ASPECTS OF INTERPHASE BOUNDARY STRUCTURE IN DIFFUSIONAL PHASE TRANSFORMATIONS

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Abstract—Distinctions among fully coherent, partly coherent and incoherent interphase boundaries are presented. Introduction of a single linear misfit compensating defect is concluded to represent the most useful definition of the transition between fully and partly coherent interfaces. The limit between partly and fully incoherent interphase boundaries is taken operationally as the absence of detectable misfit accommodating defects (i.e., localization) at the interface by high-resolution transmission electron microscopy. An answer to the question of whether or not a precipitate crystal can be fully or partly coherent at one or more boundary orientations and incoherent at others is developed. © 2000 Acta Metallurgica Inc. Published by Elsevier Science Ltd. All rights reserved.

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1. INTRODUCTION

The structure and properties of interphase boundaries have been of scientific interest for many years due to their importance in fields such as phase transformation and composite materials [1, 2]. In this paper, the principal types of interphase boundary structure at interfaces between crystalline solids, namely fully coherent, partly coherent and incoherent, are described, first in summary and then in more detail. The structural differences that separate fully coherent from partly coherent, and with more difficulty, partly coherent from incoherent, are considered. Finally, the question of whether a given precipitate crystal nucleated and grown intragranularly during a diffusional phase transformation can have different types of interfacial structure at some orientations than at others is examined and answered in the affirmative.

2. THE MAIN TYPES OF INTERPHASE BOUNDARY STRUCTURE IN CRYSTALLINE SOLIDS

At the present time, three general types of interphase boundary structure are widely recognized: fully coherent (or commensurate), partly coherent (sometimes termed partially coherent, semi-coherent or discommensurate) and incoherent (also termed disordered or incommensurate). The case of commensurate in one direction only can either be semicoherent or incoherent. We consider locally planar boundaries remote from end effects to avoid the complexities in strain fields as well as of configurations at triple lines, quadruple points and surface intersections.

A fully coherent interface is one in which the first plane of the matrix phase has the same atomic configuration as would the plane in the precipitate phase which would be present if the precipitate lattice were extended by one more layer. The interface planes can differ in their physical dimensions to an extent no greater than that which can be accommodated elastically (even if such accommodation is only temporary). Thus atomic dimensions in the precipitate are always continuous through the matrix at such a boundary even though such continuity is often accompanied by a change in direction. Sutton and Balluffi [2] describe a fully coherent interface as one across which continuity of the reference lattice is maintained and from which “anticoherency” [3] or misfit dislocations are absent.† The reference lattice

† Local uniform translations of less than an interatomic distance, in or normal to an interface, are possible without disrupting the contiguity of the crystal lattices. In general, such translations, while maintaining coherent matching of lattice sites, move the lattice sites so that they no longer coincide with atom sites. This situation is discussed in detail by Bollmann [42]. A convenience in such cases, followed
can be described as a perfect bicrystal in which thermal strains and elastic gradients are suppressed. In the present context, the concept of “full subcoherency” is required for the case of oxides and other non-metallic materials whose structure is built up from two or more sublattices differing in periodicity [4]. For example, at FeO/Fe₂O₃ interfaces, the anion sublattice may exhibit subcoherency while the cation sublattice exhibits subincoherency. (Although not explicitly discussed in succeeding paragraphs on partly coherent and incoherent interfaces, the presence of the sublattice equivalent of each of the other two major categories should be taken as implicit.)

A partly coherent interface differs from a fully coherent interface only in that interruptions of continuity occur through the appearance of linear, misfit compensating defects at the interphase boundary. (Use of Christian’s [5] term “partly” is made in order to avoid possible confusion with partial dislocations engendered by the term “partially coherent” and to circumvent the problem of defining what is half-coherent when “semi-coherent” is used.) In local equilibrium, that is with no long-range strain fields, these defects comprise dislocations or disconnections [6, 7]. The dislocations include misfit dislocations, and arrays of dislocations that produce both tilt and twist in the interface. Tilt dislocations may belong to only one of the adjoining phases (as in oxidation [4]). When the disconnections have both ledge character and dislocation or disclination character, they are operationally called structural ledges (or transformation dislocations). Pure ledges may have local dipole fields but no long-range elastic strain fields.

Lastly, relaxed incoherent boundaries are those at which there is no regular continuity of directions across the interphase boundary and no discernible elastic strain fields. Extrinsic dislocations can enter such a boundary and create a local strain field prior to relaxation of the configuration to a strain-free state. Sutton and Balluffi [2] describe an incoherent interface as one in which the spacing of the misfit or anticoherency dislocations is comparable to the width of their cores, in contradistinction to partly coherent interfaces, wherein this spacing is significantly greater than the core width.

Here, we follow the Sutton–Balluffi [2] definitions. However, we add to their work by showing that there are three classes of incoherent interfaces between two phases. We also discuss transitions from one type of interface to another and show that transitions among the types are functions not only of lattice misfit, but also orientation relationship and apparent habit–plane orientation.

3. TYPES OF PARTLY COHERENT INTERPHASE BOUNDARIES

The various types of partly coherent interphase boundaries are now discussed from the standpoint of their crystallographic description. In respect of the conjugate habit planes, apparent rather than atomic habit planes are employed for convenience in defining conjugate habit planes. Discussions of partly coherent boundary structure are conducted within this framework. This approach is particularly useful in a practical sense since crystallographic descriptions are often used to discuss the structure of these boundaries in the absence of any TEM evidence on their actual structure.

3.1. Rational orientation relationship (OR) and rational conjugate habit planes (CHPs)

When both of these characteristics can be described with rational or low-index parallel planes whose atom patterns and spacings match closely enough so that they be made coherent by inserting at least two arrays of periodically and appropriately spaced misfit dislocations into the planar boundary, the boundary exhibits this type of partial coherency. The simplest type of partly coherent interphase boundary obtains when both matrix and precipitate have either the fcc or the bcc structure (or a minor variant thereof). In this situation, the OR is such that all planes and directions in both phases are parallel, with pairs of identical (hkl) planes forming the CHPs. When the lattice parameters of the two phases differ, the misfit is compensated by (usually) two arrays of misfit dislocations. The boundaries between (fcc-CaF₂) UC₂ and (fcc-NaCl) UC [8], at which the misfit dislocations are of type a<100>, provide a good example of this type of partial coherency. (This also appears to have been the first publication of an interphase boundary structure formed during precipitation from solid solution.) A more recent example is furnished by the precipitation of a (fcc) Ag-rich phase from a (fcc) Ag–Cu matrix [9].

For pairs of lattices which have different stacking sequences (the category of primary interest in this paper), fcc and bcc lattices with the Kurdjumov–Sachs (K–S) OR, i.e., {111}fcc/⟨110⟩bcc and ⟨110⟩fcc/⟨111⟩bcc and whose CHPs are the same as the parallel planes of the OR [10], is an example of this type, in which the misfit dislocations are again emplaced in a planar boundary. Precipitation of bcc Cr-rich crystals from dilute fcc Cu–Cr alloys [11] provides a possible example of this type of partly coherent structure under different-stacking-sequence conditions. In none of the examples cited are ledges an intrinsic component of the interphase boundary structure.

3.2. Rational OR and irrational CHPs

In this situation, the irrational CHPs tend to decompose, when examined with TEM of sufficient resol-
tion, into a ledge structure. The broad faces of ferrite sideplates in steel provide a good example of this type of fcc:bcc partly coherent structure [12, 13]. This structure consists of one array of misfit dislocations and one of structural ledges. The structural ledges are of constant height, three {111} layers, and have a sufficiently uniform spacing so that they yield well-defined irrational CHPs. When the parallel {111}bcc and {110}bcc planes are rotated with respect to an axis defined irrational CHPs. When the parallel {111}fcc of constant height, three {111} layers, and have a sufficient structural consists of one array of misfit dislocations of fcc:bcc partly coherent structure [12, 13]. This sideplates in steel provide a good example of this type.

In all such cases, the apparent habit plane is irrational. Another example of this type is provided by the precipitation of (B2) TiAl from (hcp) α Ti–Al–Mo solid solution [14]. Lenticular precipitates perforce have variable irrational CHPs and may fit into this category in many cases.

3.3. Irrational OR and rational CHPs

No example of this type is presently known to us for precipitation from solid solution. However, during the massive transformation in near-TiAl alloys, where (hcp) α→(fcc) γm TiAl, a {111}γm plane is sometimes found in contact with an irrational α plane [15, 16].

3.4. Irrational OR and irrational CHPs

Plates of the (9R) α, transition phased formed in the partially B2 ordered β matrix of Cu–Zn and Cu–Zn–X alloys have a (2 11 12)β habit plane [17, 18] and an irrational OR: (009)0<009> 5.5° from (101)0, (141)0<141> 5.5°((011)0, (115)0<115> 5.5°(0.5°) from (110)0. However, this interface is initially fully coherent, acquiring dislocations at a later reaction time [20]. Probable examples of this situation were found in a study of hcp grain-boundary α allotriomorphs precipitated at bcc β grain boundaries in a Ti–Cr alloy [21]. Each of the many allotriomorphs examined at β grain faces had an exactly or nearly rational OR with respect to one β grain forming a face and an irrational OR with respect to the other grain. The apparent habit plane at the irrationally oriented interface was especially variable. However, the types of defect structure found at both the rationally and irrationally oriented interfaces were the same; both were usually based upon CHPs consisting of {110}β//{0001}α, <111>β=<1120>α. During current research [22], a clear-cut example of this situation was discovered in the hcp α→fcc γm massive transformation in a near-TiAl alloy. In a particular example of an interface which was planar when studied with CTEM, the OR was near: (221)0<221>γm and [012]0<210>γm and the apparent habit plane varied from (242)γm to (241)γm, displaying various degrees of one-dimensional commensurability. In both this massive transformation [23, 44] and in the crystallographically equivalent massive transformation of τ MnAl [24], a large proportion of the many interfaces examined fell in this category (when the apparent CHPs were determined with CTEM).

These descriptions should make clear that while a rational OR can correctly identify partly coherent interphase boundaries (most if not all of which are presumably fully coherent during the early stages of growth), an irrational OR and/or CHPs cannot reliably predict the presence of an incoherent boundary. A considerably more intensive TEM study of interfacial structure is required before a possibly incoherent boundary can be unambiguously identified.

From the standpoint of diffusional phase transformations, all of the variants of partly coherent interfaces which require a change in stacking sequence across the interphase boundary, e.g., a significant shape deformation of the lattice, have at least one characteristic in common: they act as significant barriers to growth. Such barriers must be surmounted by some form of ledge mechanism. The barriers are provided by the coherent regions between misfit compensating defects. Movement of an atom (or group of atoms) off lattice sites to form the adjacent crystal structure requires a substantial increase in strain energy [25], which, except when the crystal structure is the same on both sides of the boundary, requires a very high activation enthalpy for movement. When first proposed, the coherent regions were taken to consist of accurately matched rational planes. However, the finding just noted that irrational habit planes can also serve as a barrier to growth, as demonstrated by their faceted shape, requires broadening of this statement to include any pair of planes with a sufficiently high atomic density and sufficiently good matching between them so that they still form an essentially impenetrable barrier to atomic movement through them.

4. THE DISTINCTION BETWEEN FULLY AND PARTLY COHERENT INTERPHASE BOUNDARIES

For widely spaced defects, the consequences for misfit reduction are the same whether a dislocation is of the misfit type or is part of a disconnection. We consider such defects first, without regard to the particular dislocation type. For a small, fully coherent precipitate with the same crystal structure as the matrix (or a long-range ordered version thereof) but sufficient misfit and size so that its free energy is reduced by the incorporation of, say, a single dislocation loop [26], the effect of introducing this loop upon the TEM image of the precipitate is remarkable. In the absence of the loop the strong coherency strain associated with the precipitate is often sufficient to make its outline difficult to discern [26, 27]. The Ashby–Brown [26] contrast developed in this situation exhibits a relatively thick line of no-contrast across a diameter.
of the precipitate under two-beam diffracting conditions. However, once a single dislocation loop with prismatic character is incorporated into the interface and girds the particle, the Ashby–Brown contrast disappears and the size and shape of the precipitate are readily discerned, even though misfit compensation is incomplete. The same situation applies for plate-shaped precipitates, when a loop girds the particle so that each planar interface contains a single misfit dislocation [28]. Hence, introduction of a single, bounding dislocation loop is considered to convert a fully to a partly coherent interphase boundary.

5. THE TYPES OF INCOHERENT INTERPHASE BOUNDARIES

As in the case of partly coherent boundaries, different types of incoherent boundaries can be identified. Although different in their atomic details, the three types of boundary to be described should offer no significant barrier to migration over most if not all of their area.

5.1. Irrational OR, no rational CHPs

For this type of boundary, illustrated in Fig. 1, most or all of the atoms are unmatched across the interface, both parallel and perpendicular to the viewing direction. In general, boundaries such as that in Fig. 1 have no periodic structural repetition. In special cases, the boundary may have periodic structural repetition but the misfit is so large that there is core overlap of the misfit dislocations and most of the atoms are unmatched: the dislocations are smeared into a vernier configuration. Ledges are unnecessary at such boundaries from the standpoints of both energy minimization and migration. This type of boundary is expected to have a high energy, in a manner parallel to that of a random high-angle grain boundary [29].

5.2. Irrational OR, rational habit plane only in one phase

This type of incoherent boundary is illustrated in Fig. 2. There may be some periodic structural repetition at the boundary but the strain is likely to be large and one expects the dislocations present to be spread out into continuous infinitesimal dislocations, so that a planar interface would have no discernible strain field. This type of interface may have a lower energy than the preceding type of incoherent boundary, primarily because of the reduced energy associated with the low-index interface plane. Crystallographically, it is similar to an asymmetrical high-angle grain boundary.

5.3. Rational OR in at least one direction, ill-matched rational habit planes

This type of incoherent boundary, illustrated in Fig. 3, displays no atom matching even though low-index rational planes are parallel across the boundary in both phases. In the example shown in Fig. 3, the juxtaposition of low-index planes requires the phases to have a rational orientation relationship in the direction parallel to the interface normal, even though there may be no parallel low-index directions within the interface, as also shown in Fig. 3. This type of boundary is similar in a sense to a high-angle twist grain boundary. However, because the matrix and
Fig. 3. Geometric atomic model of an incoherent interphase boundary between the same bcc and fcc crystals as in Fig. 1, but with a rational orientation relationship in the direction perpendicular to the low-index (011)_{bcc} and (111)_{bcc} conjugate habit planes. The orientation relationship between the two crystals is: (011)_{bcc}//(111)_{fcc} and [511]_{bcc}//[347]_{fcc}, the interface plane is (111)_{fcc} and the viewing direction is [347]_{fcc}. The (011)_{bcc} and (111)_{fcc} planes are parallel so $q=0^\circ$, as indicated in the figure. Note that $\theta$ does not represent the angle of twist in the plane of the interface, but the angle of inclination between the close-packed planes in the two crystals.

product planes may have different symmetries and lattice parameters across the boundary, simple coincident site orientations that may occur with rotation are often far apart or only quasiperiodic [2] at best, so that atomic matching is minimal and complete relaxation of the phases across the boundary leads to incoherency. This is illustrated in Fig. 4, where the two ill-matched planes across the interface in Fig. 3 are viewed normal to the interface. It is tempting to speculate that such a boundary may not remain confined to a single interface plane with little atomic matching, but instead, is spread over a finite width, so that one phase transitions into the other. This has been shown to occur at a martensite interface [30]. It may also be possible that a liquid-like phase forms at the interface at high temperatures, as predicted by molecular-dynamics simulations for high-angle tilt/twist grain boundaries in fcc metals [31]. In any case, this boundary is expected to have a relatively high energy, although possibly lower than the previous two types of incoherent interphase boundary.

Another point of interest in Fig. 3 is that if the two crystals forming the interface are rotated so that they have parallel low-index directions, as illustrated in Fig. 5, the boundary is still incoherent but is now rational.

6. THE DISTINCTION BETWEEN PARTLY COHERENT AND INCOHERENT INTERPHASE BOUNDARIES

The problem of distinguishing between partly coherent and incoherent interphase boundary structures is difficult. It parallels the problem of distinguishing between low-angle, high-angle and random grain-boundary structures [2, 32–34], though it is often more complicated because there may be different lattice types across the interface. Where then
should the boundaries between the various partly coherent and incoherent structures described in the preceding sections be drawn?

In the case of low-angle grain boundaries, primary dislocations with lattice translation Burgers vectors are readily discernible by strain contrast TEM. As the misorientation between two grains increases and a high-angle grain boundary forms (at approximately 15° misorientation), the primary dislocation cores approach one another and become indistinguishable by TEM [34]. High-angle grain boundaries can be described by coincident site lattice (CSL) or structural-unit models, where secondary dislocations with displacement shift complete (DSC) Burgers vectors accommodate the mismatch in the grain boundary as a function of misorientation. These defects are also discernible by strain contrast TEM until the misorientation increases such that they too become invisible. In order to determine if there is still atom matching or some structural periodicity in the grain boundary, one must employ HRTEM techniques [29, 34, 35]. Eventually, when there is no structural periodicity within the limits of HRTEM observation, a grain boundary may be considered random or incoherent. By analogy, for interphase boundaries the limit to a partly coherent structure might thus be set as that corresponding to the minimum discreteness in the Burgers vector distribution for detectability with HRTEM.* An alternate HRTEM-based definition is the absence of detectable misfit localization at the interface. Because of the periodicity of atomic planes on opposite sides of the boundary, dislocations might be considered to be present in a formalistic Burgers vector or vernier sense; however, if local relaxations do not attend these dislocations then the interface may be regarded as structurally incoherent. However, the question of how little local relaxation is required in order that the boundary may be regarded as incoherent makes this alternative criterion of lesser operational value than the former one.

7. CAN AN INTRAGRANULAR PRECIPITATE BE FULLY OR PARTLY COHERENT AT SOME BOUNDARY ORIENTATIONS BUT INCOHERENT AT OTHERS?

An important aspect of interphase boundary structure that is directly related to the discussion of incoherent structures above, is whether a precipitate crystal can be fully or partly coherent at one or more boundary orientations and incoherent at others. This has been a topic of controversy in the phase transformations literature [36–40] and may be particularly important with regard to the massive transformation, where the product phase often has an irrational OR with the matrix and is bounded by a variety of interface planes. As demonstrated by comparison of Fig. 3 and Fig. 6, it is possibly to cause an interface plane between two phases to vary from incoherent, as in Fig. 3, to commensurate in one (the x) direction, as in Fig. 6, by rotating the interface plane approximately 40° counterclockwise with the OR held constant. In this example, the atom matching in the z direction remains incommensurate so that the interface remains incoherent. However, by varying the bcc/fcc lattice parameters, one can create an interface analogous to that in Fig. 6 that is commensurate in the x direction and has patches of coherent regions separated by misfit dislocations with lines parallel to the x direction to remove misfit in the z direction. Hence, such an interface would be partly coherent. This example illustrates the point that atom matching across the interface depends on the interface plane, and not just on the orientation relationship between the two phases. This change in boundary structure is possible because the interfacial structure varies with boundary orientation. In the case of an intragranular precipitate with a low-symmetry crystal lattice, possibly only one boundary orientation would support full coherency during nucleation and the early stages of growth and partial coherency later in the transformation process, whereas other boundary orientations would mainly be represented by some form of partly coherent or incoherent structure. A useful analogue to this problem in homophase boundaries is that of a Σ3 twin [41], with a coherent (111) interface, and a partly coherent (112) interface that can be considered incoherent (in the real crystal lattice because of twinning dislocation core disruptions [2]) or coherent (in

* Even when the OR is irrational, it is usually possible to align the interface parallel to the electron beam and to image some lattice planes in both phases.
the DSC lattice [42]). We find the latter definition more appealing. In the real crystal lattice the (112) interface still has one lattice site in three in coincident positions so, rather than strictly incoherent, it could be thought of as having another form of subcoherence. The DSC coherent definition is unambiguous and reflects the Σ3 matching. The coherent (111)hcp/(0001)hcp interface and partly coherent (112)hcp/(1010)hcp interface that is coherent in the DSC reference lattice in the fcc to hcp transformation [43] is a similar example for an interphase interface. Thus we conclude that it is possible for a precipitate to be fully coherent at some boundary orientations while being only coherent in the DSC lattice when its crystal structure differs from that of the matrix phase.

A related question is whether a precipitate (or interface) can be considered incoherent based on only the orientation relationship between two crystals. In other words, is it correct to conclude that a precipitate (or interface) is incoherent based on a random orientation relationship between two phases in a selected-area diffraction pattern in the TEM, as is often done in the literature? Examination of Fig. 6, where there is an irrational relationship between all but the x direction (i.e., the two crystal directions [011]bcc and [111]bcc), but the interface is clearly commensurate along one direction (in this case [703]), suggests that such a conclusion is not definitive. The degree of coherency depends on the orientation of the interface plane with respect to the two crystals when their lattices are different, and it is not possible to evaluate coherency without accounting for this relationship and the corresponding interfacial structure of the boundary.

8. CONCLUSIONS

The distinctions among fully coherent, partly coherent and incoherent interphase boundaries are presented. Three types each of partly coherent and of incoherent boundaries are identified. The partly coherent boundaries always contain significant areas of coherency whereas the incoherent boundaries do not. The main operational differences among these three classifications when a difference in stacking sequence occurs across the interphase boundary, i.e., when a shape change accompanies the transformation, is that fully coherent boundaries completely halt growth, partly coherent boundaries hinder growth when growth ledges are present and halt growth in their absence, and incoherent boundaries allow essentially unimpeded growth.

Introduction of a single linear misfit compensating defect is concluded to represent the most useful definition of the transition between fully and partly coherent interfaces. The limit between partly and fully incoherent interphase boundaries is taken operationally as the absence of detectable misfit accommodating defects (i.e., localization) at the interface by HRTEM.

The question of whether or not a precipitate crystal can be fully or partly coherent at one or more boundary orientations and incoherent at others is resolved. The dependence of interfacial structure on boundary orientation can cause a transition from fully to partly coherent to incoherent for a constant orientation relationship between two phases.

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