2} \alpha [11\bar{1}]\), \(0 \leq \alpha \leq 1\). The resulting fault is equivalent to that obtained by a displacement of \(\frac{1}{4} (n + \alpha) [11\bar{1}]\), where \(n\) is any positive or negative integer. The physical shear associated with the deformation twinning process is in the opposite sense to the displacement used here, arising when \(n = -1\) and \(\alpha = \frac{7}{3}\). The unrelaxed fault energy \(\gamma_\text{f}\) was determined as a function of \(\alpha\) using the Johnson \(J_0\) potential for iron (Johnson 1964). The resulting curve which is shown in figure (4.2), is symmetric about \(\alpha = 0.5\) and contains no local minima. The faulted model crystals, which consisted of 23 \((112)\) planes each containing 18 atoms, were then allowed to relax using the DEVIL lattice handling routines described in Chapter 2. During the relaxation process the outer boundaries parallel to the \((112)\) fault planes were kept rigid whilst cyclic
boundary conditions were imposed on the other surfaces. It was anticipated that for each value of $\alpha$ the relaxed structure would be an elastically strained, but otherwise perfect, single crystal as shown schematically in figures (4.1b) and (4.1c) for $\alpha < 0.5$ and $\alpha > 0.5$ respectively. In practice this occurred for all values of $\alpha$ except $0.38 < \alpha < 0.48$ when the metastable structure shown schematically in figure (4.1d) was obtained. This surprising configuration may be interpreted as a twin nucleus consisting of one layer of cells in twin orientation bounded by interfaces with a structure represented by isosceles triangles in the projection shown in the diagram.

The energies of the relaxed configurations are shown in figure (4.2) which demonstrates that $\gamma_t$, the energy of the metastable twin structure is considerably larger than $\gamma_c$, the corresponding energy of the strained single crystal, which is again symmetric about $\alpha = 0.5$. The energy is of course inversely proportional to the number of (112) planes used in the model and it was most fortuitous that the relaxation procedure was able to locate this interesting structure. It will be noted from figure (4.2) that the curve $\gamma_t$ has a symmetric minimum at $\alpha = \frac{2}{3}$ corresponding to a configuration involving zero elastic strain. However for this particular value of $\alpha$ the relaxation process did in fact produce the lower energy configuration of a strained perfect single crystal. The total energy of the unstrained microtwin was determined to be $0.516 \text{ J m}^{-2}$ ($516 \text{ erg cm}^{-2}$). For the ideal case the total shear displacement of $\alpha = \frac{1}{2}$ can be resolved into component shears of $-\frac{1}{6}$, $-\frac{1}{6}$, $\frac{1}{6}$ between the pairs of planes $(0,1)$, $(1,2)$ and $(2,3)$ which are labelled in figure (4.1d).

Before discussing the relaxed boundary structures predicted in this study, it is interesting to consider the significance of the
symmetric form of the energy $\gamma_f$ of the unrelaxed faults. This energy is plotted in figure (4.2) which demonstrates that equal and opposite displacements on the (112) [11\bar{1}] shear system produce identical changes in bond length, at least for the first and second nearest neighbours which fall within the range of the Johnson potential. A glance at figure (4.1a) indicates that this result is unexpected as nearest neighbour bonds, joining adjacent atoms on either side of the fault, clearly become shorter for small displacements of the upper half-crystal to the right and longer for displacements to the left. However, these differences are exactly compensated by distortions of the other nearest neighbour bonds which cross the interface and join atoms on planes separated by 2$d$, where $d$ is the (112) interplanar spacing. Thus the changes in energy in the two cases is identical.

The same effect occurs for second nearest neighbours and indeed further analysis has demonstrated that the result is general for all neighbours, and hence all 2-body potentials. A detailed account of this analysis illustrating for which crystallographic planes, directions and structures this result holds is given in §4.3.

The composite curve $\gamma_e$ of figure (4.2) representing the energy of the elastically strained perfect single crystal of figure (4.1b) ($\alpha < 0.5$) and figure (4.1c) ($\alpha < 0.5$) is also symmetric. This arises because both parts of this curve are parabolae, the energies being proportional to $\alpha^2$ and $(1 - \alpha)^2$ respectively. The energy $\gamma_e$ is also inversely proportional to the number of (112) planes used in the model crystal and if more had been used in the present calculation the metastable configuration of the single layer microtwin might not have been discovered. The curve $\gamma_e$ of figure (4.2) giving the energy of this strained microtwin is also, at least approximately, a parabola of the same form.
4.2. The Nucleation and Growth of Microtwins.

The structure of the twin boundary predicted by this work confirms the numerical calculations of Vitek (1970), namely that a mirror image orientation relation is not satisfied and there is an additional displacement of \( \frac{1}{12} [\overline{1}11] \) at the interface. However Vitek unfortunately plotted his results incorrectly and thus did not fully appreciate the symmetry of the interface as illustrated in figure (4.1d) and more clearly in figure (4.3) where two twin boundaries are separated. The significant feature of this interface is that it has an identical appearance when viewed from either side of the boundary. The only other \{112\} twin boundaries in bcc crystals with this property are the conventional mirror image twin of figure (4.1e) or figure (4.1f) where a localised volume increase has been allowed at the interface. This volume increase would occur if, for example, the conventional twin boundary were constructed from hard spheres in which case the expansion needed would equal \( \left( \frac{1}{4} \sqrt{2} - \frac{1}{3} \right) [112] = 0.0202 [112] \), if the reflection orientation relation is to be retained. The schematic illustrations of figure (4.1d) and figure (4.3) involve no expansion perpendicular to the interface. The numerical results did however involve a small expansion of about 0.0064 [112] concentrated at the boundary. A hard sphere model of this boundary requires a rather larger expansion of \( \left( \frac{1}{24} \sqrt{70} - \frac{1}{3} \right) [112] = (0.0152) [112] \), which is about 75\% of the corresponding value for the conventional twin. Thus the relaxed computer simulated boundary corresponds satisfactorily with that suggested by the hard sphere approximation. However it is interesting that the structure of this boundary was not anticipated prior to the discrete lattice calculations and as this structure appears to be the most likely one to occur in practice the results help to validate the use of 2-body empirical potentials.
In order to investigate whether the unstrained microtwin of figure (4.1d) might be induced to grow, additional faults were now produced on adjacent (112) planes. In particular translations of \( \alpha/2 [11\overline{1}] \), \( 0 \leq \alpha \leq 1 \), were made on planes separated by 2d and 3d from the original fault. Upon relaxing these structures various configurations were obtained, depending on the fault separation and \( \alpha \). In some cases the microtwin effectively grew so that 2, 3 or 4 layers of cells were in true twin orientation, rather than the single layer of the original structure. An example of an unstrained 4-layer twin, produced when the fault separation was 3d, is shown in figure (4.3). In other cases the microtwin remained 1-layer thick or was annihilated. In general all of the relaxed configurations did of course involve elastic strains. However it was possible to deduce the energy of the unstrained twins and this was found to be 0.516 J m\(^{-2}\) as given above for the 1-layer twin and 0.540 J m\(^{-2}\) for the thicker twins.

It is an interesting fact that microtwins have been effectively nucleated and induced to grow from stacking faults. In particular a 1-layer twin was produced upon relaxing a single translation fault. However this fault is unlikely to arise in a real crystal so that no nucleation mechanism is being implied here. In practice nucleation is expected to be associated with dislocation dissociation mechanisms and calculations of this kind are discussed in Chapter 6. In this computer study the growth of a microtwin has been induced by generating an appropriate second fault in a neighbouring parallel plane although again no real growth mechanism is implied. Alternatively this process may be considered to be the nucleation of a second microtwin followed by the interaction of the two nuclei to give a twin of up to 4-layers in thickness. The mechanism could clearly be extended to produce
broader twins but when using the Johnson potential the maximum
spacing of the faults must be no greater than 3d in order that the
nuclei may interact with each other. Once this has occurred the
remaining two twin boundaries do not interact under this potential
and thus the energy of the unstrained twins of thickness greater
than d consists solely of the self energy of the two boundaries. Thus
the twin boundary energy as determined in this study is 0.270 J m$^{-2}$
which compares with an experimental value of 0.160 J m$^{-2}$ obtained
by Nilles and Olson (1970) using thermal growing techniques. For
the cases of the 1-layer twin the two boundaries do interact in such
a way that the total energy of the twin is reduced by about 4½%.
Thus at this separation there is a small negative interaction energy
between the boundaries, or equivalently a small attractive force
between them.

4.3. Discussion on the Symmetric Variation of Fault Energies.

In §4.1. 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 ± [111] directions.
In addition the interatomic pair potential used to evaluate their
energy terminated between second and third nearest neighbours. The
aim of that 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 sheared positions to equilibrium configu-
trations. 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 bcc fault in fig. (4.4).
It suggests the following general problem: Given a crystal which
undergoes a rigid-body shear on a plane \( h_1 = (h_1, h_2, h_3) \) 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 \( h_1 \) cuts this bond the
vector becomes \( p^i \pm a u^i \) in the faulted crystal. Here \( a \) is a para-
meter defining the magnitude of the displacement and the two signs
correspond to the two senses of the shear. The length of the bond
is thus changed from \( \lambda = (p^i p^j c_{ij})^{1/2} \) to

\[
\lambda^\pm = \left[ (p^i p^j + a^2 u^i u^j \mp 2 a u^i u^j) c_{ij} \right]^{1/2}
\]

(4.1)

where \( c_{ij} \) is the direct metric tensor. Clearly \( \lambda^+ \neq \lambda^- \) 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 \( L^\pm = \lambda^\mp \) for all values of \( a \). For this to
occur \( p^i \) and \( q^i \) must be crystallographically equivalent variants \( r^i_1 \)
and \( r^i_2 \), of a particular vector form \( r^i \), which satisfy
\( r^i_1 u^j c_{ij} = - r^i_2 u^j c_{ij} \). Matched pairs of this kind must of course arise
for all possible variants \( r^i_\alpha \) of \( r^i \). In addition, as indicated in
fig. (4.4) for the bcc fault, for each \( r^i_\alpha \) there will be \( r^i_\alpha h_1 \) parallel
bonds which cross the fault for each atom in the plane \( h_1 \). Hence
to obtain identical distributions of bond lengths for opposite shears
the condition

\[
\sum_\alpha (r^i_\alpha h_1) (r^i_\alpha u^j c_{ij}) = 0
\]

(4.2)

must be satisfied for all lattice vectors \( r^i \). However, although this
condition is necessary it is not sufficient. Clearly, for pairs of bonds to match across the fault \( \sum_{\alpha} \mathbf{r}^i \mathbf{h}_i \) must be even.

There are two groups of solutions to equation (4.2). The first arises when the shear plane \( \mathbf{h}_i \) is perpendicular to an \( n \)-fold axis. The vectors \( \mathbf{r}^i_\alpha \) then occur in groups of \( n \) with \( (\mathbf{r}_\alpha^i \mathbf{h}_i) \) constant, as shown for the case of \( n = 3 \) in fig. (4.5a). Thus equation (4.2) reduces to

\[
\sum_{\alpha=1}^{n} (\mathbf{r}^i_\alpha \mathbf{u}^j_c) = 0 \quad (4.3)
\]

which is equivalent to the identity

\[
\sum_{\alpha=1}^{n} \cos \left( \theta + \frac{2(\alpha-1)\pi}{n} \right) = 0 \quad (4.4)
\]

where, as shown in Fig. (4.5b), \( \theta \) is the angle between \( \mathbf{u}^i \) and the projection of \( \mathbf{r}_1^i \) on to the plane \( \mathbf{h}_i \). Thus equation (4.2) is satisfied by each group of \( n \) vectors and hence by all vectors \( \mathbf{r}^i \) crossing the fault plane. Similarly the second group of solutions arises when the shear direction \( \mathbf{u}^i \) is parallel to an \( n \)-fold axis. The term \( (\mathbf{r}^i_\alpha \mathbf{u}^j_c) \) is then constant so that equation (4.2) reduces to \( \sum_{\alpha=1}^{n} (\mathbf{r}_\alpha^i \mathbf{h}_i) = 0 \), which is equivalent to the above identity if \( \theta \) is now the angle between \( \mathbf{h}_i \) and the projection of \( \mathbf{r}_1^i \) on to the plane normal to \( \mathbf{u}^i \). Obviously this result is just a special case of the initial proviso that \( \sum_{\alpha} (\mathbf{r}^i_\alpha \mathbf{h}_i) \) be even. Note also that within this proviso the second shear elements \( \mathbf{u}^i \) and \( \mathbf{h}_i \) appearing in the two solutions, are unrestricted, as is the number of crystallographically distinct bonds \( \mathbf{r}^i \). 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) [111] faults in bcc crystals, it is now seen that they produce symmetric variations in fault energies because the shear direction is a three-fold 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 bcc as long as the shear direction remained a three-fold axis. Finally in the bcc structure symmetric unrelaxed fault energies must also arise for shears in any direction on \{110\} planes and for shears on any plane in the <110> direction.
CHAPTER 5 The Structure of Twin Boundaries in BCC Crystals

5.1. Introduction

It is well known that mechanical twinning is an important deformation mode in body-centred cubic metals, particularly at low temperatures. The crystallography, which was described formally in Chapter 1, has also been established for some time. The twins form as bands on \{112\} planes and are associated with a homogeneous shear in the \langle111\rangle direction, the shear strain being $2^{-\frac{1}{2}}$. Until the recent computer simulation studies by Vitek (1970) and also those of Chapter 4 of the present work (both describing generalised \{112\} stacking faults) it was assumed that these twins satisfied the classical orientation relation of reflection in the interface. Also it was supposed that this occurred both at a macroscopic and at an atomic level where, it was presumed, the interface coincided with a plane of atoms. Thus a (112) bcc twin boundary was assumed to have the atomic configuration shown schematically in fig. (5.1.a). However the simulation studies have shown that the most stable \{112\} twin boundary in bcc crystals does not have the mirror image structure of fig. (5.1.a) but involves an additional displacement of about $\frac{1}{12} \langle-\bar{1}1\bar{1}\rangle$ at the interface. The resulting structure is shown schematically in fig. (5.1.b) where, unlike the microtwin depicted in fig. (4.3), a single interface is illustrated. It consists of parent and twin bcc crystals separated by an interface consisting of a layer of cells which, in the projection shown in the diagram, are represented by interlocking isosceles triangles. Thus, if the interface is to be associated with a plane, it must be considered to lie mid-way between planes of atoms.
Unfortunately experimental techniques capable of distinguishing between the two proposed twin boundary structures, by detecting at least qualitatively the different displacements at the interface, have only just become available (Pond and Smith 1974) and have not yet been applied to this problem. Thus as the predicted structure of the isosceles boundary is so unexpected it was decided to investigate its properties further using the computer simulation method and the results of these investigations are reported in this chapter. In particular it was felt desirable to study a single isolated twin interface rather than the pair of interfaces associated with a micro-twin. Also it was considered important to try to obtain comparative relaxed energies for the two types of interface and to do this using different interatomic potentials. In the earlier work a relaxed boundary of the reflection type was not found although Bevis and Vitek (1970) obtained a value for the energy of a partially relaxed boundary artificially restricted to be of this kind. Finally it was thought that the volume increase associated with the twin boundaries (see Chapter 4) required further study as this had been restricted in the previous investigations by effectively imposing rigid boundaries to the model crystal.

5.2. Present Model

As with the simulations described in the previous chapter the model bcc crystal used in the calculations consisted of a rectangular block with (110), (111) and (112) faces. A (112) twin boundary can readily be introduced into this model, without essentially altering its shape, as these planes in the parent crystal are parallel to their counterparts in the twin. However, small changes in shape must be allowed in order to investigate translations parallel to the
interface, strains perpendicular to the interface and even irregularities in the interface. In practice model crystals were used with up to 8 (110) planes, 33 (111) planes and 100 (112) planes of atoms, but usually much smaller crystals were found to be satisfactory. The twin boundary was always located, at least approximately, at the centre of the model in its unrelaxed state.

The twinned model crystals were allowed to relax to their minimum energy configurations using the lattice-handling techniques described in Chapter 3. During a given relaxation process the outer boundaries parallel to (112) were kept rigid, although between different relaxations their relative positions were changed by displacements both parallel and perpendicular to (112). Cyclic boundary conditions were imposed on the (110) and (111) faces. Note that the minimum energy configurations obtained correspond to atoms at rest so that the method simulates equilibrium structures at a temperature of 0 K.

Three interatomic potentials $\phi(r)$ were used in the calculations, the Johnson $J_0$ potential for iron (Johnson 1964), a molybdenum potential developed by Kenny and Heald (1974) and a potential for tungsten due to Stabell and Townsend (1974). Their characteristics have already been described in Chapter 3 and they have been plotted in fig. (3.1). It may be commented however that the three potentials used have rather different characteristics and therefore any structural features predicted by all three might be considered to be essentially correct.
5.3. Results

The basic results to be reported here were obtained using a model bcc crystal consisting of 24 (112) planes and containing a reflection twin as shown in fig. (5.1.a). The upper part of the crystal was initially translated by \( \alpha/2 \) \([11\bar{1}]\), \( 0 \leq \alpha \leq 1 \), relative to the lower part. Note that this displacement is in the opposite direction to the deformation twinning shear. The unrelaxed boundary energy \( \gamma_u \) was then determined as a function of \( \alpha \) using the iron potential, and is plotted as the upper curve in fig. (5.2.a). As expected it has a period of unity in \( \alpha \), corresponding to the inter-atomic spacing in the \([11\bar{1}]\) direction. It is also symmetric about its minimum at \( \alpha = \frac{1}{6} \) and its maximum at \( \alpha = \frac{2}{3} \). These points correspond respectively to the isosceles triangle boundary structure of fig. (5.1.b) and an unfavourable configuration in which the boundary consists in projection of a layer of rectangular cells. Thus the unrelaxed boundary energy clearly favours the isosceles structure (\( \alpha = \frac{1}{6} \)) rather than the reflection structure (\( \alpha = 0 \)).

The model crystals were now allowed to relax to their minimum energy configurations. During this process the outer (112) boundaries were kept fixed so that no additional macroscopic shear and no volume change were allowed. However free rearrangements of atoms within the computational cell were of course permitted. For all values of \( \alpha \) the relaxed boundary structures were found to be either the reflection twin or the isosceles twin, although in general the ideal configurations were slightly distorted due to the long-range elastic strain fields imposed by the rigid (112) outer boundaries. The relaxed boundary energy \( \gamma_r \), which includes this elastic contribution, is plotted as the lower curve in fig. (5.2.a). This curve varies very little with \( \alpha \).
indicating that the reflection and isosceles boundaries have very similar energies and that the elastic contribution to the energy is very small. The curve does in fact have a period of $\frac{1}{3}$ with undistorted reflection boundaries at $\alpha = 0, \frac{1}{3}, \frac{2}{3}$ and undistorted isosceles boundaries at $\alpha = \frac{1}{6}, \frac{1}{2}, \frac{5}{6}$. This arises because the relaxation procedure minimises the elastic strain by moving the twin boundary perpendicular to itself by $+1$ and $-1$ (112) interplanar spacings for $\alpha = \frac{1}{3}$ and $\frac{2}{3}$, respectively. The boundary energy $\gamma_r$ is plotted at an expanded scale for $0 \leq \alpha \leq \frac{1}{3}$ in fig. (5.2.b). This shows that the curve consists of parabolic segments and is symmetric about a local minimum at $\alpha = 0$, which is equivalent to $\alpha = \frac{1}{3}$, and the true minimum at $\alpha = \frac{1}{6}$. Thus for this particular model the isosceles configuration ($\alpha = \frac{1}{6}$) is more stable. However, this result could be misleading and it depends critically on the size of the model. In particular the parabolic increases in $\gamma_r$ on either side of the minima arise from the stored elastic shear strain in the crystal. The strain energy is proportional to the square of this strain and hence to $\alpha^2$ and $(\alpha - \frac{1}{6})^2$, respectively, for the two minima. It is also proportional to the inverse square of the number of (112) planes in the model. Thus for a sufficiently large number of planes the parabolae would effectively become a pair of horizontal lines. In this case the relaxation procedure would only locate the lower line and it appears from fig. (5.2.b) that this would correspond to the isosceles structure. However, this need not be the case as increasing the number of (112) planes also reduces the stored elastic energy associated with long-range compressive strains in the model. These arise from the volume increases which, as discussed in Chapter 4, are expected to occur at both types of interface. Because, as shown in fig. (5.2.a), the energies of the two relaxed boundaries are so
similar, slight differences in the stored elastic energy in the two cases could then result in the reflection twin being more stable.

In practice the elimination of the long-range strains by increasing the number of (112) planes in the model would use an excessive amount of computer time and, as indicated above, would result in the less stable boundary structure being lost. An alternative procedure was therefore used. This consisted of allowing volume increases by initially moving outwards by ±ν [112] the rigid (112) faces of the model, together with the nine outer (112) planes of the computational cell on either side of the interface. The results are illustrated in figs. (5.3.a) and (5.3.b) for the reflection (α = 0) and isosceles (α = \(\frac{1}{2}\)) twins. In these calculations a model containing 24 (112) planes was retained for the isosceles twin but 25 (112) planes were used for the reflection twin in order that the interface should be symmetrically located in the model. Curves A in fig. (5.3) give the relaxed normal displacements \(v_n\) of successive (112) planes away from the interface for the case \(ν = 0\), corresponding to no volume change. For both boundaries there is indeed an expansion, indicated by steep positive slopes of the displacement curves, near the interfaces. The associated long range compressive strains in the outer parts of the models are indicated by negative slopes. Curves B give the corresponding displacements for the cases of \(ν = 0.0164\) and \(ν = 0.0082\) respectively, which result in excessive volume increases, indicated by positive slopes remote from the boundaries, so that the model crystals are in tension. Finally curves C, corresponding to \(ν = 0.0090\) and \(ν = 0.0041\) respectively for the reflection and isosceles twins, have zero slopes remote from the interfaces and thus zero long-range strains. Hence these critical values of \(ν\) define the correct
relaxed boundary structures and energies for the two twins. They compare with the values of 0.0101 and 0.0076 respectively suggested by the hard sphere model.

As the equilibrium iron potential is being used in these particular calculations, the critical values of $v$ corresponding to zero long range strains can also be determined from the calculated energies of the boundaries. These pass through minima at $v = 0.0091$ and $v = 0.0041$ for the reflection and isosceles twins, respectively, as shown in fig. (5.4). These values confirm the true equilibrium structures predicted by the displacement curves of fig. (5.3). The most striking feature of fig. (5.4) however is that it demonstrates that the further relaxation of the boundaries that has been allowed results in the reflection twin having a slightly lower energy than the isosceles twin, thus reversing the situation depicted in fig. (5.2.b).

The actual energies obtained are $\gamma = 264.2 \text{ mJm}^{-2}$ for the reflection twin and $\gamma = 265.6 \text{ mJm}^{-2}$ for the isosceles twin. The significance of the fact that these values are so close is discussed in §5.4. Detailed numerical values for the locations of atoms near the two unstrained boundaries are presented in table (5.1). These are given as displacements relative to the perfect geometrical structures illustrated in fig. (5.1). Note that as expected the calculated displacements on either side of the interface are symmetric so the labels reflection and isosceles are still appropriate. The displacements $v_n$ normal to (112) duplicate the information provided by curves C of fig. (5.3) but are of course far more accurate. Apart from the $n = 0$ plane for the reflection twin the coefficients $u_n$ of the displacements $u_n$ parallel to the interfaces are all less than $10^{-2}$. There were no displacements perpendicular to the (110) mirror planes.
The above results were all obtained using the equilibrium potential for iron. The calculations were repeated using the molybdenum and tungsten potentials and similar results obtained. Thus for models consisting of 25 or 24 (112) planes both reflection and isosceles boundaries are stable. When no volume increase was allowed the energies of the relaxed boundaries in molybdenum were 1129 mJm⁻² and 800 mJm⁻² respectively so that again the isosceles structure appears to be more stable. The same result holds for tungsten where the corresponding energies were found to be 1189 mJm⁻² and 1026 mJm⁻². The difference between the reflection and isosceles boundary energies in these metals are now quite significant compared with those for iron. Since non-equilibrium potentials were used in the molybdenum and tungsten calculations the energies they give for the model crystal do not have a minimum at the true crystal structure. Thus the volume changes giving zero long range strain could not be obtained from the plots of γ against ν corresponding to fig. (5.4). However normal displacement plots similar to those of fig. (5.3) could still be derived and used to deduce the critical values of ν. In molybdenum these were + 0.0037 and −0.0012 for the reflection and isosceles twins respectively and in tungsten + 0.0073 and 0.00002. Most of these values are considerably less than the corresponding ones found for iron. However as indicated in table (5.1) where detailed numerical values of the locations of atoms near the boundaries are again given, the normal displacements for planes ± 1 are similar for the three metals. Also apart from plane 0 the displacements parallel to [111] in molybdenum and tungsten are all about twice as large as those for iron. The main difference between the three sets of results however is that the isosceles twin in molybdenum is associated with a small volume decrease rather than the expected increase which occurs in all other cases.
The energies of the unstrained boundaries in molybdenum were found to be 877 mJm$^{-2}$ and 882 mJm$^{-2}$ for the reflection and isosceles twins respectively. The corresponding values for tungsten were 861 mJm$^{-2}$ and 1025 mJm$^{-2}$. Thus in both metals the volume changes have resulted in significant corrections to the interfacial energies and now the reflection twin is apparently preferred although only slightly in the case of molybdenum. These comparatively large changes in boundary energies arise because the tungsten and molybdenum potentials do not hold the structure in equilibrium and thus, unlike the iron potential, do not give an energy minimum, insensitive to volume change, for the predicted structures. There is however an additional contribution to the energies of the unstrained interfaces in molybdenum and tungsten as the second part of the total potential, simulating the contribution of the electrons, is volume dependent. In the present model this potential gives rise to a pressure on the outer (112) planes which exactly balances the outwards normal pressure arising from the forces between atoms in the computational cell. For an unstrained bcc crystal this pressure $p_{(112)}$ is given by

$$p_{(112)} = (b_3) r_2^{-1} [r_1^{-1} \phi'(r_1) + r_2^{-1} \phi'(r_2)]$$  (5.1)

where $r_1$ and $r_2$ are first and second nearest neighbour distances. Allowing for work done by this pressure as the volume of each model crystal is changed to give the unstrained configurations the energies of the reflection and isosceles boundaries in molybdenum become 752 mJm$^{-2}$ and 923 mJm$^{-2}$ respectively while those in tungsten become 706 mJm$^{-2}$ and 1025 mJm$^{-2}$. Thus in both metals the reflection twin is finally seen to have an appreciably smaller energy which is still however about three or four times larger than the corresponding value for iron where no correction of the kind was necessary.
5.4. Discussion

Before discussing the relaxed (112) twin boundary structure for bcc metals predicted by this study, it is interesting to consider first the symmetric form of the energy $\gamma_u$ of the unrelaxed interfaces. This energy is plotted in fig. (5.2.a) as a function of the displacement $a[\mathbf{11\bar{1}}]$ and significantly has a minimum at the isosceles configuration shown in fig. (5.1.b). A similar symmetric curve was obtained in the previous chapter for unrelaxed generalised (112) stacking faults in bcc crystals, the minimum occurring at the perfect single crystal configuration. A detailed study of this result given in §4.3 showed that it arose because the distribution of inter-atomic distances across these unrelaxed faults is independent of the sense of the [11\bar{1}] fault vector. Furthermore it was demonstrated that the same result occurs for any crystal structure if, with certain restrictions on the value of $n$, the shear plane is perpendicular to an $n$-fold axis or if the shear direction is parallel to an $n$-fold axis. In the case of the bcc faults the shear direction is of course a 3-fold axis. The symmetry of the curve $\gamma_u$ in fig. (5.2.a) must also arise because the same set of distorted bonds is produced by equal and opposite shears of the isosceles twin boundary structure. That this is indeed the case is demonstrated by the two crystallographically equivalent bonds $b_1$ and $b_2$ shown bold in fig. (5.1.b). These bonds cross the interface and satisfy the equations

$$
(b_1 + b_2) \cdot (112) = (b_1 - b_2) \cdot [11\bar{1}] = 0 \quad (5.2)
$$

Thus the distorted lengths of $b_1$ and $b_2$ produced by a shear $a[11\bar{1}]$ equal the distorted lengths of $b_2$ and $b_1$ produced by the opposite shear $a[\bar{1}1\bar{1}]$. All bonds crossing the boundary in fig. (5.1.b) can be
paired in this way and the symmetry of the curve \( \gamma_u \) about this structure follows. The same result is not obtained for the reflection twin of fig. (5.1.a) as bonds joining planes 0 and 1 in the diagram, such as bond \( b \), cannot be paired. This situation arises because the plane on which the shear actually occurs lies between planes 0 and 1 of fig. (5.1.a) and thus does not coincide with the composition plane of the twin. Alternatively in fig. (5.1.b) the shear plane and the effective composition plane of the isosceles twin do coincide. This is also true for the interface structure corresponding to the symmetric maximum of the \( \gamma_u \) curve of fig. (5.2.a). This structure is similar to that of fig. (5.1.b) except that the band of isosceles triangles is replaced by one of rectangles. Indeed it is this structure which has the highest symmetry about the true shear plane, at least in projection. Thus the isosceles structure may be considered to lie at the minimum of \( \gamma_u \) because it is mid-way between adjacent symmetric maxima corresponding to the energetically unfavourable rectangular structure. This argument can clearly be extended to twins in other crystal structures but this will not be discussed here.

The basic computational method used in this study is the same as that used throughout this thesis. It is described fully in Chapter 3 and requires little elaboration here. However, it is worth emphasizing the fact that many aspects of the results obtained indicate that the simulation procedures are working reliably. For example as shown by table (5.1) identical results have been found for atomic displacements on either side of symmetric boundaries. Also the energies of the predicted structures as shown by figs. (5.2) and (5.4) all varied smoothly as a function of various displacements. Again some unexpected results, such as the period of \( \gamma_r \) in fig. (5.2.b), are, when considered
carefully, clearly correct. It is nevertheless important that the results can if necessary be checked and therefore they have been quoted numerically to more significant figures than can be justified physically. One interesting aspect of this particular simulation is that exact compliant boundary conditions have been applied on the (112) faces of the computational cell. In other simulations it has been necessary for example (Kenny and Heald 1974) to use average isotropic values for the pressure associated with the free electron gas but here, because the simulation is essentially one-dimensional, the correct anisotropic value of $p_{112}$ could be readily adopted. The success of the method used is demonstrated by curves C of fig. (5.3) which are accurately horizontal, demonstrating zero strain for $n > 8$ and have been shown to continue this way using models containing up to 100 (112) planes.

The results on the equilibrium structures and energies of (112) twin boundaries in iron, molybdenum and tungsten which have been obtained in this study are summarised in table (5.2). It should be remembered that these results correspond to a simulation at 0 K, but as twinning is primarily a low temperature phenomenon in these metals this would seem to be appropriate. The results for the isosceles (I) twin in iron are different from those given in earlier studies using the same potential and it is instructive to consider the reasons for this. The value of $\gamma = 282 \text{ mJm}^{-2}$ given by Vitek (1970) is high because no overall volume change was allowed ($v = 0$), the model was small and, as a slightly asymmetric boundary was found, the relaxation incomplete. Similarly the value of $\gamma = 270 \text{ mJm}^{-2}$ obtained in Chapter 4 of the present work is also a little high, probably because it was deduced from the energy of a microtwin in a small model again with $v = 0$. 
Even the $v = 0$ value of 267 mJm$^{-2}$ given in table (5.2) is dependent on the size of the model, although it is very close to the value of 266 mJm$^{-2}$ which arises when the correct volume increase, defined by $v = 0.0041$, is allowed. These changes are however all minor compared with the fact that an equilibrium reflection (R) twin was not obtained in the earlier work, whereas in the calculations described in this chapter it is stable, having slightly the lower energy of 264 mJm$^{-2}$ in the fully relaxed state corresponding to $v = 0.0090$. The failure to discover a reflection twin in the calculations of the preceding chapter is perhaps not surprising as even the occurrence of a metastable isosceles twin nucleus was fortuitous. It is however strange that Vitek (1970) who examined single twin interfaces, failed to observe this structure which seems to have been precluded by his computational procedures. The high value of 348 mJm$^{-2}$ for the energy of the reflection boundary quoted in the related work of Bevis and Vitek (1970) appears to have arisen because the structure was not fully relaxed. In any case it is now clear that the unstrained (112) reflection and isosceles twins in iron have very similar energies and thus, if the iron potential is reliable, both structures are likely to occur in practice.

The second and third potentials were used in the present study mainly to provide a check on the predictions for iron. The results are again summarised in table (5.2). The isosceles twin is highly favoured when no volume increase is allowed, although this is dependent on the size of the model. However on allowing a volume change, to eliminate the long-range strains in the crystal, the reflection twin becomes preferred. Indeed the changes in energy are very striking and perhaps disturbing, suggesting that defect simulations involving
volume changes may be unreliable when non-equilibrium potentials are used. These strains could have been relaxed by using a much larger model without allowing a volume change in creating the interface. Thus the fact that the simulated reflection twin has a lower energy does not depend on the volume changes which are suggested here. The additional energy changes, associated with the work done by the forces simulating the pressure of the free electron gas, do arise directly from the volume changes, but are smaller than the strain energy corrections, and simply confirm that the reflection interface is preferred, the ratio of the final energies of isosceles and reflection boundaries being 1.23 for molybdenum and 1.45 for tungsten. The magnitudes of these energies are 3 or 4 times as large as those for iron and this may be related to the relative frequencies of twin formation in these metals. In general however the results on molybdenum and tungsten do tend to confirm those for iron, both twin boundaries being possible in the model and having comparable energies. One surprising result of the molybdenum calculations is the volume decrease necessary to give an unstrained isosceles twin. Although unexpected this decrease is small and is supported by the tungsten calculation which gives a virtually zero volume increase in this particular case.

It thus appears that two distinct types of (112) twin boundary may arise in some bcc metals. This conclusion has important consequences in the study of the corresponding twinning dislocations. A formal description of twinning dislocations is given in Chapter 6 but can be considered here as essentially steps in the twin boundaries. Figs. (5.5.a) and (5.5.b) show schematic diagrams of edge twinning dislocations in the reflection and isosceles boundaries, respectively. In both cases the height of the step is one (112) interplanar spacing
and using isotropic elasticity theory the long-range strain field would be the same as that of a slip dislocation of Burgers vector \( \frac{1}{6} [\overline{1}11] \). Now twinning dislocations like slip dislocations may in principle dissociate into partials although this possibility is not normally considered as the structure of the resulting stacking fault superimposed on that of the twin boundary would be unacceptable. However, in some structures such as that of \( \beta \)-tin it has been suggested (Ishii and Kiho 1963) that dissociation of twinning dislocations does take place and results in two types of interface which are effectively defined by two classical orientation relations, reflection in the interface and rotation of \( \pi \) about the shear direction. These orientations relations are distinct in \( \beta \)-tin, as the structure consists of atoms at the points of two interpenetrating lattices, but are identical for single lattice structures like the bcc metals. However, dissociation of the \( \frac{1}{6} [\overline{1}11] \) twinning dislocation in the (112) bcc reflection twin boundary into two equal \( \frac{1}{12} [\overline{1}11] \) partials produces a ribbon of isosceles boundary. Similarly symmetric dissociation of a twinning dislocation in the isosceles boundary produces a ribbon of reflection type boundary. These dissociations are illustrated schematically in fig. (5.5.c) which shows a (112) twin boundary containing three partial \( \frac{1}{12} [\overline{1}11] \) twinning dislocations. The two partials to the left represent a dissociated dislocation in a reflection type boundary and separate a ribbon of isosceles structure. Similarly the two partials at the right represent a dissociated dislocation in an isosceles type boundary and define a ribbon of reflection structure. Note that the interface is displaced by one-half of a (112) interplanar spacing at each partial. This means that formally the perfect twinning dislocation may be considered to be a stack of two partials which, using elasticity theory, is a
localised metastable configuration. The partial separation is, however, so small that elastic calculations are not valid and in any case the dissociation energy must be very small.

If the energies of the two interface structures were identical the equilibrium spacing of the partials would be uniform. This situation is suggested for example by the present results for iron so that the Burgers vector for the twinning dislocation may effectively be considered to be $\frac{1}{12} [\overline{111}]$. When the energies of the two boundaries are different, naturally the dissociations will result in narrower bands of the structure with the higher energy. Thus if the molybdenum and tungsten results presented here are realistic the reflection boundary will predominate. However, due to effects of applied or internal stresses substantial areas of the isosceles boundary may still occur.

It must be emphasised that the foregoing discussion on twinning dislocation dissociations is, at this stage, purely speculative. Nevertheless many of the remarks made here are borne out in the following chapter which attempts to quantify the properties of the twinning dislocation using the computer simulation technique. As suggested here it is found that these properties, like the width of the partial twinning dislocation, are quite naturally potential dependent. The possibility that twinning dislocations in bcc metals may be dissociated means that many theories of the deformation and fracture of these materials, in which twinning plays an important role, need to be reconsidered. The present simulation studies will clearly provide a useful basis for such new theories.
### TABLE (5.1) Locations of Atoms near Reflection (R) and Isosceles (I) type (112) Twin Boundaries in Iron, Molybdenum and Tungsten

<table>
<thead>
<tr>
<th></th>
<th>IRON</th>
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<th>MOLYBDENUM</th>
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<th></th>
<th>TUNGSTEN</th>
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<td>n</td>
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<td>+431</td>
<td>±168</td>
<td>+812</td>
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<td>+795</td>
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<td>-11</td>
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<td>+144</td>
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<td>+5</td>
<td>±426</td>
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<td>±402</td>
<td>+7</td>
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<td>+1</td>
<td>±415</td>
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<td>±333</td>
<td>+14</td>
<td>±123</td>
<td>-2</td>
<td></td>
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</tbody>
</table>

The atomic locations are given for successive (112) planes (n) by the coefficients $v_n$ and $u_n \times 10^5$ of the vectors $v_n[112]$ and $u_n[111]$ defining displacements relative to the geometric configurations of fig. (5.1).
TABLE (5.2) Summary of Results on the Energies of (112) Twin Boundaries in Iron, Molybdenum and Tungsten.

<table>
<thead>
<tr>
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<th>v</th>
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<tbody>
<tr>
<td>Fe</td>
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</tr>
<tr>
<td>R</td>
<td>0</td>
<td>270</td>
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<tr>
<td></td>
<td>90</td>
<td>264†</td>
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<tr>
<td>I</td>
<td>0</td>
<td>267</td>
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<tr>
<td></td>
<td>41</td>
<td>266†</td>
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<tr>
<td>Mo</td>
<td></td>
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<tr>
<td>R</td>
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<td>1129</td>
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<tr>
<td></td>
<td>37</td>
<td>877*</td>
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<tr>
<td></td>
<td>37</td>
<td>752†</td>
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<tr>
<td></td>
<td>-12</td>
<td>923†</td>
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<td>W</td>
<td></td>
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<tr>
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<td>1189</td>
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<tr>
<td></td>
<td>73</td>
<td>861*</td>
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<td>706†</td>
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<td>I</td>
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<td>1026</td>
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<tr>
<td></td>
<td>~0</td>
<td>1025*</td>
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<tr>
<td></td>
<td>~0</td>
<td>1025†</td>
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</tbody>
</table>

The energies \( \gamma \) are given in mJm\(^{-2}\) for the reflection (R) and isosceles (I) twins for volume increases defined by the coefficient \( v (\times 10^4) \) of the displacement vector \( \pm v[112] \). Energies are given for zero volume change and zero long range strain (†). For Mo and W energies uncorrected for the work done by the forces simulating the pressure of the free electron gas are also given (*).
CHAPTER 6 The Core Structure of BCC Twinning Dislocations

6.1. Introduction

The previous two chapters of this thesis were concerned primarily with the determination of the detailed structure of the coherent twin boundary in various bcc metals. Since the occurrence of apparently perfect twin lamellae has been experimentally observed in many metals, for instance iron where the straight lamellae are called Neumann bands, such determination is clearly worthwhile. In general, however, the lamellae are observed to be distorted, i.e. the twin boundary deviates from its composition plane. This distortion normally presents itself as non-uniform tapering of the lamellae which obviously could have occurred only via a pile-up of steps or dislocations in the boundary. It has been shown by Sleeswyk (1962) that around the blunt tip of the taper there exists a high stress concentration which if not relieved would be large enough to nucleate a microcrack when the twin encountered an obstacle e.g. a grain boundary. Clearly it is of some importance now to determine the detailed structure of the incoherent twin boundary. In particular it would be useful to obtain information about the core structure of the steps, or twinning dislocations, their equilibrium separation and self energy. Because the effective width of the twinning dislocation determines the lattice resistance to nucleation and growth of the twin, some light may also be thrown upon the important problem of how the twinning dislocation was created. The source of twinning dislocations, various mechanisms for twin nucleation and growth and their interpretation in view of the present work, is discussed in further detail in §6.4. Additionally other approaches to the problem of fully describing a twinning
dislocation are reviewed. In particular elastic analyses given by Yoo and Loh (1970) and Mendleson (1970) are compared with the atomistic approach. The remainder of this Introduction is devoted to a formal characterization of the twinning dislocation.

Consider initially a general but rational planar interface of unit normal $\mathbf{y}$. An infinite or a closed step of height $\mathbf{yH}$ may be introduced into the interface by a series of virtual operations as shown in fig. (6.1). The structure is analogous to the formation of a lattice dislocation so that such a step, which is sharp, will have a similar long range stress field falling off as the inverse of distance. The Burgers vector of the stepped interface is simply

$$b_T = g\mathbf{e}$$  \hspace{1cm} (6.1)

where $g$ is a scalar and $\mathbf{e}$ a unit vector describing the invariant plane strain between the two lattices. The step is called a twinning dislocation when $\mathbf{y}$ represents a coherent twin boundary. Obviously in this case $\mathbf{e}$ will lie in the plane of the interface and in general the twinning dislocation will be of mixed type, with edge and screw components. Movement of this dislocation will clearly result in a shear of the lattice and a corresponding change of shape. It also provides a possible mechanism for growth of the twin. These possibilities are considered further in the discussion but it emphasises here that $b_T$ must be strictly defined, unambiguous and fixed by the twinning crystallography.

An elastic analysis of the stepped boundary may be made but there exists an inherent discontinuity at the step. The present discrete calculations can overcome this difficulty and obtain, at least in principle, the local stresses and strains as well as the atomic
configuration around the dislocation. There is also another difficulty in calculating the elastic field of a step in that the effective elastic properties of the crystal may be different in the vicinity of the twin and in particular the shear modulus may be different. For example a low shear modulus could result in a wide core structure and hence raise doubts about the stability of the step. However this problem can be avoided in the case of a tapered twin lamella containing closely separated steps. Each step will then have a narrow core structure whose elastic field (long range) can be calculated.

Returning to the crystallography of the twinning dislocation it is well known that in some twinning modes shuffles are required in order that the correct crystal structure and orientation relationship be obtained. However even after these shuffles have been applied it is possible that when a twinning dislocation is present non-equivalent boundary structures may exist on either side of the step. When this occurs the twinning dislocation has been called elementary (or unit). In such cases the step height may be chosen so that the structure of the boundary is equivalent on both sides of the step and this has been described by Thompson and Millard (1952) as a zonal twinning dislocation. Although the terms elementary and zonal have been used many times in the literature (see e.g. Westlake 1961 or Mendelson 1969) their general application to all twinning dislocations is clearly limited. Indeed it is possible to fully describe any incoherent twin boundary in terms of the perfect twinning dislocation whose Burgers vector has been defined in eq. (6.1.) and the partial twinning dislocation that has already been postulated in Chapter 5. This nomenclature is preferred by the author and will be the only one used in the present
work. The dissociation then of a perfect twinning dislocation of
Burgers vector $b_T$ into $s$ partial twinning dislocations or partials
of Burgers vector $b_{TP}$ may be represented thus

$$b_T \rightarrow \sum_{i=1}^{s} b_{TP}^i \quad |b_T| > |b_{TP}^i| \forall i \quad (6.2)$$

The mutual separation of the partials will, of course, depend
on the energy of the intermediate "twinned stacking fault". Experimental results have suggested that the twinning dislocation line is
sharp. However Vitek using the computer simulation technique in a
preliminary calculation has shown that the width of the dislocations
of the bcc twin is large, thus assisting growth (Christian 1974).
Similar calculations presented in this chapter suggest however that this
result will depend, as indeed it must, upon the chosen interatomic
interaction.

To conclude this introduction the Frank circuits around the
twinning dislocations are presented. Consider first the perfect
twinning dislocation of Burgers vector $\frac{1}{6} [11\bar{1}]$ that is illustrated
schematically in real crystal in fig. (6.2.a). When the dislocation
occurs in a reflection boundary the interface is displaced downwards,
from right to left in the direction of the twinning shear, by one (112)
interplanar spacing. This configuration is labelled RR since the
structure of the interface on both sides of the step is the same.
Similarly when the dislocation occurs in an isosceles boundary the
interface is again displaced downwards by one (112) interplanar spacing
and is labelled II. It is seen from the diagrams that although the
Burgers vector of RR and II is the same their core structure is
different. The equality of the Burgers vector may be demonstrated by
drawing Frank circuits around RR and II in real crystal and drawing the equivalent circuits in the reference crystal. The reference crystal contains a coherent twin boundary that may be of either isosceles I or reflection R type. Clearly in the RH/FS sense the closure failure FS of the circuits in both reference crystal is the same and equal to $\frac{1}{6} [\overline{1}11]$. The situation in which the Burgers vector of the perfect twinning dislocation lies in the opposite direction is now considered. Fig. (6.2.b) shows schematically in real crystal a twinning dislocation of Burgers vector $\frac{1}{6} [\overline{1}11]$. This time when the dislocation occurs in either a reflection or an isosceles boundary the interface is displaced upwards, from right to left in the direction of the twinning shear, by one (112) interplanar spacing. The labelling clearly remains the same and, as before, the core structures are seen to be different. When the Frank circuits are drawn the closure failure FS in the reference crystals are again both found to be equal to the Burgers vector which, of course, are lying in the opposite direction to those of fig. (6.2.a). It must be deduced from this that the RR structure of fig. (6.2.a) is identical to that of fig. (6.2.b) and similarly for the II structure. In fact this is obvious since the structures in fig. (6.2.b) are just the mirror image of those in fig. (6.2.a).

The construction of Frank circuits around partial twinning dislocations may be performed in exactly the same way as for perfect twinning dislocations. Fig. (6.2.c) shows schematically in real crystal a partial twinning dislocation of Burgers vector $\frac{1}{12} [\overline{1}11]$. When the partial occurs in a reflection boundary the interface is displaced downwards, in the direction of the twinning shear, by one half of a (112) interplanar spacing. The structure of the interfaces on either side of the step is now different and, from right to left, changes.
from isosceles to reflection type. This configuration is thus labelled IR. In a similar manner the partial twinning dislocation in an isosceles boundary will displace the interface downwards by one half of a (112) interplanar spacing which, in the direction of the twinning shear, changes the interface structure from reflection to isosceles type. This configuration is correspondingly labelled RI. The core structures of IR and RI are not equivalent but, as can be seen from the Frank circuits, their Burgers vectors, equal to the closure failure FS, are identical and equal to \( \frac{1}{12} [11\bar{1}] \). When the direction of the Burgers vector of the partial is reversed the structures labelled IR and RI in fig. (6.2.d) are found. As with the perfect twinning dislocations these structures are just the mirror image of those in fig. (6.2.c). It can be concluded that only two structurally distinct perfect twinning dislocations can occur (RR and II) which themselves are composed of two distinct partials (IR and RI).

6.2. Present Models

The model body centred cubic crystal was set up using the lattice handling techniques described previously in Chapter 3 and essentially had the same orientation as in the calculations on faults and twins described in Chapters 4 and 5. The computational cell consisted then of a rectangular block of atoms with (110), (111) and (112) faces. However, due to the long range strain field of the defect to be studied the actual dimensions of the block were changed. Also it was felt desirable to have an especially large \(<111>\) dimension due to the wide dissociation separation tentatively predicted by Vitek. In practice then the model was used with up to 200 (11\bar{1}) planes, 25 (112) planes and a minimum of 2 (1\bar{1}0) planes. The same relaxation procedure was
used as in the calculations described earlier however the boundary conditions had to be changed. Since a step was to be inserted in the twin boundary it was no longer possible to keep cyclic boundary conditions on the (111) face. These were replaced by rigid boundary conditions and, as before, cyclic boundary conditions were imposed on the (110) face and the outer boundaries parallel to (112) were kept rigid. Three potentials, which were identical to those described in Chapter 3, were used in the calculations so that it could be determined how sensitive the results were to the interatomic interaction.

Some consideration had to be given to the problem of actually inserting the defect, a twinning dislocation, into the model. Preliminary calculations in which a reflection twin boundary was introduced into the centre of the model by shuffling (112) planes and then dislocated by rigid body translations of the lattice were unsuccessful. It was then considered more appropriate to introduce the twin boundary (of either reflection or isosceles type) by the shuffling process and then superimpose an edge dislocation whose displacements were calculated from anisotropic elasticity theory. The order in which the twin boundary or edge dislocation were inserted into the model in fact does not matter. Clearly the Burgers vector of the edge dislocation had to be in the <111> direction and the line of the dislocation along <110>. The actual magnitude of the Burgers vector could be experimented with so as to produce the required twinning dislocation and indeed so could the actual number of edge dislocations introduced. The origin of the edge dislocation was chosen arbitrarily to be as near the centre of the (110) face of the model as possible. The model was chosen large enough so that any small deviation from this chosen origin had negligible effect upon the relaxation. If
more than one edge dislocation was introduced then they were placed symmetrically within the model. Several test calculations were performed to ensure that parameters in the model like the origin of the dislocation(s) and size of the computational cell did not prejudice the relaxation. The types of boundary condition chosen here were unavoidable but it can be seen that the introduction of an anisotropic displacement field has effectively improved the rigid boundary condition by making it elastic. It should be noted that the atoms in the elastic region are still fixed and that the term elastic should not be confused with compliant. Test calculations were also performed to check whether imposing an anisotropic elastic displacement field on a crystallite containing a reflection twin in which half the model is clearly in the wrong orientation substantially affected the results. This was done by reversing the sign of the Burgers vector of the dislocation. It was found that in such calculations the energy of the crystallite did not differ by more than 1.5% and that because of the large size of the model used any mis-orientation of the boundaries had negligible effect on the relaxed core structure of the twinning dislocations.

The differential equation defining the displacement field \( u_k \) of a straight dislocation in an anisotropic medium is well known: see for example Hirth and Lothe (1968). It is given by

\[
\begin{align*}
\frac{\partial^2 u_k}{\partial x_i \partial x_\alpha} = 0 & \quad i = 1, 2, 3 \\
\alpha, \beta = 1, 2
\end{align*}
\]

(6.3.)

and has solutions of the type

\[
u_k = A_k f (x_1 + px_2)
\]

(6.4)
where $c_{\alpha k}, A_k, p$ are constants.

The exact solution will involve solving a sextic in $p$ and will not, in general, be possible analytically. The present work makes use of routines developed at A.E.R.E., Harwell which solve the sextic numerically in a manner similar to that of Teutonico (1961). The values of the elastic constants $c_{\alpha k}$ used in the calculations are the same as those from which the potentials for iron, molybdenum and tungsten were derived, (see Johnson 1964, Kenny and Haald 1974, Stabell and Townsend 1974).

6.3. Results and Interpretation

As pointed out by Basinski et al. (1971) there is an inherent difficulty in presenting the core structure of dislocations obtained from atomistic calculations in a way which is not only unique and represents something physically real but also may be related to continuum theory. It appears that there are currently three methods of interpretation, each however having its disadvantages. Several authors, for example Bullough and Perrin (1968a), have presented their results in the form of a displacement field which clearly has physical significance. However the displacement field is many valued and nonlocal at the dislocation core. The differential displacement method first presented by Vittek et al. (1970) and subsequently used by Vittek in much of his later work relies on mapping the displacement of neighbouring atoms relative to the perfect lattice. The result, which is essentially a pseudo strain field, is good at showing up prominent features of the core structure such as symmetries or asymmetries but in some respects needs careful interpretation since, for instance, relative displacements give no unique distinction between tension and compression.
Basinski et al. (1971) have plotted the stress tensor at each atom which is possible if a small homogeneous deformation is applied to the dislocated crystal. However the resulting expression for the stress tensor can only be applied with ease to screw dislocations where the atomic volume at each atomic site varies by only a few percent from the perfect lattice. As expressed by Vitek and Yamaguchi (1973) application of this method to nonscrew dislocations would be complicated which is unfortunate in view of the fact that stress has real physical meaning and that many authors, for example Yoo and Loh (1970) in the case of edge twinning dislocations, have been able to plot the elastic stress fields.

The method adopted in the present work is an adaptation of Vitek's differential displacement mapping. The only basic difference between the two approaches is that in the present work the reference lattice from which relative displacements are calculated is taken to be the perfect reflection twin instead of the perfect lattice. Additionally, in order to display a quantity which is small far from the core but has large magnitude at the core centre, the difference between adjacent relative displacements was also taken. A second technique, also developed by Vitek in his study of nonscrew dislocations, has been applied to the present study. It involves calculating the density of the Burgers vector along a plane in which the largest displacements are mostly confined. Strictly speaking this method can only be applied to dislocation core structures that are planar. As will become evident from the detailed results given later in this chapter, appreciable displacements around a twinning dislocation can extend over four (112) planes especially near the centre of the core; however a plot of the continuous distribution of the Burgers vector (equal to the derivative
of the disregistry of the lattice relative to perfect reflection twin) along carefully selected planes serves the extremely useful purpose of revealing the exact location of the centre of the core.

Both these techniques may be illustrated in a calculation performed for α-iron in which a partial twinning dislocation is simulated. As explained in §6.1 only two structurally distinct partials can occur and have been labelled IR and RI in fig. (6.2). In these calculations the actual partials simulated had Burgers vector $\frac{1}{12} [11\bar{1}]$ and are shown in fig. (6.2.c). Figures (6.3.a) and (6.3.b) give the relaxed configurations for these two partial twinning dislocations. They were obtained by superimposing an edge dislocation of Burgers vector $\frac{1}{12} [11\bar{1}]$ onto a reflection and isosceles type boundary respectively. The relaxed energies of the model crystals in both these simulations were found to be within 0.05% of each other. It is obvious from both diagrams that the transition from reflection to isosceles type boundary occurs over many $[11\bar{1}]$ atomic sites or that the width of the partials is large. This becomes more apparent if the displacement, or disregistry, of the lattice relative to perfect reflection twin orientation is plotted along $[11\bar{1}]$. This may be done both parallel to the Burgers vector and perpendicular to (112) for adjacent (112) planes throughout the model crystal. In practice however it was found that for example in figs. (6.3.a) and (6.3.b) the largest displacements occurred between planes (1) and (0) and also (0) and (-1). Moreover displacements parallel to the Burgers vector were in general found to be at least four times as great as those perpendicular to (112). It was therefore considered sufficient to plot only the disregistry $D_x$ parallel to $[11\bar{1}]$, along $[11\bar{1}]$, between planes (1)-(0) and (0)-(1). This is shown in fig. (6.4.) for the partial twinning dislocation given
in fig. (6.3.a). Similar curves were found for the partial illustrated in fig. (6.3.b). The disregistry may be written algebraically thus

\[ D_\mathbf{x} = (x^n_q - x^n_{q-1}) - (x^p_q - x^p_{q-1}) \quad (6.5.) \]

where the \( x^p \)'s are the positions of the atoms in perfect reflection twin orientation.

Clearly fig. (6.4) has several interesting features. The fact that both curves converge to the left of the diagram means that atoms are mirror imaged in this region but because they do not converge to zero disregistry the mirror image or reflection twin is slightly distorted. This can also be seen from the results given in table (5.1) for the coherent reflection boundary so that this non-convergence to zero is not surprising. To the right of fig. (6.4) the curves are separated by approximately \( \frac{1}{12} [111] \). It is obvious that this represents the region of isosceles type twin although again the configuration is not perfect.

In order to locate the centre of the dislocation core a plot of the continuous distribution of the Burgers vector is made. As stated previously this is equal to the derivative of the disregistry of the lattice relative to perfect reflection twin along a specific direction. The direction chosen here is parallel to the Burgers vector so that by plotting the gradients \( \sigma_x \) of the curves shown in fig. (6.4) the desired quantity is obtained. Clearly

\[ \int_{-\infty}^{+\infty} \sigma_x(x) \, dx = b_{TP} \quad (6.6) \]
Figure (6.5) shows how $\sigma_x$ varies with $x$ for the two sets of (112) planes considered. It is seen that the extrema, corresponding to the centre of the core, coincide at least approximately a few atomic sites to the left of the centre of the model (in the (110) projection). This demonstrates that the size of the model crystal has not been such as to constrain the dislocation from moving. It also shows that there is a tendency for more isosceles type boundary to exist in this situation than reflection. This is reasonable when it is realised that under no volume expansion the boundary energy of the isosceles type twin in $\alpha$-iron is lower than that of the reflection twin (see table (5.2)).

Yamaguchi and Vitek (1975) were able to obtain plots analogous to fig. (6.5) for the case of non-screw $\frac{1}{2} <111>$ dislocations on {112} planes in bcc metals. However, because they found from their displacement maps that the non-screw dislocation cores were always virtually confined to one plane they could interpret their results directly in terms of a Peierls-Nabarro model. Such interpretation in the present work would be inappropriate since the twinning dislocations cores were always found to be spread over two to four (112) planes. This spread of the core is illustrated for the $\frac{1}{12} [11\bar{1}]$ partial in $\alpha$-iron in figs. (6.6.a) and (6.6.b). The mapping was obtained by taking the relative value of adjacent disregistries of the lattice both parallel to the Burgers vector and perpendicular to (112). Algebraically, the $x$ and $y$ components of the vectors may be expressed as

$$\Delta x = \left[ \left( x_{q_n}^{n+1} - x_{q-1}^{n+1} \right) - \left( x_{q_n}^p - x_{q-1}^p \right) \right] - \left[ \left( x_{q_n}^n - x_{q-1}^n \right) - \left( x_{q_n}^p - x_{q-1}^p \right) \right]$$

$$= \left[ x_{q_n}^{n+1} - x_{q_n}^n \right] - \left[ x_{q-1}^{n+1} - x_{q-1}^n \right]$$

(6.7)
The vectors (*50) are drawn at the centre of the parallelograms formed by atoms in the (110) projection and their direction is determined by a sign convention which is indicated in the figures. It can be concluded then from the displacement maps and the plots of the distribution of the Burgers vector that although the core of the \( \frac{1}{12} [11\bar{1}] \) partial twinning dislocation in \( \alpha \)-iron is well defined, the transition between reflection and isosceles type boundaries is diffuse, occurring over about thirty (111) planes, and therefore implying that the repulsive force is large or that the dissociation energy is small. These implications were confirmed when the simulation of a perfect twinning dislocation of either type RR or II was attempted. It was found that the perfect twinning dislocation of, for example, Burgers vector \( \frac{1}{6} [11\bar{1}] \) always dissociated into two partials each of Burgers vector \( \frac{1}{12} [11\bar{1}] \). In iron then the RR and II configurations of fig. (6.2) may be considered as unstable.

All the computations described above were repeated using the interatomic potentials for molybdenum and tungsten. However it was found that the partial twinning dislocation of Burgers vector \( \frac{1}{12} [11\bar{1}] \) simply ran out to the edge of the model crystal leaving behind a coherent isosceles twin boundary. It was concluded from this that, using these two potentials, the boundary was energetically highly in favour of the isosceles configuration when no volume expansion was allowed. A glance at table (5.2) confirms that this is indeed the case. It must also be concluded that the transition from isosceles to reflection type boundary for these two metals is quite sharp or

\[
\Delta y = \left( y_{q+1} - y_q \right) - \left( y_{q-1} - y_{q-1} \right)
\]
that the separation of \( \frac{1}{12} [111] \) twinning partials is small. To verify this the calculation was performed, first for molybdenum, by superimposing two edge dislocations of Burgers vector \( \frac{1}{12} [111] \) onto an isosceles type boundary. The dislocations were placed symmetrically within the model crystal but to ensure that their origin did not prejudice the relaxation an equivalent calculation was also performed by superimposing one edge dislocation of Burgers vector \( \frac{1}{6} [111] \) onto the isosceles boundary. The resulting relaxed structure which was identical in both calculations is shown in fig. (6.7). It is seen that only one pair of atoms (in this projection) can be said to be in true reflection orientation so that the width of the partials is indeed extremely small. This calculation corresponds to simulating the configuration labelled II in fig. (6.2.a). However when the alternative perfect twinning dislocation RR was simulated a negative result was once more obtained in so much as the dislocation ran out to the edge of model leaving behind a coherent isosceles boundary.

The differential displacement map for the II twinning dislocation in molybdenum is shown in fig. (6.8) (displacements \( \times 10 \)). It is seen that the core is highly localised and well defined and because of this it was thought unnecessary to plot the disregistry of the lattice or the density of the Burgers vector.

Unfortunately when the computation was repeated for tungsten even the twinning dislocation of Burgers vector \( \frac{1}{6} [111] \) ran out to the edge of the model. However it was possible to simulate a stable core structure very similar to that obtained for molybdenum by superimposing an edge dislocation of Burgers vector \( \frac{1}{2} [111] \) on a perfect isosceles boundary. The dislocation dissociated during relaxation leaving a \( \frac{1}{6} [111] \) twinning dislocation of type II near the centre of
the model. However the outer regions of the model crystal then became highly distorted so that a twinning dislocation obtained in this way could be said to be highly constrained and not represent a true situation. This calculation was also performed for $\alpha$-iron and the surprising configuration of fig. (6.9.a) was found near the centre of the model upon relaxation. Also on both sides of this configuration were two twinning partials of IR and RI type and each, of course, have Burgers vector $\frac{1}{12} [\overline{1}1\overline{1}]$. Frank circuits around the configuration of fig. (6.9.a) reveal that the closure failure FS shown in the reference isosceles crystal of fig. (6.9.b) is equal to $\frac{1}{6} [\overline{1}1\overline{1}]$. The original slip dislocation of Burgers vector $\frac{1}{2} [111]$ has thus interacted with the isosceles twin and dissociated into five twinning dislocations, one of Burgers vector $\frac{1}{6} [111]$ and four of Burgers vector $\frac{1}{12} [111]$. However the $\frac{1}{6} [111]$ twinning dislocation cannot be labelled II for two reasons: firstly the dislocation displaces the interface by two (112) inter-planar spacings and secondly this displacement is upwards (and not downwards as in fig. (6.2.a)) in the direction of the twinning shear. This unusual conjugate configuration, which may be termed a zonal twinning dislocation, has thus been labelled II* and the dissociation reaction is shown schematically in fig. (6.9.c). In this figure the $T$ symbol indicates that the II* dislocation originated effectively from the superposition of the edge dislocation and a twinning dislocation of Burgers vector $\frac{1}{3} [\overline{1}1\overline{1}]$. A similar dissociation reaction occurred when the edge dislocation was superimposed upon a reflection boundary although this time the dissociation was not so symmetric as can be seen from fig. (6.9.d). Obviously an RR* type configuration must also be structurally possible but none of preliminary calculations of the present kind have revealed it. Additionally twinning dislocations of Burgers vector $\frac{1}{6} [111]$ which displace the interface by more than two (112) interplanar spacings could exist but further calculations are
needed to test this proposal. Indeed it is suggested that a complete investigation of this unusual type of twinning dislocation should be undertaken especially to determine the stability of the structures under applied stress and whether the dissociation reactions are realistic. Moreover it would be useful to see whether such dislocations have been observed experimentally and if so under what conditions. Many future studies are suggested by the results of this chapter but it is evident that at least one dominant feature in these studies may be predicted immediately: the dependence of the structures of the twinning dislocations on the chosen interatomic potential. If any reliance can be placed in the simulation technique then this feature clearly demonstrates the dangers of making plausible assumptions about the widths or self-energies of such dislocations without reference to physical models and the use of discrete atomic calculations.

Finally it is considered appropriate here to formally present some of the hard copy output on twinning dislocation structure obtained on the visual display unit using the Atlas SCFOR routines. They are illustrated in figs. (6.10) and (6.11). This particular facility has proved invaluable for rapidly analysing relaxed defect structures obtained with DEVIL. The manual plotting of such structures can be extremely tedious.

6.4. Discussion

In this discussion it is hoped to relate some of the foregoing computer simulation results on twinning dislocations to some of the many nucleation and growth theories that have evolved over the past twenty years. These theories fall into two categories - those in which the twin originates from a lattice defect, e.g. a dislocation
(heterogeneous nucleation) and those in which the twin is created from a perfect lattice, (homogeneous nucleation). In the case of cubic metals, however, the latter mechanism may be dismissed immediately since the relatively large Burgers vectors of the twinning dislocations would require stresses of the order of the theoretical shear strength of the lattice. As a preamble to this discussion it would seem appropriate to describe the origin of twinning dislocations in general, initially from a purely crystallographic point of view and then in terms of more sophisticated elasticity theories.

With the absence of any obvious physical source of twinning dislocations it is natural to look for and take advantage of any crystallographic symmetries that may be present. Lattice dislocations have always been considered a possible source of twinning dislocations so that, for instance, the dissociation of a glissile slip dislocation into a twinning dislocation on the same plane leaving behind a residual dislocation is clearly feasible. If, however, by a crystallographic coincidence the slip and twinning planes are the same, as the (112) planes are in the bcc structure, then the lattice dislocation line need not be straight since it is not required to lie along the line of intersection of two planes. Similarly in the bcc structure if a screw dislocation lies along the line of intersection of three crystallographically equivalent twinning planes then it may dissociate into three twinning dislocations on these planes each of equal Burgers vectors, so that no residual dislocation remains. Clearly it would be tempting to say that these crystallographically convenient situations controlled the formation of a deformation twin however this may not necessarily be the case. Computer simulations and experiments have been inconclusive to date in this respect.
Mendelson (1970) has applied elasticity theory to the dissociation of a dislocation into \( s \) glissile partial twinning dislocations each separated by a width \( w \) from the sessile residual dislocation in order to determine when a dissociation will be energetically favourable and when it will be spontaneous. He gave the maximum repulsive force \( \gamma_{mi} \) on the \( i \)th partial as

\[
\gamma_{mi} = \left( K_i / 2 \pi \right) b_R \cdot b_i + \frac{1}{2} \sum_{j=1}^{s} b_i \cdot b_j \tag{6.9}
\]

where \( K_i \) is the elastic energy factor for the \( i \)th dislocation on its slip plane, \( b_j (j = 1, 2, \ldots, s) \) are the Burgers vectors of the twinning partials and \( b_R \) is that of the residual dislocation. When all \( \gamma_{mi} > 0 \) a dissociation is considered favourable. If \( \gamma_i \) denotes the twinning fault energy of the \( i \)th partial then a dissociation is considered spontaneous if \( \gamma_{mi} > \gamma_i \). The total dislocation energy \( E \) is obtained by summing the self energies of partials \( E_i \), their interaction energies \( W_{ij} \), their interaction with the residual dislocation \( W_{Ri} \) and the self energy of residual dislocation \( E_R \):

\[
E = E_R + \sum_{i=1}^{s} E_i + W_{Ri} + \gamma_i W_{Ri} + \frac{1}{2} \sum_{i,j=1}^{s} W_{ij} \tag{6.10}
\]

The equilibrium separation \( r_{Ri} (\equiv w) \) is found by minimising \( E \). Since experimental values for \( \gamma_i \) have not been determined it is difficult to make constructive use of equations (6.9) and (6.10). This is especially the case when it is required to test whether a particular dissociation mechanism is stable under the application of stress. However Mendelson (1970) was able to conclude by using theoretical estimates of \( \gamma_i \) given by Wasilewski (1967) that twinning in many metals could be rationalised in terms of non-planar dissociation of dislocations.
Heterogeneous nucleation of a deformation twin could in theory take place in any crystal structure by two general mechanisms: the formation of identical partial dislocations on each twinning plane or the motion of one twinning dislocation from twinning plane to twinning plane through the crystal. Although it has been postulated that the former mechanism could occur by reflection of twinning dislocations from surfaces or grain boundaries it is generally believed that the latter mechanism is more probable. Within this particular type of mechanism there exist various different models. For body-centred cubic crystals they may be placed in the following chronological order.

Cottrell and Bilby (1951) proposed that the growth of a twin could occur from a single layer fault by what is now known as a pole mechanism. Basically it involves the dissociation of a $\frac{1}{2} [111]$ slip dislocation into a single twinning partial and a residual sessile dislocation in the following way:

$$\frac{1}{2} [111] + \frac{1}{6} [11\bar{1}] + \frac{1}{3} [112]$$  (6.11)

The single layer fault is formed by the revolution of the screw component of the $\frac{1}{6} [11\bar{1}]$ partial, which cross glides on to the (121) plane, around the $\frac{1}{3} [112]$ pole dislocation. A twin is formed on the (121) plane since as it spirals the dislocation moves forward by $\frac{1}{\sqrt{6}}$ along the [121] direction.

Sleeswyk (1963) suggested that a $\frac{1}{2} <111>$ screw dislocation could dissociate into three $\frac{1}{6} <111>$ twinning partials on the three {112} crystallographically equivalent planes in a manner previously described in this section. According to elasticity theory this arrangement of partials is unstable and could nucleate a three layer twin which
would grow by a pole mechanism. The dissociation reaction is represented thus

\[
\frac{1}{2} \langle 111 \rangle_{\text{screw}} + 3 \times \frac{1}{6} \langle 111 \rangle
\]  

(6.12)

A similar reaction for \( \frac{1}{2} \langle 111 \rangle \) edge dislocations was proposed by Ogawa (1965).

Sleeswyk (1974) has suggested an adaptation to the Cottrell–Bilby pole model in which the pole dislocation is perfect. This, according to Sleeswyk, would not impede the growth of the twin. Basically the perfect pole dislocation results from a mechanism nucleated from a jogged \( <001> \) dislocation. The jog produces an extrinsic fault on the \( (121) \) plane which is bounded on one side by a \( \frac{1}{3} [112] \) partial and on the other side by two \( \frac{1}{6} [11\bar{1}] \) partials. Under an appropriate stress the two \( \frac{1}{6} [11\bar{1}] \) partials become connected so that a twin lamella can grow on each side by motion of a single twin partial. The dislocation reaction is described below:

\[
[00\bar{1}] \rightarrow \frac{1}{3} [\overline{1}12] + 2 \times \frac{1}{6} [11\bar{1}]
\]  

(6.13)

This model however has met with some controversy and indeed several criticisms have been made of all the nucleation and growth mechanisms described here from both an experimental and theoretical standpoint. Some however are more serious than others. Experimentally there is no direct support for a pole mechanism originating from either an imperfect or perfect dislocation. In fact it is observed that the Burgers vector of twinning partials is always parallel to the Burgers vector of the parent glide dislocation, and that dislocations with
other vectors are not present. This would tend to support the proposal of Sleeswyk (1963). Indeed experimental work by Mahajan (1972) has produced evidence that screw dislocations are the source of the twins, although because these dislocations were located within a slip band no pole mechanism was necessary. Recent work by Mahajan (1975) tends to confirm this. From a theoretical point of view it has long been realised that the initial dislocation dissociation reaction of the Cotterell-Bilby pole model is energetically unfavourable. It also has the disadvantage of being particular to the bcc structure although adaptation to other structures has met with some success (see e.g. Venables 1961). Atomistic calculations of screw dislocations under stress by Duesbery et al. (1973) have shown that, using some interatomic potentials, the core of the dislocation can change so that three or four (112) planes are in twin orientation.

It is clear from the foregoing experiments and theoretical evidence currently available that, despite the elegance of the Cotterell-Bilby pole mechanism, Sleeswyk's screw dislocation model is the most realistic. This model must now be examined and interpreted in the light of the present results. Obviously the existence of both reflection and isosceles type boundaries found in the present calculations has a relatively minor effect on the dissociation reaction. As pointed out by Christian (1974) the screw dislocation would still dissociate into three $\frac{1}{6} <111>$ partials but then one of these partials would itself dissociate again into two equal $\frac{1}{12} <111>$ partial dislocations. The twin could then be thought of as nucleating now not from a three layer but a four layer fault thus:

$$\frac{1}{2} <111>_{\text{screw}} + 2 \times \frac{1}{12} <111> + 2 \times \frac{1}{6} <111> \quad (6.14)$$
It must be remarked, however, that the splitting of a $\frac{1}{6}$ <111> twinning dislocation into two equal $\frac{1}{12}$ <111> partials would not essentially alter any dissociation reaction from a theoretical point of view. Indeed this splitting could equally well be applied to the nucleation mechanisms visualised by either Ogawa (1965) or Sleeswyk (1974). Indeed some of Ogawa's schematic diagrams show twins in both isosceles and reflection orientation although this is not explicitly mentioned in the text nor a dislocation dissociation reaction given. It must be concluded therefore that only a combination of experimental investigations, atomistic calculations and crystallographic theories will lead to a deeper understanding of twinning dislocations. Moreover the experimental techniques may well have to resolve dislocations of small Burgers vector as indicated in Chapter 5. Preliminary results using weak beam electron microscopy applied to twins in other structures have detected a non-coincidence across the boundary thus lending support to the existence of the type of boundary, like the present isosceles twin, in which there is a relative translation of the crystal at the interface. This in turn, of course would support the idea of a twinning dislocation itself dissociating into smaller partials in a way similar to the reaction given in eqn. (6.14).

Finally as a result of the discrete lattice calculations performed on twinning dislocations in body-centred cubic crystals described in this chapter the following conclusions can be drawn. It is fairly simple to describe the core structure of a twinning dislocation in terms of an adapted differential displacement map. The mapping of a physical quantity more easily related to elasticity theory, such as the stress tensor, proves to be complicated. To merely locate the centre of the core however a plot of the disregistry of the lattice across the core is
adequate. To determine the separation of the twinning dislocations it is only necessary to plot the crystal structure along the boundary. The schematic core structures of twinning dislocations shown in Chapter 5 are borne out, i.e. the perfect edge twinning dislocations of Burger vector $\frac{1}{6} [111]$ dissociates so that ribbons of isosceles and reflection type twins are obtained. The relative width of these ribbons, or in other words the width of the twinning partials, is potential dependent. In the case of $\alpha$-iron the width is large and the step diffuse corresponding to zero lattice resistance to the nucleation and growth of a new layer. For molybdenum and tungsten however the width is small and the step sharp suggesting that the dissociation energy is very small and that the dislocations are sessile. These results, of course, just reflect the relative energy of the isosceles and reflection type boundaries for the three metals and could have been predicted from table (5.2). Further it was found that although the self energy of a step from isosceles to reflection type boundary was the same as a step in the same direction from reflection to isosceles type boundary the structures were different. However even the existence of such steps resulting from the dissociation of twinning dislocations had not been postulated before the application of the computer simulation method.

The encouraging results on edge twinning dislocations presented here clearly indicate that the work could be extended without difficulty to include the application of shear stresses to test for stability of the structure and also, of course, a study of screw twinning dislocations. It is envisaged that provided the potentials, models and relaxation techniques are chosen with care than this type of discrete calculation will in future progress and reveal many more important characteristics of interface structure.
CHAPTER 7 The Interaction of Vacancies with BCC Twin Boundaries and Twinning Dislocations

7.1. Introduction

With the exception of the work on interacting boundaries of microtwins described in Chapter 4 and the study of groups of partial twinning dislocations in Chapter 6 this thesis has been concerned with the properties of a single isolated crystal defect. However, such isolated defects are seldom observed in practice so that any physical property of the crystal must be explained in terms of the mutual interaction of these defects, in addition to their own characteristic properties. In a polycrystalline material, therefore, it is the influence of grain boundaries on other defects that is important whereas in a single crystal the interaction of dislocations and point defects controls physical processes.

The interaction of a vacancy or cluster of vacancies with a boundary has been of considerable interest for some time. A large number of experiments have established that boundaries can, under certain conditions, act as both sources and sinks for vacancies. In addition some special kinds of boundaries have been found to be good conductors of vacancies. Clearly results such as these are particularly valuable in formulating theories for phenomena like swelling due to irradiation or diffusional creep. Sophisticated transport mechanisms now exist for creep but to determine their reliability a quantitative knowledge of several atomistic parameters is required including the formation energy of a vacancy in the vicinity of a boundary. Although experimental estimates can be made it is obvious that another method, the discrete computer calculation, is readily available and able to deal with the problem.
As a first step in a more general program of work on the interaction of point defects with interfaces this chapter describes how, using the computer simulation technique, the formation energy of a vacancy and divacancy may be calculated in the neighbourhood of a \{112\} twin boundary in a bcc metal representing \(\alpha\)-iron. The relative binding energy of a vacancy to a reflection and isosceles type boundary is determined and for a divacancy the most stable configuration is found and an estimation of the three-body effect made.

7.2. Previous Work

In order to put the present work into perspective a brief review is now given of some of the theoretical calculations and experimental evidence for the interaction of vacancies with twin boundaries. For a more comprehensive review of the interaction of crystal defects with grain boundaries see Gleiter (1972).

7.2.1. Experimental

The vast majority of experimental observations made to date have been on the interaction of vacancies with grain boundaries. It is generally agreed that grain boundaries can act as sources for vacancies, although in most of the experiments (see e.g. Barnes 1960, Ells and Evans 1959 or Cahn 1965) this is done by force, i.e. heating or irradiation. Similarly a number of experiments have shown that grain boundaries act as sinks for vacancies. Kelly and Nicholson (1963) have, for instance, observed denuded zones near boundaries in precipitation processes, and Balluffi (1969) has shown that the introduction of boundaries can enhance the kinetics of vacancy equilibration. Results on twins, however, remain remarkably sparse.
Barnes (1960) has demonstrated that coherent twins in copper and beryllium are not sources of vacancies and that non-coherent twin boundaries act as vacancy conductors. Segall (1964) has provided evidence that coherent twins in gold may, under certain conditions, be good sinks. He observed that within a region about 0.5 μm wide around the coherent twin there were no defects, suggesting that vacancies may annihilate at the boundary. This result is surprising since it is generally believed (see e.g. Ashby 1972) that when any boundary emits or absorbs vacancies it is really climbing boundary dislocations which are the sinks or sources. Segall's results can then only be explained by assuming that vacancy absorption occurred at pre-existing monatomic steps causing the steps to move in the boundary plane.

The idea that emission or absorption of vacancies occurs only when the boundary is incoherent, i.e. around boundary dislocations or regions of severe misfit, has been examined further theoretically.

7.2.2. Theoretical

Weins et al. (1970, 1971) have considered the proposal that steps sweeping across boundaries can generate or absorb vacancies using a geometrical ball model. They considered initially the diffusion of a vacancy to a step in an interface between two crystals. Such diffusion would, of course, occur naturally in practice on purely energetic grounds to relieve the local strain in a region of misfit. The step would then occupy the vacant site by translating laterally across the interface. The reverse process would of course generate vacancies.
The only significant computer simulation study of the interaction of vacancies with boundaries has been made by Dahl et al. (1972) (or Dahl 1970). They calculated the formation and migration energy of vacancies in and near a 6° tilt grain boundary in γ-iron. The conclusions they drew from their studies may be summarised as follows:

(i) The formation energy of a vacancy in a region of misfit was considerably lower than in the perfect crystal (or a region of good fit). These regions may then be considered as sinks or sources for vacancies.

(ii) The vacancy formation energy and hence the activation energy for migration was lower at sites approaching the sinks along close-packed directions than along any other direction. Thus close-packed directions are preferred for vacancy diffusion.

(iii) The interaction zone in which the vacancy formation energy differed from that of the perfect crystal by up to a few percent extended about 7a₀ (a₀ = lattice parameter) from the boundary.

(iv) Under pressure it was found that regions subjected to compressive stresses (good fit regions) became sources for vacancies. Misfit regions remained vacancy sinks.

Unfortunately there appears to be little work done on the interaction of vacancies with high coincidence site boundaries. The results on {112} twin boundaries presented in this chapter are the first of their kind. Both the coherent and incoherent twin are considered and, in general, the results agree with current experiment and theory.
7.3. Results and Interpretation

The crystal used for the study was α-iron partly because of its technological importance but primarily because a well-established potential is available for this metal. This Johnson J₀ potential has been used extensively to investigate the properties of vacancies and divacancies in bcc metals (see Johnson 1964, 1966). In particular it predicts a vacancy formation energy $E_v^F$ of 1.37 eV and stable first and second nearest neighbour divacancies with binding energies of 0.095 and 0.146 respectively in units of $E_v^F$. Other potentials which have been developed for bcc metals give similar results and in particular confirm that the second nearest neighbour divacancy is more stable than the first. The preliminary calculations to determine the formation and binding energies of vacancies in a single crystal confirm in detail the original work of Johnson (1964) and demonstrate that at least for these defects and for the Johnson J₀ potential the minimisation procedure based on conjugate gradients being used here converges to the same values as the slower procedures used earlier.

7.3.1. Vacancy-Twin Interactions

The procedure used to investigate the interaction of a single vacancy and a bcc twin boundary involved removing an atom from the model crystal containing either a coherent isosceles or reflection type boundary. The boundary was approached along a close-packed direction and atoms were removed in turn from each of the (112) planes. This procedure was carried out for up to eight (112) planes from the boundary. In the calculations the outer (112) boundaries were displaced outwards by ± v [112], where v is the critical volume expansion for the twin, and then held rigid while the relaxation
proceeded in the computational cell. As cyclic boundary conditions were used on the (1\overline{1}0) and (1\overline{1}1) faces of the crystal, the model actually simulates the interaction between a rectangular array of vacancies, lying in (112), and the twin. However tests using models of different sizes indicated that there was no effective interaction between the vacancies if the crystal contained as few as four (1\overline{1}0) planes and six (1\overline{1}1) planes. No models smaller than this were used and indeed in order to test for boundary instabilities 33 (1\overline{1}1) planes and 8 (1\overline{1}0) planes were normally used. In the [112] direction 24 planes were used for the isosceles boundary interaction and 25 for the reflection boundary interaction. As expected no marked changes in the twin boundary structure were observed for any of the vacancy locations and there was no vacancy migration. However there were marked differences in the energy $E^\text{T/V}$ of the crystal for different locations of the vacancy relative to the twin. Here and elsewhere the italic $E$ indicates that the energy is a function of the size of the model crystal. Now

$$E^\text{T/V} = E^\text{T} + E^\text{F} + E^\text{I}_{TV} \quad (7.1.)$$

where $E^\text{T}$ is the energy of the crystal containing only the twin and $E^\text{I}_{TV}$ is the interaction energy of the vacancy and the twin. This interaction energy is the negative of the binding energy $E^\text{B}_{TV}$ which is given in table (7.1) for both the isosceles and reflection type boundaries. Note that $E^\text{B}_{TV}$ is small, and in some cases negative. For the isosceles boundary the maximum occurs at plane 2 (or equivalently -2) where $E^\text{B}_{TV}$ is approximately + 0.2 eV or 0.14 $E^\text{F}_V$. In the case of the reflection boundary the maximum occurs at plane 1 (or -1) where $E^\text{B}_{TV}$ is approximately + 0.15 eV or 0.11 $E^\text{F}_V$. These results are displayed graphically in fig. (7.1). Thus as expected there is no long range interaction between
vacancies and twin boundaries. However there is an appreciable binding energy when the vacancy is adjacent to, but not in, the interface. This preferred location is at first surprising but the result follows from curves C of fig. (5.3) for the reflection and isosceles twins which indicate that this part of the crystal is the most highly compressed.

The effect of stress on the binding energy of a vacancy to a twin may be considered in an approximate way by examining the models corresponding to curves A of fig. (5.3). These involve rigid outer boundaries parallel to (112) and no overall volume increase. Thus, because of the volume increase associated with the formation of the twin, the whole crystal is in elastic compression. Therefore the compressive strain associated with plane 2 (for isosceles boundary) or plane 1 (for reflection boundary) increases progressively from model C to model A. This is reflected in the binding energies, which are maxima for this plane and increase by about two per cent. Note however that these results do not correspond to an applied uniaxial stress as no expansion is allowed perpendicular to the [112] axis.

The effective zone of interaction remains the same and, as stated earlier, is short range extending about six (112) planes (or $\sqrt{6} a_0$) from the boundary.

7.3.2. Divacancy-Twin Interactions

Both first and second nearest neighbour divacancies were considered in this study. In a single crystal these both have appreciable positive binding energies, the latter being the more stable. When orientation relative to the (112) twin boundary is taken into account these divacancies have 3 and 2 crystallographically distinct variants respectively. Examples of these five variants are illustrated in fig. (7.2).
The model crystal used for the calculations was identical to that described in §7.3.1. The twin boundary structure was in all cases basically unchanged by the divacancies but there were appreciable changes in the total energy $E_{TVV}$ of the crystal for different relative positions of the twin and the two vacancies. This energy may be written

$$E_{TVV} = E_T + 2E_V + E_{TVV}^I \quad (7.2.)$$

where $E_{TVV}^I$ is the total interaction energy of the twin and the two vacancies. Now,

$$-E_{TVV}^I = E_{TVV}^B_{TV_1} + E_{TVV}^B_{TV_2} + E_{VV}^B + E_{TVV}^B,$$

where $E_{TVV}^B_{TV_1}$ and $E_{TVV}^B_{TV_2}$ are the binding energies of the two individual vacancies to the twin and $E_{VV}^B$ is the binding energy of the isolated divacancy. These three results are already known from preliminary calculations on a single crystal or from the results of §7.3.1. The remaining term $E_{TVV}^B$ is an additional binding energy arising from the mutual interactions between the three defects and could be called a three-body effect. This correction term was found to be less than 0.02 $E_V^F$ except for cases in which the divacancy straddled the twin boundary when neither the first or second neighbour values for $E_{VV}^B$ are strictly appropriate. However it could be concluded from the values obtained for the total interaction energy that $E_{TVV}^I$ is a minimum when the divacancy lies directly across the boundary (for a reflection twin) or lies parallel to the boundary in plane 2 for the isosceles twin. These configurations correspond to the most tightly bound and hence most stable divacancy variants in the neighbourhood of a {112} boundary.
7.3.3. Vacancy-Twinning Dislocation Interaction

Due to the importance of boundary steps in the process of emission or absorption of vacancies it was decided to determine how the binding energy of a vacancy varied in the region of a $\frac{1}{12}$ [11̅1] partial twinning dislocation in α-iron. The twinning dislocation was created in a manner similar to that described in Chapter 6, in a model containing 200 (11̅1) planes, 20 (112) planes and 4 (110) planes. The outer (112) planes were kept rigid and no volume expansion allowed. The outer (11̅1) planes also remained rigid but cyclic boundary conditions were imposed on the extreme (110) faces. As described in Chapter 6 there are two distinct structures having approximately the same energy for a $\frac{1}{12}$ [11̅1] partial twinning dislocation and have been denoted RI and IR. These are shown in figs. (6.3.a) and (6.3.b) and, in the notation of those figures, a single vacancy was introduced on the (112) plane, q. The variation of the binding energy across the partials could then be determined by moving the vacancy from one [11̅1] atomic site to the next on plane q, for $q = 0, \pm 1$ and $\pm 2$. This gives a total of ten curves which can in effect be joined end to end so as to simulate the variation of the binding energy along a single (112) plane that lies through ten $\frac{1}{12}$ [11̅1] partials (or five $\frac{1}{6}$ [11̅1] perfect twinning dislocations). This composite curve is shown in fig. (7.3) along with a schematic diagram of the ten $\frac{1}{12}$ [11̅1] partials. The (112) plane along which the binding energy varies is shown bold. The curve has a number of striking features. Firstly it is noticed that the matching is quite good, (any large mismatch must be attributed to boundary effects at the edge of the model) and that the value of the binding energy at all the joins agrees well with the results shown in table (7.1) for the coherent twins. Secondly it is seen that there
are just two localised maxima (labelled A and B), and that the rest of the curve either monotonically increases or decreases to form plateaux. A careful check for other maxima, however small, was made but surprisingly none were found. It is assumed that this effect is caused by the large differential in binding energy that occurs between adjacent plateaux, and which in some cases is so overwhelming that the curves connecting the plateaux can only be steep and monotonic. The two maxima that were found and which are also labelled on the schematic diagram of the dislocation structure must correspond to the positions where a vacancy is most tightly bound to the dislocation. They have binding energies of 0.16 and 0.24 eV respectively and coincide approximately with the centres (indicated by $\gamma$) of both partial dislocation structures whose displacement maps are given in figs. (6.6.a) and (6.6.b) The fact that these regions are in compression agrees with the predictions of elasticity theory. Finally fig. (7.4) gives all equivalent positions (shown as circles) of binding energy maxima that occur for the two types of twinning dislocations that advance in the $[\{11\}]$ direction either by stepping up or by stepping down.

7.4. Discussion

The computational method, interatomic potential used and the overall validity of this type of calculation have been discussed in depth elsewhere in this thesis and will not be explained further here. However since this discussion will be devoted to relating the results of the present work to experiment and to such important phenomena as thermal creep it is again worth emphasising that all the simulations have effectively been performed at absolute zero. With this borne in mind several important conclusions may be drawn from the calculations.
Firstly it is clear that the vacancy formation energy is, in general, lower in the immediate vicinity of an isosceles twin than in the immediate vicinity of a reflection twin. An isosceles twin can thus be considered more likely to capture a vacancy than a reflection twin. This is in accord with conclusion (i) of Dahl et al. (1972) although here, strictly speaking, the isosceles twin cannot be called a sink for vacancies since it is a quasi-coherent boundary; rather it is the twinning dislocation that acts as the vacancy sink (or indeed source). This conclusion is confirmed by the work on vacancy-twinning dislocation interactions. The binding energy of a vacancy to the dislocation is highest around two particular regions so that it is expected that a vacancy will preferentially diffuse towards those regions. It must be emphasised, however, that this result is true only within the framework of the present model and that under conditions of temperature and pressure different results may well be obtained. Nevertheless the diffusion of vacancies to specific regions of the dislocation and their subsequent growth into voids will have an important effect on creep phenomena. The results on divacancy twin interactions clearly indicate the most stable configurations of vacancy pairs from which these voids could nucleate.

Experiments performed to date have demonstrated that in at least some fcc and hcp metals coherent twins do not act as either vacancy sources or sinks but an incoherent twin can act as a vacancy conductor. Although the present work could agree with the former result it would have difficulty confirming the latter because, as can be seen from fig. (7.1), an energy barrier of at least 0.1 eV needs to be overcome in order to cross the boundary. However since different twin boundaries in different metals are being compared the disagreement is hardly surprising.
Many studies are suggested by the preliminary calculations on the interaction of vacancies with twin boundaries reported in this chapter. Clearly it would be desirable now to determine the interaction of vacancy clusters with the boundary and also to see what effect pressure has on the binding energy. Indeed work has already begun on determining the variation of the binding energy of a single vacancy to a twin with uniaxial stress (Ingle 1975). Under certain conditions transformation changes can occur and again this will have important consequences on mechanisms for creep failure. To fully understand these thermal and irradiation effects on metals however future work must also be aimed at determining the interaction of interstitials and impurities with interfaces.
Table (7.1)

The Binding energy (in eV) of a vacancy in the vicinity of a reflection (R) and an isosceles (I) type (112) twin boundary in iron (n denotes the number of (112) planes from the composition plane).

<table>
<thead>
<tr>
<th>n</th>
<th>R</th>
<th>I</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-0.0981</td>
<td>-</td>
</tr>
<tr>
<td>±1</td>
<td>0.1480</td>
<td>0.0195</td>
</tr>
<tr>
<td>±2</td>
<td>0.0880</td>
<td>0.1913</td>
</tr>
<tr>
<td>±3</td>
<td>-0.0029</td>
<td>-0.0133</td>
</tr>
<tr>
<td>±4</td>
<td>0.0059</td>
<td>0.0164</td>
</tr>
<tr>
<td>±5</td>
<td>0.0035</td>
<td>-0.0020</td>
</tr>
<tr>
<td>±6</td>
<td>0.0022</td>
<td>0.0033</td>
</tr>
<tr>
<td>±7</td>
<td>0.0025</td>
<td>0.0001</td>
</tr>
</tbody>
</table>
CHAPTER 8 General Discussion and Conclusions

8.1. Discussion

Motivated by a desire for a better understanding of several metallurgical phenomena attributed to interfacial effects, this thesis has described the application of a technique that is capable of determining physical parameters hitherto out of reach using standard experimental and theoretical procedures. In particular the atomistic technique fulfils the need to know the microstructure and energy of such interfaces and thereby can contribute to achieving the ultimate aim of controlling the phenomena. However the discrete lattice calculation requires critical assessment and it is the purpose of this final discussion to examine several factors within the model which could affect the reliability of the results and also to relate the work to what little experimental information is available. The limitations of the calculations are clearly stated and it is within these confines that the details of the present work on twinning in bcc metals are summarised in §8.2.

The validity of computer simulation results rely to varying degrees on the chosen interatomic interaction, the boundary conditions and the relaxation procedure. Probably the most important of these is the choice of a semi-empirical interatomic interaction since to some extent it is a fairly arbitrary quantity and can only be as accurate as the data from which it was constructed. It is usually desirable in computer experiments to use a potential which is as simple in form as possible and which does not have an excessively long range. The only criterion which must of necessity be fulfilled is that the potential ensures a stable crystal lattice with respect to small
deformations and rigid body displacements (Born and Huang 1954). When applied to bcc structures this means that the inflexion point in the potential must lie beyond the second nearest neighbour distance, which it does for the Johnson-type potentials used in the present work. It is this emphasis on predicting the correct lattice structure that usually results in more confidence being placed in the relaxed atomic configuration than in the relaxed energies. However at least the limitations of simple potentials are quite clear. The interpretation of results obtained from the use of more complex potentials, which might include quantum mechanical effects due to electronic redistribution in the vicinity of severely distorted defect cores, would be difficult. So far general empirical potentials of this nature have not been constructed. Moreover present potentials have usually been designed for particular classes of defects, e.g. vacancies and interstitials. It is gratifying to show that these potentials may also be applied successfully to interfaces. Indeed in order to test the results it would seem necessary in any computer simulation calculation to use at least two different interatomic interactions. It would be useful if one of these interactions was a pseudopotential but this is not always practical. If the same or similar defect configuration results from such calculations then it could be said to be characteristic of that particular crystal structure even though the magnitude of the relaxed energies may be greatly different. In addition it is unusual to place much significance on the actual metal the potential represents. It is clear that more accurate potentials, however complicated, will only come from increased experimental information concerning the bulk properties of the material. It is expected that this data will come from new atomic and neutron scattering measurements, positron annihilation and NMR techniques.
The extent to which the boundary conditions and relaxation procedure effect the computer results is difficult to assess. The fact that their exact nature is frequently never stated indicates that some authors consider them to be of relatively minor importance. It is, however obvious that the boundary conditions, for instance, must be chosen to suit the type of defect to be studied. Similarly the choice of numerical minimisation method may depend on whether it is considered an advantage or not to locate metastable configurations. Experience gained from the present work has suggested the following combination of boundary conditions for particular kinds of defect. It is usually always desirable to have as large a computational cell as possible, however for extended defects the size of the cell may be reduced by applying cyclic or periodic boundary conditions along directions in which the defect must repeat itself. Thus for a twin boundary these directions would lie in the plane of the interface, and for a dislocation along its line. Normally rigid boundary conditions are then applied to the other face(s) of the cell but in the case of a dislocation a better approximation is achieved by incorporating the appropriate displacement field calculated from anisotropic elasticity theory. The resulting elastic boundary may be improved further by including non-linear effects in the dislocation core but since this complicates the calculation considerably it is seldom thought to be worthwhile. The use of cyclic boundaries in the simulation of point defects is only useful if an infinite array of such defects is required. Therefore when simulating a single point defect or even a small cluster of point defects it is probably better to use a large computational cell with rigid boundary conditions in all directions. In this way the possibility of spurious effects due to the mutual interaction of defects within the array is excluded. It
is obvious from the foregoing discussion that to avoid prejudicing the relaxation, care must be taken in choosing the best size computational cell in conjunction with the most suitable boundary condition. This is particularly important for defects with long range strain fields. In the present work where rigid, cyclic and elastic boundary conditions have all been used it is believed that the correct matching across the boundary has been obtained. It seems unlikely that the numerical relaxation procedure, provided it is programmed accurately, will have a serious effect on the final configuration and energy. Nevertheless if metastable configurations are to be avoided the quasi-dynamic or dynamic techniques are recommended. It must also be remembered that molecular statics calculations always simulate a defect structure at absolute zero whereas any desired temperature (or pressure) may be simulated using the molecular dynamics method (see Chapter 2). In addition only real space models have been used or summarised in the present work.

Harmonic reciprocal space or lattice statics calculations (Kanzaki 1957) have been applied extensively to point defects (see e.g. Kenny 1973). However, although the method has the advantage of minimising the potential energy of the model crystal without the use of an iterative relaxation process, it would be difficult to apply to extended defects. This is principally because the strength of these defects and also the imperfect lattice Green function are not known.

One of the most interesting results of the present studies is the finding that the orientation relationship for twinning in bcc metals can involve not just one but two basic components, namely reflection (or rotation) and translation. The magnitude of this translation, when coupled with reflection, has been found to be
\frac{1}{12} [\overline{1}1\overline{1}] in the antitwinning direction and the resulting structure called the isosceles twin. A glance at the asymmetric curve of fig. (5.2.a) shows that the complementary translation of \frac{5}{12} [\overline{1}1\overline{1}] in the twinning direction is energetically unfavourable, at least when no relaxation is allowed. Alternatively, the structure of the isosceles twin may be described in terms of a sequence of stacking faults on (112) planes. These stacking faults can be produced by the passage of a partial dislocation with \frac{1}{12} [\overline{1}1\overline{1}] Burgers vector on the first (112) plane of the product crystal plus the passage of partials with \frac{1}{6} [\overline{1}1\overline{1}] Burgers vector on successive (112) planes. Note that these vectors are in the twinning direction. Complementary \frac{5}{12} [\overline{1}1\overline{1}] and \frac{1}{3} [\overline{1}1\overline{1}] Burgers vectors are geometrically possible but have never been observed. There is thus a twinning - antitwinning asymmetry on (112) planes in both the perfect and reflected crystals. The formation of an isosceles type twin from the perfect crystal is easier by translations in the twinning direction than in the anti-twinning direction whereas the converse is true for the formation of this type of boundary from the reflected crystal. This asymmetric feature of (112) planes was first noticed in a computer simulation study by Vitek (1968) while investigating intrinsic stacking faults in bcc crystals. However although his (112) \gamma-surfaces displayed a definite asymmetry, no local minima were found. The possibility of stable stacking faults in bcc crystals was discussed further by Eichler and Pegel (1969) who, using similar computer techniques, found that a minimum in the \gamma-surface could exist at \frac{1}{12} [\overline{1}1\overline{1}] if the interatomic interaction was terminated close to the second nearest neighbours. Such a short cut-off, however, would lead to an unstable crystal structure and the calculation could not be considered realistic. Indeed, the result approximates to the 'hard-sphere' model which
predicts a local minimum with translation vector equal to
\[ \frac{1}{2} [\overline{1}11] \pm \frac{5-\sqrt{15}}{16} [\overline{1}10], \]
allowing no expansion perpendicular to the fault plane (Vitek 1970a). Although the existence of a single layer stacking fault on (112) planes is therefore doubtful Vitek (1970) showed that n-layer faults (n ≥ 3) with fault vectors
\[ \frac{1}{12} [\overline{1}11], \]
\[ \frac{1}{6} [\overline{1}11], \ldots, \frac{1}{6} [\overline{1}11], \frac{1}{12} [\overline{1}11] \]
were stable. In addition Vitek postulated that an infinite twin of the isosceles type would also be stable and this has been confirmed in the present study. However, the present work has also shown that the reflection twin can exist, and moreover is likely to predominate because of its lower interfacial energy. Nevertheless in practice quasi-coherent boundaries, i.e. boundaries which are translated away from exact coincidence, have been detected. In particular, twins in aluminium and stainless steel have been examined using weak-beam electron microscopy. To detect rigid body translations between coincidence related crystals the specimen is oriented into a two beam diffracting condition using planes which would be continuous through the twin boundary if there were no translation. Such planes are then invisible, but Pond and Smith (1974) found that stacking fault like fringes appeared when the twinning plane was apparently interrupted by segments of another plane. The appearance of these fringes is believed to be due to a relative translation between adjacent grains caused by a need to relieve the 'severe crowding' in the immediate vicinity of a coincidence (or reflection) twin boundary. The actual magnitude and direction of these translations is not yet known but work is reported to be in progress.

Dispite the experimental evidence for the existence of translated, non-coincidence site boundaries, sophisticated theories have developed
in favour of the concept of atom sharing. Notably a general mathematical formulation of the coincidence site and O-lattice have been made by Bollmann (1970) which has underlined the importance of lattice coincidence. Furthermore these theories have emphasised the significance of such geometrical quantities as the reciprocal density of coincidence sites or Σ function and related them to the frequency of occurrence of particular boundary orientations. In addition several authors (see e.g. Ishida and McLean 1972 or Grimmer et al. 1974) have developed prescriptions for calculating the coincidence site lattice (CSL) vectors, the complete pattern-shift lattice (DSL) vectors and the Burgers vectors of boundary dislocations for cubic lattices up to Σ = 49. Studies of this kind are clearly useful when attempting to rationalise the results of theoretical and experimental investigations on translated boundary structures. As discussed in Chapter 2 the deviation from coincidence orientation found in grain boundaries by several workers using computer simulation methods could be explained in terms of the DSC lattice. The occurrence of the isosceles type twin boundary found in the present study can be explained in a similar fashion, i.e. although lattice coincidence is destroyed the overall pattern of coincidence sites remains. Moreover it is possible, at least in principle, to determine the magnitude of the translations which result in a DSC lattice.

Unfortunately for the simple case of a {112} bcc twin boundary where Σ = 3 there exist an infinite number of such translations. Therefore direct comparison with the present work, in which the translation vector \( \mathbf{t} = \frac{1}{12} [111] \) was obtained, cannot be made. Nevertheless, as discussed in Chapter 1, the fact that \( \mathbf{t} \) is non-zero is significant since the resulting boundary, which has been termed quasi-coherent, has not previously been considered as a minimum energy configuration and
consequently excluded from many theories involving crystalline interfaces.

8.2. Conclusions

The results obtained in the present study from the computer simulation of \{112\} twin boundaries and twinning dislocations in body centred cubic metals representing \(\alpha\)-iron, molybdenum and tungsten may be summarised as follows:

(i) In a study of generalised \{112\} stacking faults in \(\alpha\)-iron a stable fault has been found which may be regarded as a twin nucleus. From this nucleus a stable microtwin has been induced to grow although no formal nucleation or growth mechanisms are proposed. The twin boundaries have an unexpected but characteristic, symmetrical structure which is distinct from that associated with the conventional mirror image orientation relation. The twin boundary energy was deduced to be 0.270 Jm\(^{-2}\).

(ii) The distribution of interatomic distances across unrelaxed stacking faults is, under certain conditions, 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.
(iii) Two distinct \{112\} twin boundary structures have been found to be stable or metastable in all the models used. These were the conventional twin boundary defined by a reflection orientation relation and a twin in which the boundary consisted of a layer of cells which project on the \{110\} plane as interlocking isosceles triangles. In the case of iron the two boundaries, when fully relaxed, are found to have almost identical energies but for molybdenum and tungsten the reflection boundary is preferred. The twin boundary energies for these two metals are three or four times as large as those for iron. Volume increases are predicted for the reflection twins in all three metals but for molybdenum a surprising volume decrease arises for the isosceles twin. The results suggest that in some bcc metals both types of boundary may arise in which case each twinning dislocation is likely to be dissociated into two partials, each with Burgers vectors $\frac{1}{12} \langle \overline{111} \rangle$.

(vi) The core structures of bcc edge twinning dislocations with Burgers vectors $\frac{1}{12} \langle \overline{111} \rangle$ and $\frac{1}{6} \langle \overline{111} \rangle$ have been examined using differential displacement mapping techniques. In molybdenum and tungsten the perfect twinning dislocation of Burgers vector $\frac{1}{6} [11\overline{1}]$ was found to be stable and well localised suggesting that the dissociation energy of the partials is very small and that there is a high Peierls-Nabarro stress associated with the dislocations. However, in iron
the perfect twinning dislocation always dissociated into two separate partials each of Burgers vector \( \frac{1}{12} [11\overline{1}] \) so that ribbons of isosceles and reflection twin were obtained. The width of these partials was found to be large and the step diffuse corresponding to zero lattice resistance to nucleation and growth of a new layer. The separation of the partials must depend on the energy of the "intermediate twinned stacking fault" which clearly is dependent on the chosen interatomic interaction.

(v) Conventional rather than complementary twinning dislocation structures have resulted from the present studies. However, when simulating the interaction of an edge slip dislocation of Burgers vector \( \frac{1}{2} [11\overline{1}] \) with a (112) twin boundary in iron an unexpected type of twinning dislocation was obtained. The defect has the same Burgers vector as the conventional perfect twinning dislocation but is associated with a double interfacial step in the opposite sense. It therefore has a low self energy but zonal character. It is suggested that this defect may play a significant role in the interaction of slip and twin boundaries in bcc metals.

(vi) The interaction of vacancies and divacancies with \{112\} twin boundaries in iron have been investigated and the interaction energies obtained as a function of the separation of the point defect(s) from the boundary. For the single vacancy the maximum binding energies for
the two boundaries are similar in magnitude and occur when the vacancy lies adjacent to but not in the interface. These binding energies are equal to 0.15 and 0.19 eV for the reflection and isosceles boundaries respectively. Pairs of vacancies, whose mutual separation did not exceed the second nearest neighbour distance, were considered in all possible orientations relative to the twin boundaries. The most stable types were found to a nearest neighbour divacancy adjacent and parallel to the isosceles boundary and a vacancy pair straddling and perpendicular to the reflection boundary.

(vii) The variation of the binding energy of a single vacancy in the region of a partial twinning dislocation of Burgers vector $\frac{1}{12}[11\bar{1}]$ in iron has also been studied. It was found that the vacancy was most tightly bound to the dislocation around two specific regions of compression close to the dislocation core. The binding energy of the vacancy in these positions was 0.16 and 0.24 eV respectively. Thus it is expected that under suitable conditions it would be towards these regions that the vacancy would preferentially diffuse.

(viii) In accord with a number of other computer simulations of intercrystalline boundaries the present work has resulted in an emphasis on periodic patterns in interface structure rather than lattice coincidence.
The contribution of discrete atomic models to our understanding of the nature of crystalline interfaces is potentially great. As always, however, the main difficulty lies in the construction of a realistic interatomic interaction. The present work on rather simple types of interfaces has nevertheless shown that sensible results can be obtained using unsophisticated potentials originally designed for other problems. Needless to say there is always room for improvement. The whole framework of the model could be elaborated upon so as to include several metallurgical variables hitherto neglected. Specifically, in relation to twinning behaviour it would be extremely valuable to simulate the effect of temperature, strain rate and alloying. However the present state of the art is such as to make interpretation of the results impossible. Future work must still be directed towards simulating simple defect systems on which meaningful results can be obtained.
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Figure Captions

Figure (1.1) The interrelationship between the twinning elements.
K denotes the twinning plane and n the shear direction.
K is the second plane undistorted, but not unrotated,
by the twinning shear.

Figure (3.1) The interatomic potentials φ(r) used in the calculations.
The iron, molybdenum and tungsten potentials were
developed by Johnson (1964), Kenny and Heald (1974) and
Stabell and Townsend (1974), respectively. The first,
second and third nearest neighbour distances are indicated
by 1, 2, 3 on the r/a axis; a is the lattice parameter.

Figure (4.1) Faults on a (112) plane of a bcc structure projected on to
a (110) plane, atoms represented by circles and crosses
lying in adjacent (110) planes. The simple twin fault
shown in (e) may be obtained by a homogeneous deformation
twinning shear of 2 in the [111] direction or by the
complementary twinning shear of 2 indicated here by the
outlined cells. In (f) this structure has been allowed to
relax perpendicular to the interface. A generalised
stacking fault involving a displacement of a/2 [111]
(0 < a < 1) is shown in (a) and various possible ways in
which this structure may relax are given in (b), (c) and
(d). In particular (b) and (c) show alternative ways in
which the resulting configuration may be an elastically
strained single crystal and (d) shows a possible twin
nucleus with unexpected interfaces.
Figure (4.2) Variation of the energy $\gamma$ of generalised faults of displacement vector $a/2$ [111] on a (112) plane of a bcc structure. The upper curve $\gamma_f$ gives the unrelaxed fault energy, the lower curve $\gamma_e$ the energy of the relaxed configurations corresponding to elastically strained single crystals and the intermediate segment $\gamma_t$ the localised metastable microtwin energy.

Figure (4.3) 4-layer {112} twin in a bcc structure projected on to {110}, atoms represented by circles and crosses lying in adjacent {110} planes. Note the structure of the interfaces.

Figure (4.4) Faults on a (112) plane in a bcc crystal projected on to a (110) plane, atoms represented by circles and squares lying in adjacent (110) planes. The nearest neighbour bonds $p = \frac{1}{2} [11\bar{1}]$ 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 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 $\frac{1}{2} [\bar{1}11]$ so that equal numbers of bonds are in fact extended and contracted.
Figure (4.5) Relationships between a triad of bond vectors $\mathbf{r}_\alpha^i (\alpha = 1,2,3)$ 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 $r_\alpha^i$ on the plane $h_i$ make angles of $\theta$, $\theta + 2\pi/3$ and $\theta + 4\pi/3$ with $u^i$. In addition their projections on $u^i$ have lengths $s_\alpha$ such that $\sum s_\alpha = 0$.

Figure (5.1) Two possible schematic structures for a (112) twin boundary in bcc crystals shown projected on to the (110) plane. Atoms represented by circles and triangles lie on adjacent (110) planes. The conventional twin shown in (a) is obtained by reflection in the (112) composition plane. The twin shown in (b) has a boundary structure consisting of a layer of cells which project as isosceles triangles. The structures are referred to as reflection and isosceles twin boundaries respectively. Successive (112) planes are numbered as indicated; the bonds $b$, $b_1$ and $b_2$ are discussed in Chapter 5.

Figure (5.2) The energy $\gamma$ of the boundary obtained by superimposing a fault $\frac{a}{2} [11\bar{1}]$ on the twin boundary of fig. (5.1a). The energies of the unrelaxed and relaxed structures are given by $\gamma_u$ and $\gamma_r$ respectively. Both curves are plotted in (a) and the latter is given at a larger scale in (b). The Johnson iron potential was used and the model consisted of 24 (112) planes. No volume increase was allowed.
Figure (5.3) Curves defining the symmetric normal displacements \( \pm v_n [112] \) of (112) planes on either side of (a) the reflection twin and (b) the isosceles twin, after relaxation using the Johnson iron potential. The models consisted of 25 (112) planes in (a) and 24 in (b) and these are numbered along the \( n \)-axis, the interfaces being at 0 in (a) and between -1 and +1 in (b) as shown in fig. (5.1). Curves A, B and C correspond to models with compressive, tensile and zero long range strains respectively. Curves C therefore correspond to the predicted equilibrium structures.

Figure (5.4) Twin boundary energy \( \gamma \) of the reflection (R) and isosceles (I) twins as a function of volume increase defined by \( \nu \), where \( \pm \nu [112] \) is the outwards displacement of the rigid (112) boundaries of the model. The results were obtained using the Johnson iron potential.

Figure (5.5) Schematic dissociation of bcc twinning dislocations. Perfect edge twinning dislocations with Burgers vectors \( \frac{1}{6} [11\bar{1}] \) are shown in reflection and isosceles boundaries in (a) and (b) respectively. Three partial edge twinning dislocations of Burgers vector \( \frac{1}{12} [11\bar{1}] \) are shown in (c) each separating a region of reflection twin from a region of isosceles twin. The two left hand and two right handpartials in (c) may be considered to be dissociated reflection and isosceles twinning dislocation respectively.

Figure (6.1) General step in interface. When \( \gamma \) represents a coherent twin boundary then the step of height \( \frac{\gamma}{h} \) is described as a twinning dislocation with Burgers vector \( b_t \).
Figure (6.2) The Frank circuits around perfect and partial twinning dislocations in a bcc structure. Both reflection and isosceles type boundaries are taken as reference crystal and the closure failure FS indicates the magnitude and direction of the Burgers vector $b_T$. Two partial twinning dislocations labelled IR and RI and also two perfect twinning dislocations RR and II are shown to be structurally distinct.

Figure (6.3) Computed structure of a partial twinning dislocation in $\alpha$-iron with Burgers vector $\frac{1}{12} [11\overline{1}]$. The two types of structure labelled IR and RI are illustrated in (a) and (b) respectively. $q$ denotes the (112) plane number and $n$ labels the $[111]$ atomic sites.

Figure (6.4) The disregistry of the lattice across a partial twinning dislocation in $\alpha$-iron of type IR. This disregistry, defined in the text, has been calculated for two sets of planes labelled (1)-(0) and (0)-(1) in fig. (6.3)

Figure (6.5) The derivative of the disregistry illustrated in fig. (6.4)

Figure (6.6) An adapted differential displacement map for the partial twinning dislocation structures of fig. (6.3). The sign convention used to illustrate tension and compression is also given. The displacements are $\times 50$. For a complete description of the mapping technique see text.

Figure (6.7) Computed structure of a perfect twinning dislocation of Burgers vector $\frac{1}{6} [11\overline{1}]$ found in both molybdenum and tungsten. $q$ denotes the (112) plane number and $n$ labels the $[11\overline{1}]$ atomic sites.
Figure (6.8) The adapted differential displacement map for the perfect twinning dislocation of fig. (6.7). Displacements $\times 10$.

Figure (6.9) Computed structure of the conjugate (or zonal) twinning dislocation labelled II*. The Frank circuit around the structure is also given where it is shown that the closure failure FS results in a Burgers vector of $\frac{1}{6}[11\overline{1}]$ for the dislocation. Schematic dislocation dissociations involving this structure are also illustrated.

Figure (6.10) Sample V.D.U. plots.

and (6.11)

Figure (7.1) Plot of the binding energy of a single vacancy to a reflection (R) and isosceles (I) type boundary versus (112) plane number $n$ in $\alpha$-iron.

Figure (7.2) The five crystallographically distinct variants labelled 1A, B, C and 2A, B of divacancy orientation at either an isosceles or reflection type boundary. Also illustrated are vacancy pairs $r$ and $i$ which straddle the boundaries and are of neither first or second nearest neighbour type.

Figure (7.3) Plot of the binding energy of a single vacancy across a series of partial twinning dislocations of both IR and RI type in $\alpha$-iron. A and B indicate the maxima in binding energy which are also illustrated in the schematic structure above. The (112) plane along which the binding energy effectively varies is shown bold.
Figure (7.4) Equivalent positions (shown as circles) of binding energy maxima that occur for the two types of twinning dislocation that advance in the [11̅1] direction either by stepping up or by stepping down.
FIG. (1.1) The Interrelationship Between the Twinning Elements
FIG. (3.1) The Interatomic Potentials for Iron, Molybdenum and Tungsten.
FIG. (4.1) Faults on a (112) Plane of a BCC Structure Projected on to a (110) Plane.
FIG. (4.2) Variation of the Energy $\gamma$ of Generalised Faults of Displacement Vector $\alpha/2$ [111] on a (112) Plane.
FIG. (4.3) A Four-Layer \{112\} Isosceles Twin in a BCC Structure.
FIG. (4, 4) Faults on a (112) Plane Showing Nearest Neighbour Bonds p and q.
FIG. (4.5) Relationships Between a Triad of Bond Vectors \( r^i_{\alpha} \)  
\( (\alpha = 1, 2, 3) \) Related by a Three-Fold Axis which is Perpendicular to a Fault Plane \( h^i_1 \).
FIG. (5.1) Two Possible Schematic Structures for a (112) Twin Boundary Shown Projected on to the (110) Plane.
FIG. (5.2a) The Energy $\gamma$ of the Boundary Obtained by Superimposing of Fault $\alpha/2$ [111] on the Twin of FIG. (5.1a).
FIG. (5.2b) Enlarged Section \((0 \leq \alpha \leq \frac{1}{3})\) of the Relaxed Energy \(\gamma_r\) of FIG. (5.2a).
FIG. (5.3a) Curves Defining the Symmetric Normal Displacements $\pm v_n[112]$ of (112) Planes on Either Side of a REFLECTION Twin.
FIG. (5.3b) Curves Defining the Symmetric Normal Displacements $\pm v_n [112]$ of (112) Planes on Either Side of an ISOSCELES Twin.
FIG. (5.4) Twin Boundary Energy $\gamma$ of the Reflection (R) and Isosceles (I) Twins as a Function of Volume Increase $\psi$. 
FIG. (5.5) Schematic Dissociation of BCC Twinning Dislocations.
FIG. (6.1) General Step in Interface.
FIG. (6.2a,b) The Frank Circuits Around Perfect Twinning Dislocations in a BCC Structure.
FIG. (6.2c,d) The Frank Circuits Around Partial Twinning
Dislocations in a BCC Structure.
FIG. (6.3a) Computed Core Structure of a Partial Twinning Dislocation of Type IR in α-iron.
FIG. (6.3b) Computed Core Structure of a Partial Twinning Dislocation of Type RI in α-iron.
FIG 6.3a: Across the IR Partial Twinning Dislocation of FIG. 6.3a
FIG. (6.5) The Derivative of the Disregistry shown in FIG. (6.4)
FIG. (6.6a) The Differential Displacement Map for the IR Partial Twinning Dislocation.
FIG. (6b) The Differential Displacement Map for the RI Partial Twinning Dislocation.
FIG. (6.7) Computed Core Structure of a Perfect Twinning Dislocation in Molybdenum and Tungsten.

\[ \begin{array}{ccc}
1 & 2 & 3 \\
(n+1) & (n+1) & (n+1) \\
(n+1) & (n+1) \\
(n+1) \\
(n+1) \\
\end{array} \]
FIG. (6.8) The Differential Displacement Map for the Perfect Twinning Dislocation of FIG. (6.7).
\[ \frac{1}{2} [111] \rightarrow \frac{1}{12} [111] + \frac{1}{12} [111] + \frac{1}{6} [111] + \frac{1}{12} [111] + \frac{1}{12} [111] \]

FIG. (6.9) Computed Core Structure and Frank Circuit Around the Zonal Twinning Dislocation II*. 

(a) 

(b) 

(c) 

(d)
FIG. (6.10) Tektronix V.D.U. Plot: A Twinning Dislocation.
FIG. (7.1) The Variation of the Binding Energy $E^B_{TV}$ of a Single Vacancy to a Reflection (R) & Isosceles (I) Twin.
FIG. (7.2) The Crystallographically Distinct Divacancy Orientations in the Vicinity of an Isosceles and Reflection Boundary.
FIG. (7.3) The Binding Energy $E_{TV}^B$ of a Vacancy Across a Series of Partial Twinning Dislocations in Iron.
FIG. (7.4) Equivalent Positions (shown as circles) of Binding Energy Maxima That Occur for the 2 Types of Twinning Dislocation That Advance Along [111] Either by Stepping Up or by Stepping Down.