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Fundamental Studies of Beta Phase Decomposition Modes in Titanium Alloys

by

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Y. Mou, Graduate Student
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31 March 1992

TABLE OF CONTENTS

Fundamental Studies of Beta Phase Decomposition Modes in Titanium Alloys

ABSTRACT

Throughout this final grant from AFOSR, the P.I. spent much of his time in the preparation of generic overviews of numerous major topics in diffusional phase transformations. These overviews dealt with homogeneous nucleation, interphase boundary structures in Ti-base alloys, effects of interphase boundary structure upon growth kinetics, shear vs. diffusional transformation mechanism (with emphasis upon linking macroscopic observations with processes proceeding at the atomic level), the mechanism (and definitions) of the bainite reaction and the influence of alloying elements upon the growth kinetics of grain boundary allotriomorphs of proeutectoid ferrite. A major overview of the ledge mechanism in vapor→crystal, liquid→crystal and crystal→crystal diffusional phase transformations, and a still broader overview of atomic mechanisms of diffusional nucleation and growth are nearing completion. Collaborative research with Dr. M. G. Hall of the University of Birmingham, U.K., on topics concerned with distinction between diffusional and shear mechanisms of transformation from the standpoints of crystallography and surface relief effects, has also made progress. The Ph.D. thesis of Yiwen Mou on the (bcc)β→(hcp)ξ_m massive transformation in a Ag-26 A/O Al alloy has just been successfully defended. A major objective of this program, established at its inception in 1973, i.e., determination of whether the structure of the interphase boundaries between the product of a massive transformation and its matrix phase is partially coherent or disordered, was accomplished through this research. Irrespective of whether the β/ξ_m orientation relationships are rational or irrational, these interfacial structures were found invariably to be partially coherent. Additionally, and perhaps even more importantly, major extensions of the Bollmann O-lattice model were made which now permit prediction, for the first time, of the structure, spacing, height and orientation of both misfit-compensating ledges and structural ledges.

1. INTRODUCTION

This report is the last on a program which began in 1973 when the P.I. was a professor at Michigan Technological University. The focus of the program from the beginning has been discernment of the fundamental mechanisms of the bainite reaction and of the massive transformation in binary metallic alloy systems. Initially, Ti-X alloys were used as vehicles for both portions of this program. Subsequently, a Ag-26 A/O Al alloy was substituted for Ti-X alloys as a model for the massive transformation studies, simply because the Ti-X alloys in which a massive transformation occurs have M_s temperatures well above room temperature--and the kinetics of the massive transformation in these alloys are uncontrollably rapid. In the present, concluding report period of this nearly 20 year program, the ultimate result of the massive transformation program is reported: as predicted 25 years ago from considerations of nucleation theory (1), the massive:matrix interfacial

structure is partially coherent, rather than incoherent or disordered as originally deduced by Massalski (2,3).

Following completion of the Hwack Joo Lee Ph.D. thesis on the bainite reaction in a number of Ti-X systems, attention has been turned toward the generic ramifications of the experimental results obtained during this and preceding studies of the bainite reaction in Ti-X alloys, mainly conducted through this program, and of the bainite reaciton in other non-ferrous alloy systems and steel, reported in the literature and from other programs previously led by the P.I. At the invitation of the Program Manager, Dr. A. H. Rosenstein, the P.I. has now devoted most of his efforts to the preparation of generic overviews on a variety of inter-related topics, all connected with either those of this Grant or other related (NSF or ARO) Grants previously held. Particularly since additional requests to prepare such overviews have appeared since this last report period began, and at least one of the efforts has grown very large--and tedious--indeed, the P.I. has spent an additional six months at CMU after this Grant's funds expired, using his own resources. This self-funded extension has also permitted Mr. Mou's O-lattice analyses and TEM observations of massive:matrix interfacial structures to be enlarged to an important extent.

One of the central interests of this Grant has been a persistent effort to contribute to resolution of the question of whether plate-shaped transformation products which are not obviously martensite plates grow by means of a diffusional or a shear mechanism at the atomic scale. Having perceived that the diffusionist experimental results and interpretation on this vital issue are not receiving adequate attention in the literature, the author, in collaboration with Prof. C. M. Wayman (Univ. of Illinois at Urbana-Champaign) in particular but also with Prof. J. P. Hirth (Washington State Univ.) and Dr. B. B. Rath (Naval Research Laboratory) has organized a symposium entirely on exactly this topic under the sponsorship of the ASM-MSD Phase Transformations Committee. This symposium will be held at the Kona Hilton Hotel, Kona, Hawaii, Dec. 18-22, 1992. The proceedings of this conference will be published in Metallurgical Transactions A through the Met. Trans. peer review system.

We finally note that, although funds for supporting Dr. Hall's research through this Grant have run out, and Dr. Hall is severely burdened by both a heavy academic load and a wife who is almost a total invalid after partially recovering from a severe stroke, he remains an active participant in efforts to probe issues central to the shear vs. diffusional growth controversy. He will present a paper at the Hawaii conference on this subject.

2. GENERIC OVERVIEWS ON FUNDAMENTAL ASPECTS OF PHASE TRANSFORMATIONS

The topics covered in these overviews and a few notes about each are now presented:

(i) Interphase boundary structures produced during diffusional phase transformations in a wide range of Ti-base alloys (4)--

A goodly proportion of all of these studies turn out to have been performed over the years with the support of this Grant. These include the proeutectoid α reaction in several Ti-X alloys and the bainite reaction as well in some of these systems. (While this review dealt only with our studies on proeutectoid α plates, subsequent work (5) has encompassed grain boundary α allotriomorphs as well, together with a HRTEM investigation of the structure of the broad faces of proeutectoid α plates (6).) Most of the remaining work encompassed titanium hydrides, with zirconium hydrides also being considered in order to flesh out "the data base". From a fundamental point of view, however, what is mainly of interest is the replacement of misfit dislocations, the sole linear misfit-compensating interfacial defect in fcc/hcp transformations (7,8,9) and one of the two such defects in fcc/bcc transformations (10-12), with structural ledges and misfit-compensating ledges, as will be discussed in section 3 of this Report.

(ii) Basic crystallographic and mechanistic features of shear and diffusional mechanism of growth (13,14)--

Growth by shear and by diffusional processes, both taking place predominantly by means of ledge mechanisms are reviewed for the purpose of distinguishing critically between them at the atomic, microscopic, and macroscopic levels. At the atomic level, diffusional growth is described as individual, poorly coordinated, thermally activated jumps occurring in the manner of biased random walk, whereas growth by shear is taken to be tightly coordinated "glide" of atoms to sites in the product phase which are "predestined" to within the radius of a shuffle. Obedience to the invariant plane strain (IPS) surface relief effect and the transformation crystallography prescribed by the phenomenological theory of martensite is shown to be an unsatisfactory means of distinguishing between these two fundamentally different atomic growth mechanisms. In substitutional alloys, continuous differences in composition *and* in long-range order (LRO) from the earliest stages of growth onward are concluded to be the most useful phenomenological approach to achieving differentiation. At a more fundamental level, however, the details of interphase boundary structure are the primary determinant of the operative mechanism (when the driving force for growth is sufficient to permit either to occur). In the presence of a stacking sequence change across the boundary, terraces of ledges are immobile irrespective of their structural details during diffusional growth. Kinks on the risers of superledges are probably the primary sites for diffusional transfer of atoms across interphase boundaries. In martensitic transformations, on the other hand, terraces containing edge dislocations in glide orientation or pure screw dislocations are mobile and accomplish the lattice invariant deformation (LID), though probably only after being overrun by a transformation dislocation. Risers associated with transformation dislocations are also mobile and cause the crystal structure change during growth by shear. The successes achieved by the invariant line (IL) component of the phenomenological theory of martensite in predicting precipitate needle growth directions and precipitate plate habit planes (Dahmen and co-workers) are here ascribed to the rate of ledge formation usually being a minimum at an interface containing an IL, primarily because nuclei formed sympathetically at this boundary orientation are likely to have the highest edge energies. Since martensite plate broad faces also contain the IL, the ability of the phenomenological

theory to predict the habit plane and the orientation relationships of both precipitate and martensite plates is no longer surprising. The IPS relief effect at a free surface can be generated by precipitate plates when growth ledges are generated predominantly on only one broad face and only one of several crystallographically equivalent Burgers vectors of growth ledges is operative. Both preferences probably result from larger reductions in transformation strain energy for the particular geometry with which a given plate intercepts the free surface. Precipitate morphology often differs significantly from that of martensite even if precipitates are plate-shaped and can readily differ very greatly. Whereas martensite morphology is determined by the need to minimize shear strain energy, that of precipitates derives from the more flexible base of the interphase boundary orientation-dependence of the reciprocal of the average intergrowth ledge spacing, as modified by both the orientation-dependence of interkink spacing on growth ledge risers and the spacing/height ratio dependence of diffusion field overlap upon growth kinetics.

(iii) The three main definitions of bainite currently in use and the mechanistic implications of each (15,16)--

The present status of the three principal definitions of bainite currently in use is reviewed. On the surface relief definition, bainite consists of precipitate plates, producing an invariant plane strain (IPS) surface relief effect, which form by shear, *i.e.*, martensitically, at temperatures usually above M_s and M_d. The generalized microstructural definition describes bainite as the product of the diffusional, noncooperative, competitive ledgewise growth of two precipitate phases formed during eutectoid decomposition, with the minority phase appearing in nonlamellar form. This alternative mode of eutectoid decomposition is thus fundamentally different from the diffusional, cooperative, shared growth ledges mechanism for the formation of pearlite developed by Hackney and Shiflet. The overall reaction kinetics definition of bainite views this transformation as being confined to a temperature range well below that of the eutectoid temperature and being increasingly incomplete as its upper limiting temperature, the kinetic B_s, is approached. Recent research has shown, however, that even in steels (the only alloys in which this set of phenomena has been reported), incomplete transformation is not generally operative. Revisions in and additions to the phenomenology of bainite defined in this manner have been recently made. Extensive conflicts among the three definitions are readily demonstrated. Arguments are developed in favor of preference for the generalized microstructural definition, reassessment of the overall reaction kinetics definition, and discarding of the surface relief definition.

(iv) The growth kinetics of disordered vs. ledged partially coherent interphase boundaries (17-19)--

Because the growth kinetics of ledged boundaries can be both complex and non-reproducibile as a consequence of complications in both ledge nucleation and growth, there is a strong tendency to try to ignore the presence of the ledge mechanism altogether (as Hillert has done (20,21)) or to degrade the importance of the operation of this mechanism (in the style of Doherty (22,23)). The advantages and disadvantages of making this simplification, i.e., of assuming that the advancing interphase boundary is disordered

and permits uniform atomic attachment and detachment over its entire area, have been assessed in an overview compiled as an invited paper provided for Prof. Mats Hillert's retirement symposium, held in Stockholm in 1989 (17). Recently, Enomoto and Aaronson (24,25) have examined this question quantitatively on the basis of Enomoto's (26,27) finite element modeling of ledgewise growth and have found that the disordered boundary approximation is good only when the ratio of the inter-growth ledge spacing to the growth ledge height is small, say of the order of 2. When this ratio is 50, long growth times may elapse before disordered boundary growth kinetics behavior is attained. These results emphasize the need to incorporate ledgewise growth directly into analyses of more complex phenomena under many circumstances.

(v) Comparison of measured homogeneous nucleation kinetics with those calculated theoretically in binary metallic alloys (28)--

A comprehensive critical review was made of all papers which could be located in the literature in which homogeneous nucleation kinetics were measured in binary metallic alloys. In nearly all of the investigations reviewed, it was found that measurements of nucleation kinetics had been seriously compromised by overlap of diffusion fields amongst adjacent precipitates and/or by coarsening. Only in Cu-Co alloys were a few valid studies made of homogeneous nucleation kinetics. In these studies, discrepancies of a few orders of magnitude were noted between calculated and measured steady state nucleation rates. These have been ascribed to the extreme sensitivity of the nucleation rate to the nucleus:matrix interfacial energy and the use of inappropriate interatomic force laws for calculating this energy. Otherwise, the theory seems basically sound. This paper will be published as one of a set in Metall. Trans. A as a tribute to the late Prof. G. Marshall Pound, a pioneering researcher and teacher of nucleation in solids.

(vi) The energetics, kinetics and mechanism of ledgewise growth from vapor, liquid and crystalline matrices --

This is intended to be a comprehensive review of the structure, kinetics and to some extent the energetics of ledgewise growth of crystals from all three common states of matter. An effort is also being made to compare key features of ledgewise growth in the various media with one another. This has disclosed a number of possibilities for cross-fertilization. Key mathematical derivations are being presented in some detail. In manuscript form, this paper (originally intended for the ASM Phase Transformation Committee's Fall 1989(!) symposium on "The Role of Ledges in Phase Transformations") is already greater than 160 pages in length. This will lead to some problems in respect of publication--particularly in Metall. Trans., the preferred journal. The P.I. intends to continue work on this 2 1/2 year old "project" at the Naval Research Laboratory until it has been completed and submitted for publication.

(vii) Overview of atomic mechanisms of diffusional nucleation and growth (29)--

This is intended to be the manuscript of the 1990 Institute of Metals Lecture! It is in preparation and should shortly be completed. This effort was repeatedly delayed because it was desired to complete the overview of ledgewise growth first. Failure to do so in timely fashion resulted in the delay in writing up this lecture. In this "super-overview", the lessons learned from a career of research and reading on diffusional nucleation and growth, and arguing about the role (if any) of shear in these processes, will be condensed into a single, relatively brief paper.

(viii) Overview of the nucleation and growth kinetics of grain boundary ferrite allotriomorphs in Fe-C and Fe-C-X alloys (30)--

Prepared for an NRL-ONR-co-sponsored applied ferrous physical metallurgy conference on low-carbon advanced ferrous alloys recently held in New Delhi, India (March 25-28, 1992), this paper overviewed work in which the P.I. has participated at the Ford Scientific Laboratory, Michigan Tech and CMU. The overall conclusion reached is that, even in Fe-C alloys, the level of understanding so far reached of both nucleation and growth kinetics is still very limited, and is even lower in Fe-C-X alloys--thereby making clear the futility of attempting to address ferrite formation kinetics in commercial low carbon steels in a scientific manner at this time. Construction of critical nucleus shapes for bcc nuclei in an fcc matrix at austenite grain faces and measurement or calculation of the relevant interphase boundary energies are the principal foci of work needed to place the situation with respect to nucleation kinetics on a sound basis in Fe-C alloys. Effects of X (a substitutional alloying element) upon interphase boundary and grain boundary energies and critical nucleus shape must be added in the case of Fe-C-X alloys. In the area of growth kinetics, the widely accepted Hillert (20)-Kirkaldy (31)-Coates (32-34) Local Equilibrium model has been repeatedly shown to be unsuccessful (35-38). The less well regarded paraequilibrium model (20,39,40) provides a better, but still inadequate accounting for the experimental data (36-38). A solute drag-like effect (SDLE) (36,41,42) is postulated to be responsible for the differences between the paraequilibrium model and experimental results. Evaluation of the SDLE will require measurements of the X concentration at kinks on the risers of growth ledges. Efforts to accomplish this with the FIM/AP technique have so far proved unsuccessful (43). This essential problem will therefore be further pursued by the author and some colleagues-to-be at NRL using advanced physics-type detection techniques.

3. MASSIVE TRANSFORMATION IN A Ag-26 AT % Al ALLOY

3.1 Introduction

This section deals with the "core" project to ascertain experimentally the structure of β:ξ_m interfaces in a Ag-26 A/O Al alloy. This is being used as a model system through which to investigate the prediction of Aaronson, Laird and Kinsman (1) that massive:matrix interfaces must, on grounds of nucleation theory, be partially or fully coherent.. Subsections 3.2 and 3.3 summarize the final, and most decisive experimental results secured with conventional and with high-resolution TEM, respectively. The remaining

subsections describe the principal results of theoretical analysis of partially coherent bcc:hcp interfaces, accomplished through further development of the Bollmann (44) O-lattice analysis. While this new analysis is applied to the experimental observations on the Ag-Al alloy, it is intended to be general, and with appropriate modifications, should be applicable to any pair of crystal structures.

3.2 Structure of Irrationally Oriented Interfaces

Fig. 1 shows an irrationally related ξ_m:β interface. On the disordered boundary hypothesis, this interface is most likely to be disordered. However, different densities of growth ledges on facets *A*, *B* and *C* can be seen in this micrograph. The existence of growth ledges on irrationally related interfaces implies the presence of a strong interfacial structure barrier, such as would derive from partial coherency (45).

Uniformly spaced ledges were observed in some cases on irrationally related interfaces. Such an interface is shown in Fig. ^. Across this interface the close-packed planes in the two phases deviate by 27°, and the close-packed directions by 9°. Growth ledges, pointed out by larger arrowheads, are distributed irregularly, though their risers are almost linear. A set of regularly arranged ledges, noted by three small arrowheads,is spaced about 6 nm apart. These ledges exhibited strong contrast under both $[0002]_\zeta$ (Fig. 2(a)) and $[10\bar{1}0]_\zeta$ (Fig. 2(b)) reflections and no contrast with the $(0\bar{1}11)_\zeta$ reflection; they were associated with a Burgers vector of $(1/3)[11\bar{1}3]_\zeta$. Another set of uniformly spaced ledges, pointed out by two medium-sized arrowheads in this figure, lay about 10 nm apart and was again found to have a (c+a)-type Burgers vector. The apparent habit plane determined by trace analysis is irrational with respect to both the β and the ζ_m phases, as shown in the $(0001)_{hcp}$ stereographic projection of Fig. 3. Since the Burger vectors of the uniformly spaced ledges have components within the apparent habit plane, these ledges may thus be able to accommodate the mismatch across this interface.

Fig. 5 shows a ζ_m crystal formed at (or associated with) a β sub-grain boundary. The orientation relationship between the ζ_m and the β_1 grain, as shown in Fig. 4, is close to the Potter orientation but with deviations of about 2° between the close-packed planes and of about 6° between the close-packed directions. Since the β_2 grain has an orientation difference of about 7° with respect to the β_1 grain, the orientation relationship between the ζ_m and β_2 is not of a rational type. Rather straight growth ledges are seen to be spaced 25-40 nm apart on the ζ_m:β_1 interface. The somewhat discontinuous contrast of the growth ledges suggests the existence of another set of (presumably) uniformly spaced ledges on this interface.

The interface between the ζ_m crystal and the β_2 grain is gently curved. In the tip area (the right hand side) of this interface, as shown in Fig. 5(a), there are growth ledges (pointed out by big arrowheads) and regularly distributed ledges (noted with two small arrowheads) and regularly distributed ledges (noted with two small arrowheads). In the remaining area, however, only regular distributed ledges can be seen with a riser direction different from that of the regularly distributed ledges in the tip area. In Fig. 5(b), the same

interface was tilted so that the tip area was at almost an edge-on position. Two sets of regularly distributed ledges are now seen in the remaining area of the interface (pointed out by two small and three medium arrowheads, respectively). Since the regularly distributed ledges in the tip and the remaining area are all associated with kinks (Fig. 5(a)), it is likely that another set of regular ledges also exists in both areas. Close examination of the left hand side of the interface in Fig. 5(a) reveals that the spacing between the regularly distributed ledges gradually changes, from about 6 nm to 10 nm, with boundary orientation. The contrast behavior of the ledges on the left hand side of the interface in Fig. 5 suggests, again, a (c+a)-type Burgers vector. Since the misfit across the ζ_m:β_2 interface gradually changes with the boundary orientation, it is understood that the interledge spacing is accordingly altered.

3.3. High-Resolution TEM Observations of Interfacial Ledges

Fig. 6 shows a high-resolution micrograph taken at the $[11\bar{2}0]\zeta//[111]\beta$ foil orientation. The close-packed planes, $(0001)\zeta$ and $(0\bar{1}1)\beta$, however, deviated by about 7° from parallelism with respect to each other. Three ledges can be seen at the interface shown in this micrograph. They are spaced about 12.5 nm apart and are 12-14 atomic layers high (in the ζ_m phase). Although the orientation relationship slightly deviates from the exact Burgers, the atomic habit plane is seen to be $(1\bar{1}00)\zeta$, identical to the hcp component of the conjugate habit planes for the Burgers relationship. This situation is thus similar to the Burgers$(1\bar{1}00)\zeta//(2\bar{1}\bar{1})\beta$ interface modeled in Section 3.4.2. The model-predicted riser height in the Burgers case is 16 hcp atomic layers (2 nm), and the predicted interledge spacing is 15.0 nm. The observed shorter interledge spacing likely arises from the deviation from parallelism of the close-packed planes in the two phases in the present situation.

To reveal the detailed structure of these misfit-compensating ledges, one of the ledges in Fig.6 is enlarged as shown in Fig. 7. At the atomic level, the riser of this ledge appears to be composed of one riser of 8 atomic layers height and some others 2 atomic layers high. This separation of risers may result, again, from the slight deviation of the close-packed planes. The atom positions in Fig. 7 were not resolved very well due to the presence of an angle of about 1° between $[11\bar{2}0]\zeta$ and $[111]\beta$. However, a Burgers circuit may still be drawn through some atom positions close to the interface. The result of this analysis indicates that a Burgers vector of $(1/2)[0001]\zeta$ is associated with the central risers. This is the Burgers vector predicted by the misfit-compensating ledge model for Burgers-related $(1\bar{1}00)\zeta//(2\bar{1}\bar{1})\beta$ interfaces.

The atomic matching across a terrace plane on this interface is shown in Fig. 8. Some `ledges' are seen at the terraces of misfit-compensating ledges, as noted with thin lines in this figure. These `ledges' may result from the deviation between the close-packed planes. It is suggested that these `ledges' can compensate for the additional mismatch produced by the deviation between the $(2\bar{1}\bar{1})\beta$ and $(1\bar{1}00)\zeta$ planes. On this basis the mismatch approximately along $[0001]\zeta$ can be accommodated by the misfit-compensating ledges just discussed.

3.4 O-Lattice Modeling of Ledged Bcc:Hcp Boundaries

3.4.1. Extension of the Bollmann O-Lattice Theory

In the Bollmann O-lattice analysis (44,46,47), as applied to modeling the structure of interphase boundaries, two crystal lattices, (1) and (2), are juxtaposed with a coincident atom position as the origin and a relative rotation defined by the orientation relationship. These two crystal lattices then become interpenetrating lattices (44,48), and a best-matching position, or an O-point is determined by the basic equation (44,46):

$$(\mathbf{I} - \mathbf{A}^{-1})\mathbf{x}^{(0)} = \mathbf{b}^{(L)} \tag{1}$$

where **I** is the identity matrix, $\mathbf{x}^{(0)}$ is the O-lattice vector defining the O-point, $\mathbf{b}^{(L)}$ can be any of the lattice vectors in crystal lattice (1), and **A** is the transformation matrix and has the form[44]:

$$\mathbf{A}=\mathbf{R}\mathbf{S}^{(2)}(\mathbf{S}^{(1)})^{-1} \tag{2}$$

where **R** is the rotation matrix determined by the orientation relationship between the two crystal lattices, and $\mathbf{S}^{(1)}$ and $\mathbf{S}^{(2)}$ are the structure matrices determined by the base vectors in the two crystal lattices.

Fig. 9 shows the hcp and bcc unit cells chosen for the O-lattice construction (49) emphasizing that there are two atoms in each of the unit cells: $\mathbf{H}_1$ and $\mathbf{H}_2$ in the hcp and $\mathbf{B}_1$ and $\mathbf{B}_2$ in the bcc unit cell. Each of the two structures can thus be divided into two subsets of atom positions. The complete matching situation between the two structures which provides information for prediction of interfacial structures is then examined by means of four subset combinations, *i.e.*, $\mathbf{H}_1$-$\mathbf{B}_1$, $\mathbf{H}_1$-$\mathbf{B}_2$, $\mathbf{H}_2$-$\mathbf{B}_1$ and $\mathbf{H}_2$-$\mathbf{B}_2$. However, Eq. 1 can be used only for the O-lattice construction of the $\mathbf{H}_1$-$\mathbf{B}_1$ combination. This is the case treated in previous investigations (49-52).

The Bollmann O-lattice theory is now extended to permit use of the other three combinations by incorporation of appropriate translation vectors in their O-lattice construction. Fig. 10 shows a simplified two-dimensional example of this situation. The **A** structure consists of only **A** positions, whereas the **B** structure is composed of two subsets of atom positions, $\mathbf{B}_1$ and $\mathbf{B}_2$. A translation vector **t** is used to express the relative positions of $\mathbf{B}_1$ and $\mathbf{B}_2$. If O_1, a coincident site of an **A** and a $\mathbf{B}_1$ position, is chosen as the origin, the O-lattice will be composed of the $\mathbf{AB}_1$ coincident sites. (Because the lattice parameter ratio in this simplified example has been chosen as a simple fraction, the O-lattice is identically a coincident site lattice (44).) However, O_2, an $\mathbf{AB}_2$ coincident site, could equally well have been chosen as the origin; thus the $\mathbf{AB}_2$ positions are also O-points.

The coincidence condition (44) for the **A-B$_2$** combination thus needs to be considered between $\mathbf{x}^{(2)} + \mathbf{t}$ (instead of $\mathbf{x}^{(2)}$) and $\mathbf{x}^{(1)}$. These are position vectors in the two crystal lattices. The new coincidence condition has the form:

$$\mathbf{x}^{(2)} + \mathbf{t} = \mathbf{x}^{(1)}) + \mathbf{b}^{(L)} = \mathbf{x}^{(0)} \tag{3}$$

P_2 is now an additional best-matching position. Under the new coincidence condition Eq. 1 becomes:

$$(\mathbf{I} - \mathbf{A}^{-1})(\mathbf{x}^{(0)} - \mathbf{t}) = -\mathbf{t} + \mathbf{b}^{(L)} \tag{4}$$

With appropriate translation vectors determined from Fig. 9, the O-lattices achieved by the other three combinations can also be obtained. The additional best-matching positions provided by these O-lattices will now be used to predict misfit-compensating ledges.

3.4.2. Modeling of Misfit-Compensating Ledges

When the additional best-matching positions thus recognized form some additional O-point planes, interfaces formed by the stepping-down of parallel O-point planes can intersect additional O-points, and a ledged interface thus forms with misfit-compensating ledges. These ledges, recently recognized for the first time (6,52), contain an additional half-plane and represent a combination of a pure misfit dislocation and a structural ledge. Fig. 11 shows the O-lattice modeling of misfit-compensating ledges on the Burgers $(1\bar{1}00)_{\zeta//}(2\bar{1}\bar{1})_{\beta}$ conjugate habit plane. The O-points A_{ij} and C_{ij} are obtained from the **H$_1$-B$_1$** combination, and B_{ij}'s are from the **H$_1$-B$_2$** combination. The flat interphase boundary formed by $(1\bar{1}00)_{\zeta//}(2\bar{1}\bar{1})_{\beta}$ as the conjugate habit planes now has an alternative: the ledged $A_{ij}B_{ij}C_{ij}$ interface in place of the flat $A_{ij}C_{ij}$ interface.

The geometry of the misfit-compensating ledges can thus be predicted. The risers of ledges are located midway between A_{ij} and B_{ij} and between B_{ij} and C_{ij}, along the planes where the two phases are most poorly matched(44,48). The interledge spacing is equal to the horizonal distance between A_{11} and B_{21} or $(1/2)A_{11}C_{11}$ $(c/2)$. The ledge height is the vertical distance between the nearest neighboring terraces A_{ij} and B_{ij} or $(1/2)$ $(a/2)$. The ledge direction is predicted to be A_{11} and A_{12} $([1\bar{1}\bar{2}0]_{\zeta//}[111]_{\beta})$ Since all of the Burgers vectors and line lengths of these misfit dislocations on the flat and ledged interfaces are known, the structural interfacial energies of the two interfaces can be calculated. The results show that the energy of the flat interface can be reduced by 12% if a ledged interface develops instead as a result of the presence of intermediate O-points such as B_{ij}.

3.4.3. Modeling of Structural Ledges

Structural ledges(6,11,52,53) are modeled by interrelating the atom positions of the two phases, on the terrace planes formed by pairs of relaxed atom layers, through a non-homogeneous matrix transformation, which is an alternative to incorporation of translation vectors. As shown in Fig. 12, the position vectors $\mathbf{x}^{(1)}$ and

$\mathbf{x}^{(2)}$, both referred to the origin O, can be expressed as difference vectors $\mathbf{x}^{(1)} - \mathbf{t}^{(1)}$ referred to O_1 and $\mathbf{x}^{(2)} - \mathbf{Rt}^{(2)}$ referred to O_2, respectively. The two difference vectors can accordingly be related through a non-homogeneous transformation:

$$\mathbf{x}^{(2)} - \mathbf{Rt}^{(2)} = \mathbf{A}(\mathbf{x}^{(1)} - \mathbf{t}^{(1)}) \tag{5}$$

With this change in transformation matrix the basic equation (Eq. 1) becomes:

$$(\mathbf{I} - \mathbf{A}^{-1})\mathbf{x}^{(0)} = -\mathbf{A}^{-1}\,\mathbf{Rt}^{(2)} + \mathbf{t}^{(1)} + \mathbf{b}^{(L)} \tag{6}$$

Three-dimensional modeling of structural ledges is now developed by means of a non-homogeneous transformation. As shown in Fig. 13, the x_1Ox_2 plane is taken as identical to the coincident A_1 and B_1 planes. When the A_2 and B_2 planes mutually relax and become the plane F (the 'compromise plane' between A_2 and B_2), the positions P on A_2 and Q on B_2 become P_r through $\mathbf{t}^{(1)}$ and Q_r through $\mathbf{Rt}^{(2)}$, respectively. The matching situation between the two relaxed positions can now be examined through the vectors $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ defining the two relaxed positions. Structural ledges may thus be predicted to step up from the A_1 terrace to the F terrace by the configuration of best-matching positions on the two terraces. The third terrace forms by another pair of parallel layers above the A_2 and B_2 layers, with a relaxation doubled from that needed for the A_2 and B_2 layers.

Fig. 14 shows the structure and misfit compensating mechanism of biatomic structural ledges on the Burgers $(1\bar{1}00)_\zeta // (2\bar{1}\bar{1})_\beta$ interface. As the pattern shift is along $[11\bar{2}0]_\zeta // [111]_\beta$, a set of ledges orthogonal to this direction is predicted. The Burgers vector **b**, associated with these ledges, can be determined as $(1/6)\mathbf{s}(\mathbf{2})$, *i.e.* $(1/18)[11\bar{2}0]_\zeta$ or $(1/12)[111]_\beta$ the same as Furuhara and Aaronson (52) obtained with the graphical technique (10).

3.5 O-Lattice Modeling of Flat Bcc:Hcp Interfaces

3.5.1. Unrotated Lines and Their Role in Interface Modeling

Unrotated lines (44,48,56) are the lines or directions in a crystal lattice which do not undergo any directional change when the crystal lattice becomes a new lattice during a phase transformation. An unrotated line with respect to the phase transformation **A**, represented by a vector **u**, is thus an eigenvector of the transformation (44):

$$\mathbf{Au} = \lambda\mathbf{u} \tag{7}$$

where λ is the corresponding eigenvalue denoting the length change along the unrotated line during the phase transformation. When $\lambda = 1$, the vector **u** in Eq. 7 corresponds to an invariant line. A difference vector $\mathbf{x}^{(2)}$-$\mathbf{x}^{(1)}$ then obtains as the mismatch between the corresponding positions surrounding an O-point:

$$\mathbf{x}^{(2)} - \mathbf{x}^{(1)} = k_1\sigma_1\mathbf{u}_1 + k_2\sigma_2\mathbf{u}_2 + k_3\sigma_3\mathbf{u}_3 \tag{8}$$

where the k_i's are coordinates on the three (generally oblique) $\mathbf{u}_i$ unrotated lines with the eigenvalues λ_i, and $\sigma_i = \lambda_i - 1$ represent the three transformation strains.

When the three unrotated lines are orthogonal, the squared mismatch, d^2, proportional to the transformation strain energy (when elastic isotropy is assumed), can be obtained by using Eq. 8:

$$d^2 = \| \mathbf{x}^{(2)} - \mathbf{x}^{(1)} \|^2 = k_1^2\sigma_1^2 + k_2^2\sigma_2^2 + k_3^2\sigma_3^2 \tag{9}$$

Since d^2 is a constant for any preset standard of best matching, Eq. 9 shows that the best-matching region around an O-point is an ellipsoid whose three principal axes lie along $\mathbf{u}_i$ and have lengths of d/σ_i, proportional to the preset standard and inversely proportional to the transformation strains σ_i.

3.5.2. Best- and Worst-Matching Directions

When the three eigenvectors are no longer orthogonal, the best- and worst-matching directions can be found by the Lagrangian multiplier method. Since $\mathbf{u}_1$ and $\mathbf{u}_2$ (consider a two-dimensional case), the squared mismatch, d^2, can now be expressed as:

$$d^2 = \| \mathbf{x}^{(2)} - \mathbf{x}^{(1)} \|^2 = k_1^2\sigma_1^2 + 2k_1k_2\sigma_1\sigma_2\cos\phi + k_2^2\sigma_2^2 \tag{10}$$

where ϕ is the angle between $\mathbf{u}_1$ and $\mathbf{u}_2$.

Consider all of the position vectors $\mathbf{x}^{(1)}$ which have the same length c before the transformation, *i.e.*:

$$\mathbf{x}^{(1)} \|^2 = \| k_1\mathbf{u}_1 k_2\mathbf{u}_2 \|^2 = c^2 \tag{11}$$

Minimization (for best matching) and maximization (for worst matching) of Eq. 10 subject to the above condition (Eq. 11) yields:

$$r^2\sigma_1\cos\phi + r(\sigma_1 + \sigma_2) + \sigma_2\cos\phi = 0 \tag{12}$$

In general Eq. 12 has two solutions respectively representing the best- and worst-matching directions. The two directions are perpendicular to each other. The angle α between the direction determined by the solution r (r_1 or r_2) and the eigenvector $\mathbf{u}_2$ can be evaluated from:

$$\cos\alpha = (r\cos\phi + 1)/\sqrt{r^2 + 2r\cos\phi + 1} \tag{13}$$

As the shape of best-matching areas in the case of two oblique unrotated lines is also an ellipse (Eq. 10), the best-matching direction must be the major axis, and the worst-

matching direction the minor axis of the ellipse. The ratio of the two axes, which now determines the shape of best-matching regions, can be obtained from the lengths of the two vectors $\mathbf{x}_2^{(1)}$ and $\mathbf{x}_1^{(1)}$ defined by the general solutions r_1 and r_2.

$$p = \frac{||\mathbf{x}_1^{(1)}||}{||\mathbf{x}_2^{(1)}||} = \frac{\sqrt{(r_1^2 + 2r_1\cos\phi + 1)(\sigma_1^2 r_2^2 + 2\sigma_1\sigma_2 r_2\cos\phi + \sigma_2^2)}}{\sqrt{(r_2^2 + 2r_2\cos\phi + 1)(\sigma_1^2 r_1^2 + 2\sigma_1\sigma_2 r_1\cos\phi + \sigma_2^2)}} \qquad (14)$$

3.5.3. Determination of the Networks of Misfit Dislocations

Fig. 16 shows how the worst-matching regions can be determined by the shape of the best-matching regions, using the Pitsch-Schrader $(0001)_{hcp}//(0\bar{1}1)_{bcc}$ interface as an example. The two unrotated lines $\mathbf{u}_1$ and $\mathbf{u}_2$ are perpendicular to each other at this interface, with the corresponding eigenvalues being λ_1 and λ_2, respectively. Eq. 9, used now in two dimensions, shows that the best-matching area around any O-point is an ellipse with the axial ratio $|\sigma_2| : |\sigma_1|$.

Two ellipses with the same strain d_2, called iso-matching contours, are centered at two adjacent O-points, O_1 and O_2. The two points of intersection between these ellipses, A and B, are then the worst-matching positions between the two O-points. The reason is that strains inside the two ellipses are all smaller than those at the two points of intersection. This procedure can be repeated for different d values, and the resultant worst-matching positions form the line segment $CABD$. Strains along this segment increase symmetrically from the midpoint or the point of tangency, E, where two ellipses touch each other at an appropriate strain, d_1, but they are all greater than the strains in their immediately adjacent areas.

A complicated misfit-dislocation structure appears at the Burgers-related $(0001)\zeta//(0\bar{1}1)\beta$ interface, as shown in Fig. 17. One unrotated line is still $[11\bar{2}0)]\zeta//[111]\beta$, but the other is irrational and makes an angle of 24.74° with respect to the first one. The best-matching direction obtained from Eqs. 12 and 13 lies at an angle of 5.57° to $[11\bar{2}0]\zeta//[111]\beta$, and the worst-matching direction is perpendicular to the best-matching one. The principal axes of best-matching ellipses are along the best- and worst-matching directions and have an axial ratio of 29.51, obtained from Eq. 14. The Burgers vectors of the two sets of misfit dislocations are $(1/3)[1\bar{2}10]\zeta$ and $(1/3)[11\bar{2}0)]\zeta$; both, however, are not perpendicular to their dislocation lines.

Fig. 18 shows the misfit-dislocation structure at the Pitsch-Schrader $(0001)\zeta//(0\bar{1}1)\beta$ interface. As has been treated in Section 3.2.5, the misfit dislocations are distributed in a hexagonal network. Three distinguishable **a**-type Burgers vectors are associated with the dislocation segments in the network; they are mismatching vectors between adjacent O-points and can be determined by the base vectors forming the $S^{(1)}$ matrix as $(1/3)[2\bar{1}10]\zeta$, $(1/3)[11\bar{2}0]\zeta$ and $(1/3)[1\bar{2}10]\zeta$ ($\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$ in Fig. 18). The

dislocation segments with the Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ have a mixed character, whereas those with $\mathbf{b}_3$ are pure edges.

3.5.4 O-Line Modeling of Flat Interfaces

Suppose that at a special orientation obtained by a critical rotation, θ, of the bcc lattice around $[0\bar{1}1]_\beta$ one of the unrotated lines becomes an invariant line. Since the matrix $(\mathbf{I}-\mathbf{A}^{-1})$ is now singular (see Eq. 7 with $\lambda = 1$), an O-line lattice (44,48) may be constructed with O-lines parallel to the invariant line. The critical rotation angle can be determined as:

$$\theta = \sin^{-1} \frac{1 + \alpha_{11}\alpha_{22}}{\sqrt{(\alpha_{11} + \alpha_{22})^2 + \alpha_{21}^2}} - \cos^{-1} \frac{\alpha_{21}}{\sqrt{(\alpha_{11} + \alpha_{22})^2 + \alpha_{21}^2}} \qquad (15)$$

where the coefficients are the elements of the matrix $S^{(1)}(S^{(2)})^{-1}$.

When $(\mathbf{I}-\mathbf{A}^{-1})$ is singular, Eq. 1 can be solved for only certain $\mathbf{b}^{(L)}$ vectors forming the so-called **b**-subspace (44). It can be shown that the $\mathbf{b}^{(L)}$ vectors which make Eq. 1 solvable lie within the plane defined by the other two unrotated lines. Two linearly independent vectors in the **b**-subspace are needed to construct an O-line lattice, and they exist only when both unrotated lines are exactly along rows of atom positions. When at least one unrotated line does not lie exactly along an atom row, the concept of coincidence of equivalent positions (44) must be extended to that of near-coincidence. As shown in Fig. 19, *B* (in the bcc lattice) and *H* (in the hcp lattice) are equivalent positions (with the same internal coordinates (44,48)) through the transformation **A**, but in general they do not coincide with each other. If the distance between them is a *lattice* vector $\mathbf{b}^{(L)}$ (say, in the hcp lattice), another position H_1, which is displaced by the lattice vector $\mathbf{b}^{(L)}$ from *H* and is thus a position equivalent to *H* and then to *B* will coincide with *B* and form an O-point. $\mathbf{b}^{(L)}$ is thus the Burgers vector between the coincident B-H_1 position and the origin *O*. In the case of a singular $(\mathbf{I}-\mathbf{A}^{-1})$, the choice of $\mathbf{b}^{(L)}$ is confined to the **b**-subspace. If a **b**-subspace vector **b** (now without the superscript L is not a lattice vector, the position H_2 displaced by **b** from *H* will not be equivalent to *H* and then to *B*. However, if **b** is close enough to some lattice vector $\mathbf{b}^{(L)}$, H_2 will be in *near*-coincidence with *B*. The difference vector $\mathbf{b}_r$ between **b** and $\mathbf{b}^{(L)}$ is a quantitative expression of the degree of nearness, may be interpreted as the relaxation of corresponding positions and is thus termed a relaxation vector.

Fig. 20(a) shows the O-line lattice of the β and ζ_m phases at the near-Burgers orientation relationship when some relaxation is taken into account. The length of the relaxation vector for the O-lines closest to the relaxation-free ones is only 0.02 nm or 7.2% of the average interatomic distance in the close-packed directions in both phases.

It is seen in 20(a) that another O-lattice plane, *i.e.*, $(0001)_\zeta // (0\bar{1}0)_\beta$, also includes the invariant line and another unrotated line $(\mathbf{u}_1)$, and it is a possible low-energy interface. As shown in Fig. 20(b), one set of misfit dislocations compensates mismatch between the two phases; the Burgers vector of these dislocations is $(1/3)(41\bar{5}0)_\zeta$.

3.5.5 The O-line Lattice and Invariant Line Models

As the difference between any two equal vectors in the **b**-subspace, the zero vector **0** allows the basic equation (Eq.1) to become:

$$(\mathbf{I} - \mathbf{A}^{-1})\mathbf{x}^{(0)} = \mathbf{0} \tag{16}$$

If both sides of Eq. 16 are premultiplied by **A** and then rearranged, the following equation is obtained in a form identical to that of the invariant line model (56,58,59):

$$\mathbf{A}\mathbf{x}^{(0)} = \mathbf{x}^{(0)} \tag{17}$$

The identity of Eqs. 16 and 17 suggests that the lattice invariant line in the invariant line model (56,58,60) is identical to the O-line intersecting the origin in an O-line lattice.

It can be shown that the matrix **D** in the invariant line model has exactly the same form as $\mathbf{S}^{(2)}(\mathbf{S}^{(1)})^{-1}$ in the O-lattice model. Because the rotation matrix **R** is the same in both models, the identity of the transformation matrix **A** in the two models is also confirmed.

The concepts of energy minimization in the two models are very similar. The most effective accommodation of strain in the invariant line model (56,61) and the minimum structural component of the interfacial energy in the O-lattice model (62) are intimately connected with optimization of lattice matching. This suggests why the mathematical form of the invariant line model is identical to Eq. 16 for the O-line intersecting the origin in the O-lattice, and why both can predict habit planes and orientation relationships.

3.6. Summary

1. Growth ledges were frequently observed by conventional TEM on irrationally oriented ζ_m:β interfaces in a Ag-26 A/O Al alloy. Closely spaced misfit-compensating ledges were also found in some irrationally oriented interfaces.

2. High-resolution TEM revealed misfit-compensating ledges and small (structural) ledges at the terraces of misfit-compensating ledges on a ζ_m:β interface, across which the orientation relationship was deviated by about 6° from the Burgers relationship.

3. The structure of ledged, partially coherent bcc:hcp interfaces has been modeled by extending the Bollmann (44) O-lattice theory to permit the matching of all atom positions in the two phases. Misfit-compensating ledges were predicted when interfaces formed by stepping-down of O-point planes intersect additional O-points.

4. Structural ledges were modeled by interrelating relaxed atom positions by a non-homogeneous transformation in the O-lattice construction. Biatomic structural ledges were predicted on Burgers $(1\bar{1}00)_\zeta // (2\bar{1}\bar{1})_\beta$ interfaces.

5. Mismatch between any corresponding positions in the product and parent lattices was expressed as an analytical function of the eigenvectors and eigenvalues of the transformation matrix. The networks of misfit-compensating defects on a general interface were determined by common tangents to the iso-matching contours.

6. When an unrotated line is also an invariant line, the O-line lattice can be solved for the $\mathbf{b}^{(L)}$ vectors within the plane defined by the other two unrotated lines. One set of misfit-compensating defects is then sufficient to form partially coherent bcc:hcp interfaces. The O-line intersecting the origin was shown to be equivalent to the lattice invariant line in the invariant line model.

7. In accordance with the prediction of Aaronson, Laird and Kinsman (1), massive:matrix interfaces in the Ag-26 A/O Al alloy studied were found to be partially coherent. No evidence at all was found for the presence of interfaces which might have had a disordered structure at the atomic scale.

4. Organization of a Pacific Rim Conference on the Roles of Shear and Diffusion in the Formation of Plate-Shaped Transformation Products.

Although considerable progress has been made both experimentally and theoretically in distinguishing between phase transformations which take place diffusionally on the atomic scale and those which occur by shear, there remains widespread disagreement about the interpretation of many key experimental observations relevant to this distinction, even though some of their observations were reported 30 or more years ago. Further, there are increasing indications that, early views by Christian (63) to the contrary, these two very different atomic mechanisms can lead, on a macroscopic scale to a large range of crystallographic and surface relief similarities. A number of researchers are more or less independently attempting to reconcile these similarities in the form of an overarching crystallographic/interfacial structure theory which will be able both to accomodate and to distinguish critically between the two mechanisms. The time accordingly appears appropriate to hold a highly focussed conference on this subject. This will be done under the sponsorship of the ASM Phase Transformations Committee from December 18 through 22, 1992 at the Kona Hilton Hotel in Kona, Hawaii. The choice of Hawaii was mainly dictated by the shift of much current work in and enthusiasm about research in this area to the Far East. While U.S. and Canadian researchers continue to be active participants, together with some Western European workers, China, Japan and, increasingly, also India are becoming "hot beds" of this type of research. Hawaii is thus an appropriate venue for this conference since it has become a now traditional meeting place for workers from opposite sides of the "Pacific Rim".

This conference has been organized mainly by the P.I., who will serve as its Administrative Chairman, and Prof. C. M. Wayman (Univ. of Illinois at Urbana-

Champaign), who will be General Chairman. (This has meant, as the P.I. had originally planned, that the P.I. would be responsible for virtually all of the "detail work" involved in assembling the conference.) The program has been worked out through detailed discussions, frequently refined, between Prof. Wayman and the P.I. Prof. J. P. Hirth (Washington State Univ.) is serving as Advisory and General Discussion Chairman. His principal functions so far have been to suggest additional speakers and to serve as an impartial referee when Profs. Wayman and Aaronson are unable to reconcile a disagreement between them. Dr. B. B. Rath (Naval Research Laboratory) is the Government Relations Chairman of the conference and has contributed valuable information on the identity of non-usual sources of funding. Travel and at-conference support has turned out to be even more of a problem than originally anticipated because so many of the speakers will require financial aid in order to traverse the huge distances involved. While the choice of a mid-Pacific site has kept down these costs, since trans-Pacific airfares tend to be greater than those associated with trans-Atlantic flights, the requests received from 20 of the 44 speakers for financial assistance have resulted in a funding requirement of nearly $60,000, a non-trivial sum--particularly in an era of worldwide economic recession. The P.I. is at presently actively pursuing U.S. sources of conference support funding. Japanese sources will be investigated next, principally by Prof. Wayman, whose connections in Japan are exceptionally good.

A copy of the conference program is attached. Note that a considerable (and largely successful) effort has been made to achieve a balance between the diffusionist and the shearist points of view. The principal model transformations are seen to be the proeutectoid ferrite and bainite reactions in steel and α_1 plate formation from variously ordered versions of β Cu-Zn. A number of other materials, however, are included. And the overall emphasis is upon generality of principles, rather than upon the details of individual alloy systems. Possibly the most important component of this conference, however, will be the two General Discussion sessions, one of 90 min. and the other 3 hrs. in length, during the final day of the conference. Both will be supervised by Prof. Hirth. Properly orchestrated, these sessions should enable a good public airing of the main points of contention left unresolved by public and private discussions held earlier in the conference.

5. Collaborative Research with Dr. M. G. Hall, University of Birmingham, U.K.

The initial part of the program consisted of a re-examination of a paper by H. K. D. H. Bhadeshia (64) in which the claim was made that tent-shaped surface reliefs formed by back-to-back pairs of ferrite plates resulted from the second plate forming with an orientation allowing a marked reduction in the strain energy associated with the first plate. The heat treatment method used to acquire this peculiar structure consisted of isothermal transformation, followed by relatively slow continuous cooling to room temperature. Since an Fe-0.4 W/O C alloy was employed, this approach virtually guaranteed further transformation during the cooling process. We accordingly suggested that the second plate

formed via sympathetic nucleation (65) at a broad face of the first plate, without reference to the assumed shear compensation.

A detailed, matrix algebra-based analysis by Dr. Hall confirmed our earlier supposition. The hypothesis that the second plate was decisively disproved. The publication resulting from this work has appeared in Scripta Metallurgica (66).

Work is now getting underway to understand the origin of tent-shaped surface relief effects associated with single ferrite plates which form through the uni-directional migration of growth ledges under diffusion control. This work will be presented by Dr. Hall at the Hawaii '92 conference on shear vs. diffusional growth.

6 List of Publications During this Report Period

1. H. I. Aaronson, D. Eylon, C. M. Cooke, M. Enomoto and F. H. Froes, "The Widmanstatten-Start (W_S) Temperature, as Affected by Matrix Grain Size, in Ti-6% Al-4% V and in Fe-C Alloys", Scripta Met., 23, 435 (1989).

2. T. Furuhara, H. J. Lee, E. S. K. Menon and H. I. Aaronson, "Interphase Boundary Structure in Ti-Base Alloys", Met. Trans., 21A, 1627 (1990).

3. M. Enomoto and H. I. Aaronson, "Reply to Doherty and Cantor and Further Work on Computer Modeling of Growth Kinetics of Ledged Interphase Boundaries", Scripta Met., 23, 1983 (1989).

4. M. Enomoto and H. I. Aaronson, "Rebuttal of Reply to Comments on 'Computer Modelling of the Growth Kinetics of Ledged Interphase Boundaries'", Scripta Met., 23, 1995 (1989).

5. H. I. Aaronson, T. Furuhara, J. M. Rigsbee, W. T. Reynolds, Jr. and J. M. Howe, "Crystallographic and Mechanistic Aspects of Growth by Shear and Diffusional Processes", Met. Trans., 21A, 2369 (1990).

6. H. I. Aaronson, W. T. Reynolds, Jr., G. J. Shiflet and G. Spanos, "Bainite Viewed Three Different Ways", Met. Trans., 21A, 1343 (1990).

7. H. Goldenstein and H. I. Aaronson, "Overall Reaction Kinetics and Morphology of Austenite Decomposition between the Upper Nose and the M_S of a Hypoeutectoid Fe-C-Cr Alloy", Met. Trans., 21A, 1465 (1990).

8. H. I. Aaronson, T. Furuhara, J. M. Howe, W. T. Reynolds, Jr. and G. Spanos, "Why Does the Phenomenological Theory of Martensite Crystallography Sometimes Quantitatively Describe the Surface Relief Effect and the Transformation Crystallography of Precipitate Plates?", "Interfaces: Structure and Properties", ed. by S. Ranganathan, B. B. Rath, C. S. Pande and D. A. Smith, Oxford & IBH Publishing Co., New Delhi, India.

9. M. Enomoto, H. I. Aaronson and T. Furuhara, "Thickening of Grain Boundary α Allotriomorphs in a Ti-Cr Alloy by Multiple Sets of Ledges", Met. Trans., 22A, 1341 (1991).

10. H. I. Aaronson, T. Furuhara and M. Enomoto, "On the Approach of Mats Hillert to the Growth Kinetics of Diffusional Phase Transformations", Scand. Jnl. of Metallurgy, 20, 18 (1991).

11. H. I. Aaronson and F. K. LeGoues, "An Assessment of Studies on Homogeneous Diffusional Nucleation Kinetics in Binary Metallic Alloys", Met. Trans., in press.

12. G. Spanos, H. S. Fang and H. I. Aaronson, "Reply to Discussion of 'A Mechanism for the Formation of Lower Bainite'", Met. Trans., 22A, 1676 (1991).

13. T. Furuhara and H. I. Aaronson, "Computer Modeling of Partially Coherent BCC:HCP Boundaries", Acta Met. Mat., 39, 2857 (1991).

14. T. Furuhara, J. M. Howe and H. I. Aaronson, "Interphase Boundary Structures of Intragranular Proeutectoid α Plates in a Hypoeutectoid Ti-Cr Alloy", Acta Met. Mat., 39, 2873 (1991).

15. T. Furuhara and H. I. Aaronson, "Crystallography and Interfacial Structure of Proeutectoid α Grain Boundary Allotriomorphs in a Hypoeutectoid Ti-Cr Alloy", Acta Met. Mat., 39, 2887 (1991).

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Pacific Rim Conference on the Roles of Shear and Diffusion in the Formation of Plates in Crystalline Solids

December 18-22, 1992

at the Kona Hilton Hotel, Kona, Hawaii, USA

Sponsored by the Phase Transformations Committee of ASM International

Thursday, December 17 (Coconut Grove)

5:30 PM — Wine & cheese welcoming reception, until about 7.30 PM

Friday, December 18 (Alii Surf Room)

8:15 AM — C. M. Wayman, Conference General Chairman (Univ. of Illinois at Urbana-Champaign, USA): Introduction to the Conference

Setting the Stage - I

Chairman: T. Ko (Beijing University of Science and Technology, PRC)

8:30 — C. M. Wayman (Univ. of Illinois at Urbana-Champaign, USA): The Phenomenological Theory of Martensite Crystallography: Interrelationships

9:05 — H. I. Aaronson (Carnegie Mellon Univ., USA) and M. G. Hall (Univ. of Birmingham, U.K.): The Formal vs. the Derivative Requirements of the PTMC as Discriminants between Transformation Mechanism

9:40 — J. W. Christian (Oxford Univ., U.K.): The PTMC, Interfacial Structure and Transformation Mechanism (provisional)

10:15 - 10:30 Refreshment Break

Setting the Stage - II

Chairman: T. Nishizawa (Tohoku Univ., Japan)

10:30 — M. Hillert (Royal Inst. of Technology, Sweden): Thermodynamic and Kinetic Aspects of Transformations by Shear

11:05 — M. Enomoto (Ibaraki University, Japan): Thermodynamics and Kinetics of Plate Formation

11:40 — T. Ko (Beijing University of Science and Technology, PRC): Comparative Studies of Bainite and Martensite Formation

1:00 PM — Board bus for "Kona Historical Tour" at entrance to Kona Hilton Hotel. Box lunch will be supplied. Return to hotel about 5:00 PM

The PTMC and Elastic Strain Energy Effects (*Alii Surf Room*)

Chairman: G. B. Olson (Northwestern Univ., USA)

8:00 PM — B. C. Muddle (Monash Univ., Australia): Applications of the Phenomenological Theory of Martensite Crystallography to Displacive Transformations in Substitutional Non-Ferrous Alloys

8:35 — J. K. Lee (Michigan Technological Univ., USA): Some Aspects of Elastic Strain Energy in Shear Versus Diffusional Transformations

9:10 — A. Khatchaturyan (Rutgers Univ., USA): Strain-Induced Pattern Formation Caused by Diffusional and Diffusionless Phase Transformations

9:45 — A. Roytburd (Univ. of Maryland, USA): Single- and Polydomain Plate-Shaped Inclusions in Diffusional and Diffusionless Transformations

Saturday, December 19* (Alii Surf Room)

The Role of the Invariant Line in Plate Formation

Chairman: K. Shimizu (Osaka Univ., Japan)

8:30 AM — U. Dahmen (Univ. of California at Berkeley, USA): Structure, Crystallography and Growth Mechanisms of Invariant Line Precipitate Plates

9:05 — G. C. Weatherly (Univ. of Toronto, Canada): The Invariant Line and Boundary Structure of Precipitates

9:40 — D. A. Smith (IBM T. J. Watson Research Center, USA): Reconciliation of the Invariant Line, O-Lattice, PTMC and Structural Ledge Interpretations of Interface Structure and Crystallography

10:15 - 10:30 Refreshment Break

The Role of Interphase Boundary Structure in Plate Formation - I

Chairman: G. C. Weatherly (Univ. of Toronto, Canada)

10:30 — G. R. Purdy (Univ. of Toronto, Canada): Role of Interphase Boundary Structure in Plate Growth by Diffusional Mechanisms

11:05 — G. B. Olson (Northwestern Univ., USA): Kinematics, Structure and Mobility of Interphase Boundaries

11:40 — J. P. Hirth (Washington State Univ., USA): Ledges and Dislocations in Shear/Diffusional Phase Transformations

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* For accompanying persons, the Cooking Demonstration will be held from 9:30 to 11:30 AM in the Discovery Room.

1:15 PM — Board bus for "Captain Cook Kealakekua Bay Cruise" at entrance to Kona Hilton Hotel. Box lunch will be supplied. Return to hotel about 5:45 PM.

The Role of Interphase Boundary Structure in Plate Formation - II (Alii Surf Room)

Chairman: J. M. Rigsbee (Univ. of Illinois at Urbana-Champaign, USA)

8:00 PM — G. J. Shiflet (Univ. of Virginia, USA): Structural Ledges as a Misfit-Compensating Linear Defect at Interphase Boundaries

8:35 — Y. Mou (Univ. of Virginia, USA): Misfit-Compensating Ledges at Interphase Boundaries

9:10 — T. Furuhara, T. Maki and K. Tsuzaki (Kyoto Univ., Japan): Interphase Boundary Structure of Ferrite and Martensite Plates in Ferrous Alloys

9:45 — W. T. Reynolds, Jr., G. Chen and T. W. Ross III (Virginia Polytechnic Inst. & State Univ., USA): The Crystallography and Kinetics of Growth Ledge Formation on Plates

Sunday, December 20 (Alii Surf Room)

Plate Formation in Steel - I

Chairman: B. C. Muddle (Monash Univ., Australia)

8:30 — J. M. Genin (Univ. of Nancy I, France): The Initial Composition of Precipitate Plates in Interstitial Alloys

9:05 — M. G. Hall (Univ. of Birmingham, U.K.) and H. I. Aaronson (Carnegie Mellon Univ., USA): Formation of Invariant Plane Strain and Tent-Shaped Surface Reliefs by the Diffusional Ledge Mechanism

9:40 — T. Maki and K. Tsuzaki (Kyoto Univ., Japan): Substructure of Plate-Shaped Ferrite in Steels

10:15 - 10:30 Refreshment Break

Plate Formation in Steel - II

Chairman: Y. Ohmori (Ehime Univ., Japan)

10:30 — G. Spanos (Naval Research Lab., USA): Interphase Boundary Structure and Formation Mechanism of Bainite in Fe-C-Mn and Fe-C-Mn-Si Alloys

11:05 — M. K. Kang, Y. Q. Yang and Q. M. Wei (Northwestern Polytechnical Univ., PRC): Aspects of the Bainite Reaction

11:40 — H. S. Fang, J.-J. Wang and C.-M. Li (Tsinghua Univ., PRC): Roles of Superledges and Boundary Structure in the Thickening of Plates in Ferrous and Non-Ferrous Alloys

1:30 PM — Board bus for ride to Hapuna Beach at entrance to hotel. Bring bathing attire--or wear it on the bus if you wish. Changing facilities are available at the beach. Bring towels from hotel--but be sure to return them! Suggest that you have lunch at the Kona Hilton Hotel. Board bus at Hapuna Beach at 4:45 PM, returning to hotel at 5:30 PM.

Plate Formation in Steel - III (Alii Surf Room)

Chairman: G. Krauss (Colorado School of Mines, USA)

8:00 PM — T. Araki (Kobe Steel, Japan), K. Shibata (Univ. of Tokyo, Japan) and M. Enomoto (National Research Inst. for Metals - Tokyo, Japan): The Growth of Low Carbon Bainite and Isothermal Martensite Plates

8:35 — Y. Ohmori, H. Ohtani and S. Okaguchi (Ehime Univ., Japan): Morphologies of Bainite and Widmanstatten Ferrite

9:10 — M. Oka and H. Okamoto (Tottori Univ., Japan): On the Transition between Upper and Lower Bainite in Plain Carbon Steels

9:45 — S. K. Liu, L. Yang and J. Zhang (Southwest Jiaotong Univ., PRC): Influence of the Solute Drag-Like Effect and Segregation upon the Formation of Ferrite in Alloy Steels

Monday, December 21

α_1 Plate Formation in Beta Cu-Zn - I (Alii Surf Room)

Chairman: M. Hillert (Royal Inst. of Technology, Sweden)

8:30 AM — T. Y. Hsu (Shanghai Jiao Tong Univ., PRC): Thermodynamic Consideration of Formation Mechanism of α_1 Plates in Cu-base Alloys

9:05 — M. Chandrasekaran (Univ. Twiente, The Netherlands) and L. Delaey (Katholieke Univ., Belgium): T_0 and the Role of Shear in the Initiation of α_1 Plates in Cu-Zn-base Alloys

9:40 — K. Shimizu and T. Tadaki (Osaka Univ., Japan): High Resolution Analytical Electron Microscopy Study of Bainite in Some β-phase Alloys

10:15 - 10:30 Refreshment Break

α_1 Plate Formation in Beta Cu-Zn - II

Chairman: T. Y. Hsu (Shanghai Jiao Tong Univ., PRC)

10:30 — J. B. Cohen (Northwestern Univ., USA): Long-Range Order in the Early Stages of Precipitation

11:05 — M. H. Wu (Memory Technologies, USA), Y. Hamada (Sumitomo Metal & Mining Co., Japan) and C. M. Wayman (Univ. of Illinois at Urbana-Champaign, USA): Transformation Characteristics of α_1 Plates in Cu-Zn-Al Alloys

11:40 — S. Sato (Sapporo, Japan): A Discussion on the Formation of α_1 Plates and α Rods in Cu-Zn and Ag-Zn Alloys

Free Afternoon

Conference Banquet: 5:00 - 7:40 PM, in Discovery Room

Chairman: C. M. Wayman (Univ. of Illinois at Urbana-Champaign, USA)

Banquet Speaker: J. W. Cahn (National Institute of Standards and Technology, USA): Out on a Ledge with the Bainite of Our Existence

α_1 Plate Formation in Beta Cu-Zn - III (Alii Surf Room)

Chairman: B. B. Rath (Naval Research Laboratory, USA)

8:00 PM — P. E. J. Flewitt (Nuclear Electric-Gravesend, U.K.) and A. G. Crocker (Univ. of Surrey, U.K.): Non-Ferrous Bainite Transformations

8:35 — K. Chattopadhyay (Indian Inst. of Technology, India): Transformation Mechanism of α_1 Plates in β Cu-Zn

Plate Formation in Other Alloy Systems - I

Chairman: A. H. Rosenstein (Air Force Office of Scientific Research, USA)

9:10 — M. Kikuchi (Tokyo Inst. of Technology, Japan): Widmanstatten Plate Formation in Chromium-rich Cr-Ni Alloys

9:45 — H. L. Fraser, B. Kad (Ohio State University, USA) and V. Vasudevan (Univ. of Cincinnati, USA): Transformation of Ti_3Al to TiAl in the Titanium Aluminides

Tuesday, December 22

Plate Formation in Other Alloy Systems - II (Alii Surf Room)

Chairman: B. A. MacDonald (National Science Foundation, USA)

8:00 — S. Banerjee (Bhabha Atomic Research Center, India): Interfaces of Plate-Shaped Transformation Produced in Zirconium-Based Alloys

8:30 — J. M. Howe (Univ. of Virginia, USA), A. Garg (Carnegie Mellon Univ., USA) and Y. C. Chang (Univ. of Virginia, USA): In-Situ High-Resolution TEM Studies of Precipitate Growth in an Al-4% Cu-0.5% Mg-0.5% Ag Alloy

9:05 — G. W. Lorimer (Univ. of Manchester, U.K.): Bainite Plate Formation in a Cu-Mn-Al Alloy

9:40 — N. Nakanishi and T. Shigematsu (Konan Univ., Japan): Bainite-like Transformations in Some Oxides

10:15 - 10:30 Refreshment Break

General Discussion - I (Alii Surf Room)

10:30-12:00 — Chairman: J. P. Hirth (Washington State Univ., USA)

General Discussion - II (Alii Surf Room)

2:00-5:00 PM — Chairman: J. P. Hirth (Washington State Univ., USA)

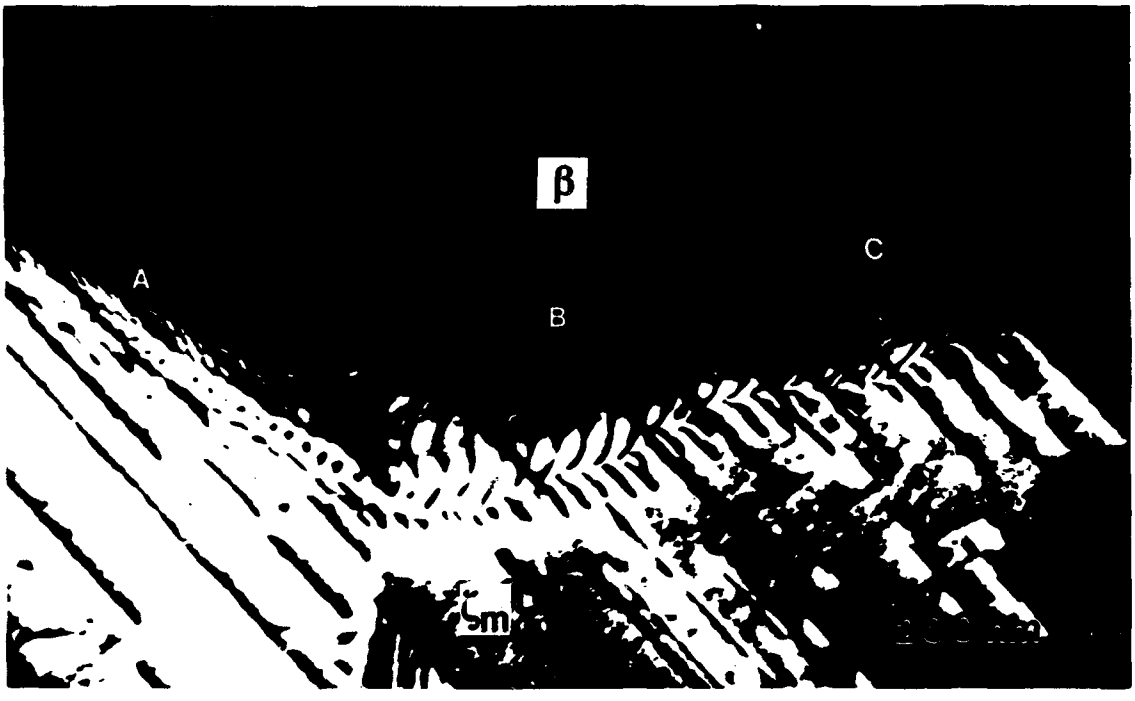


Figure 1: TEM micrograph of an irrationally oriented ζ_m:β interface, showing different densities of growth ledges at different boundary orientations.

Figure 2: TEM dark-field micrographs of an irrationally related ζ_m:β interface, imaged with (a) (0002) and (b) $(10\bar{1}0)$ ζ_m reflections, showing growth ledges and two sets of uniformly spaced ledges.

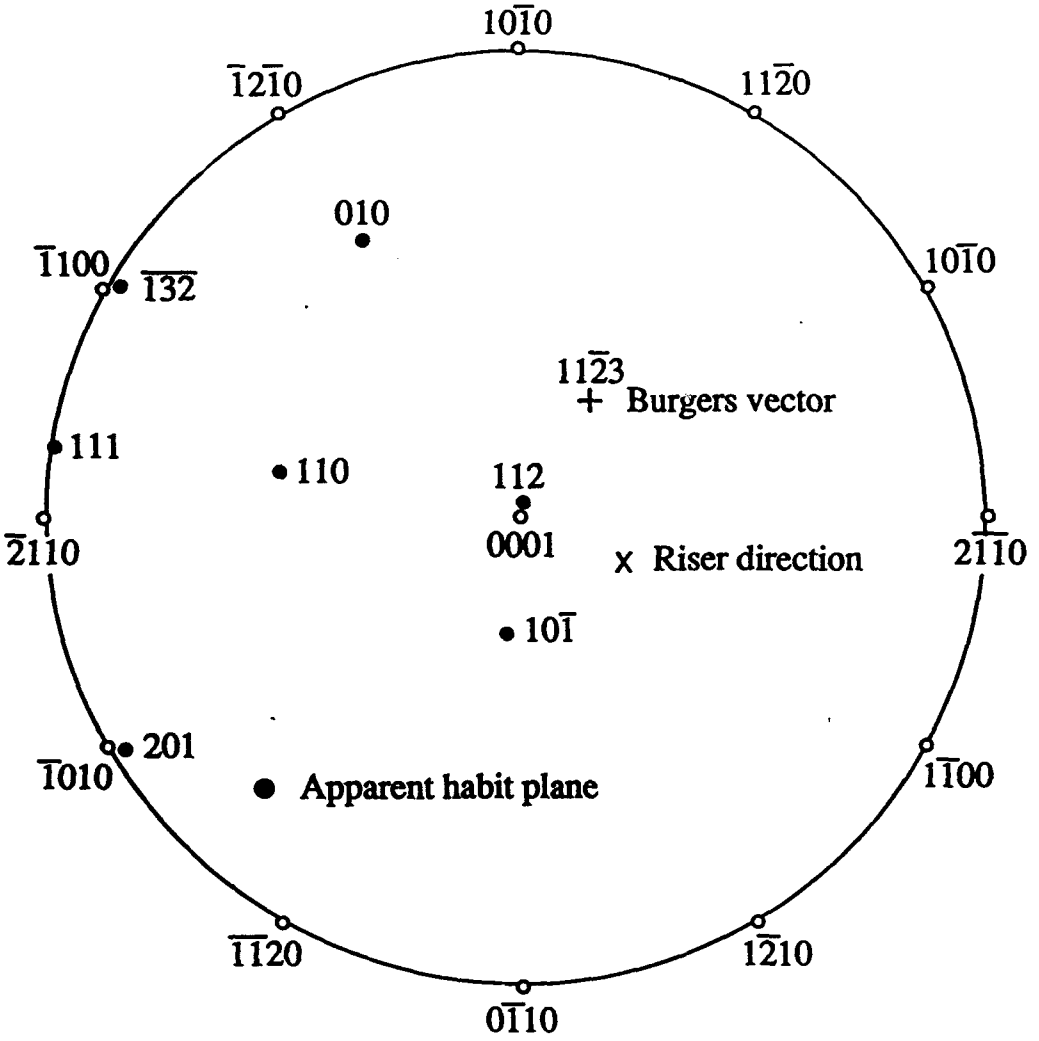


Figure 3: An $(0001)_{hcp}$ stereographic projection showing the riser direction (indicated by ×), Burgers vector (+) of the set of uniformly spaced ledges pointed out by three small arrowheads in Fig. 2(a), and the apparent habit plane (•) of the interface.

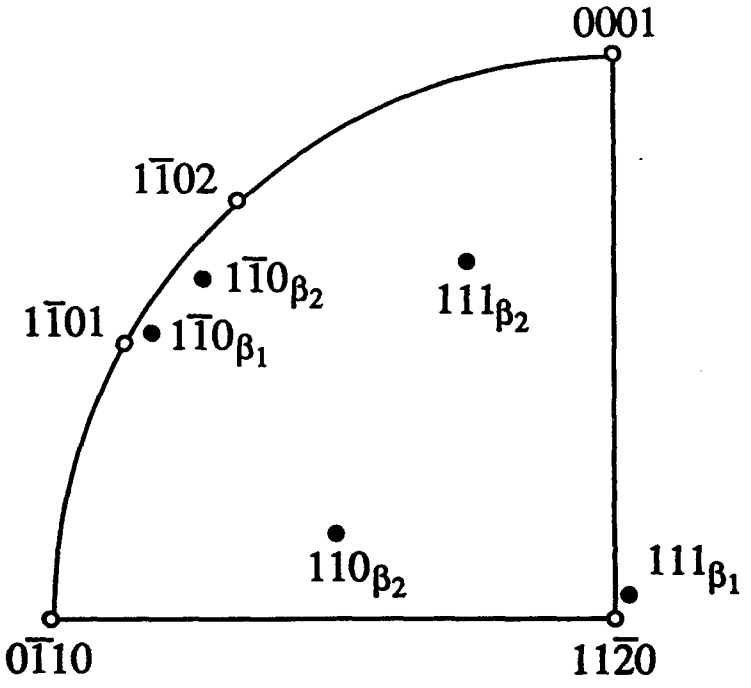


Figure 4: A quarter of an $(0001)_{hcp}$ stereographic projection, showing the orientation relationship between the ζ_m crystal and both the β_1 and the β_2 subgrains.

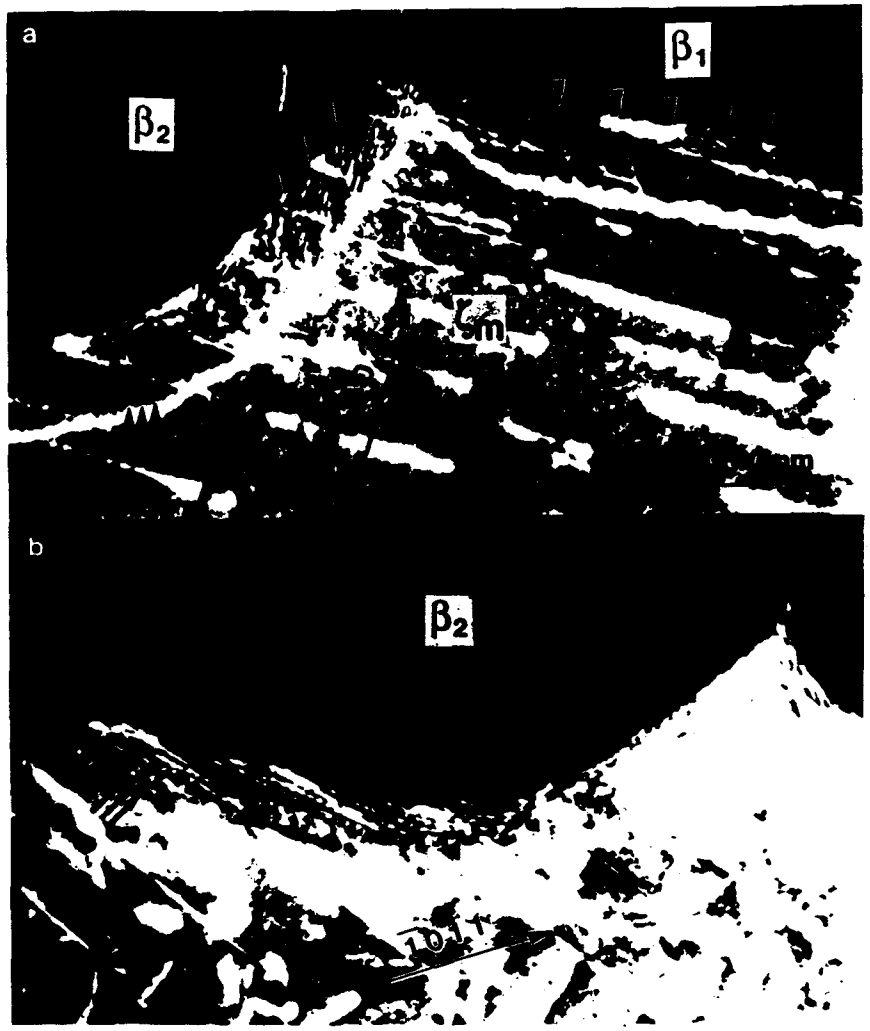


Figure 5: TEM micrographs of a ζ_m crystal bounded to two β sub-grains with a misorientation of about 7°, imaged with (a) (0002) and (b) $(1\bar{0}11)$ ζ_m reflections, showing growth ledges and a probable set of uniformly spaced ledges on the ζ_m:β_1 interface, and growth ledges and two sets of uniformly spaced ledges on the slightly irrational ζ_m:β_2 interface.

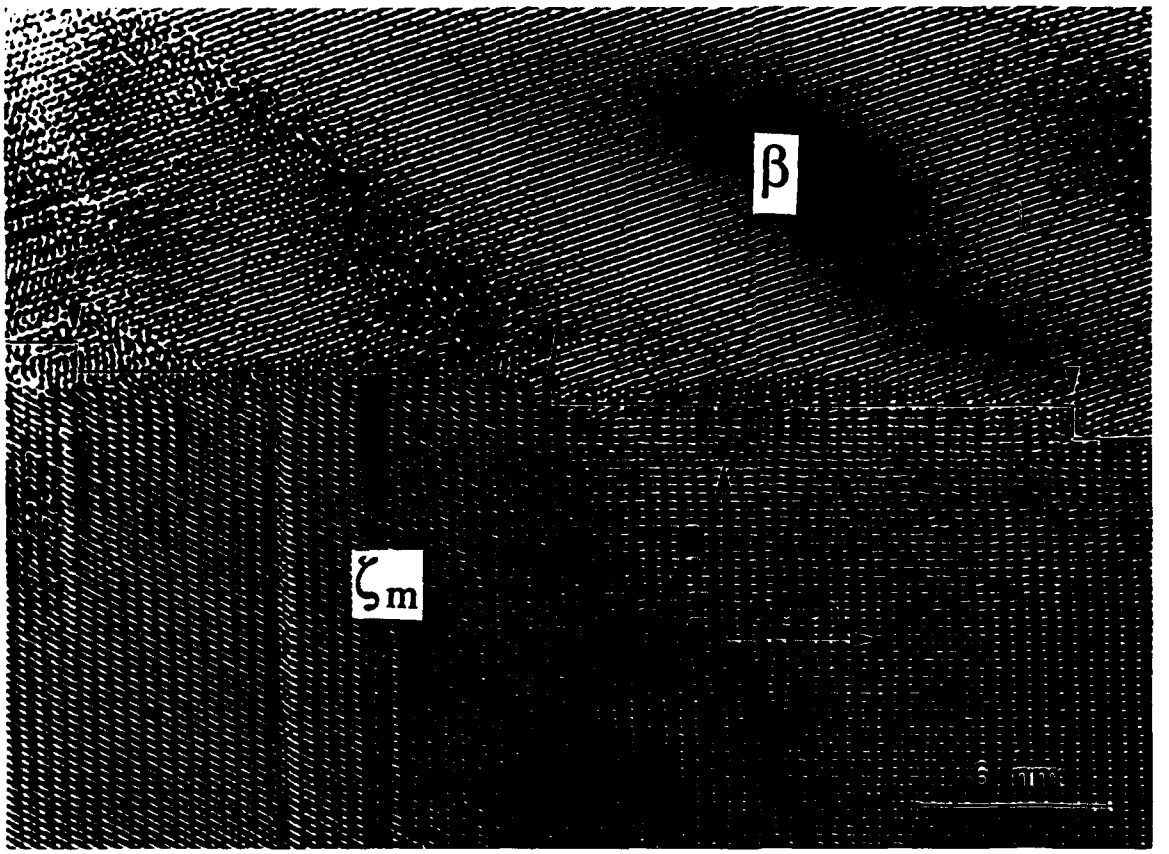


Figure 6: High-resolution TEM micrograph of a ζ_m:β interface at the $[11\bar{2}0]_\zeta$//$[111]_\beta$ foil orientation. Three misfit-compensating ledges are pointed out by large arrowheads.

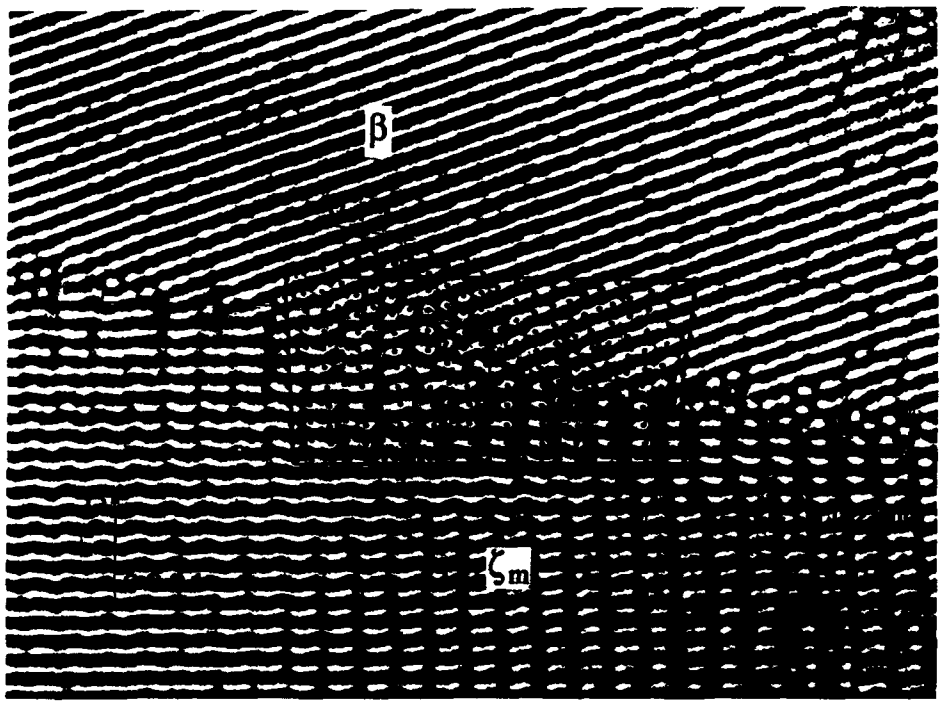


Figure 7: High-resolution TEM micrograph of a misfit-compensating ledge on the ζ_m:β interface in Fig. 6, showing that the highest ledge is associated with some three shorter ledges, and that the Burgers vector of the highest ledge is $(1/2)[0001]_\zeta$.

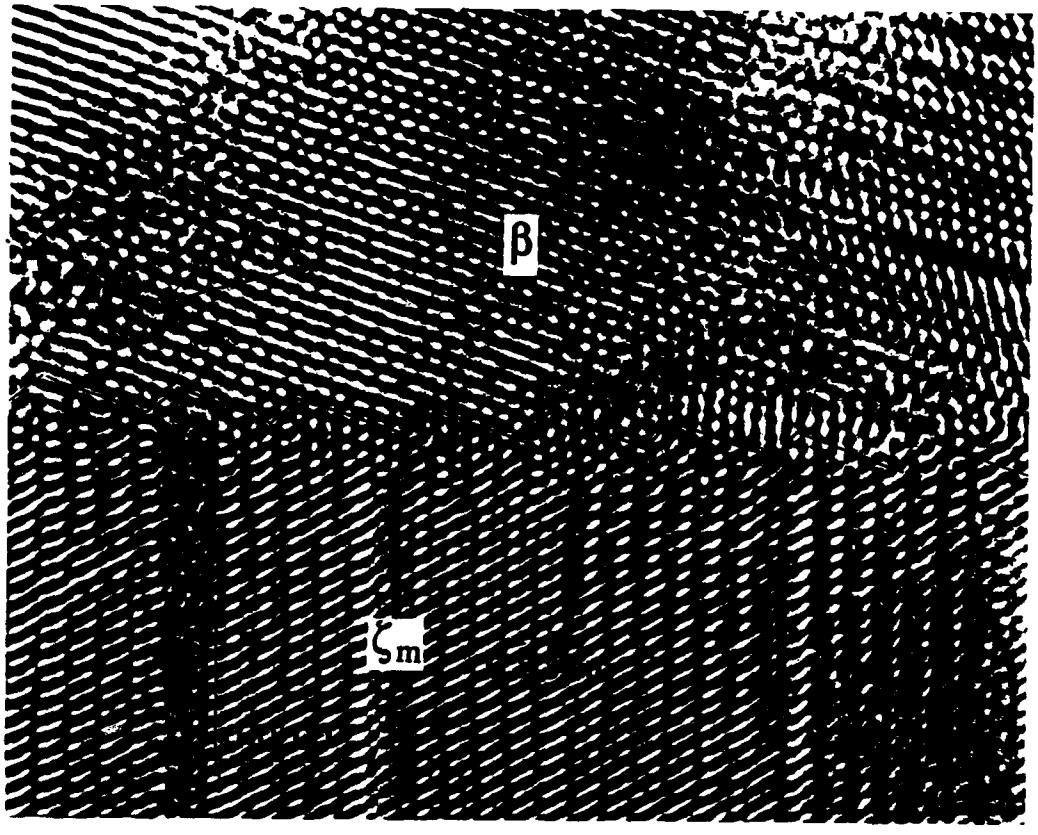


Figure 8: High-resolution TEM micrograph of atomic matching across a terrace plane on the ζ_m:β interface in Fig. 6, showing that a somewhat regular arrangement of atoms forms 'ledges' outlined by thin lines.

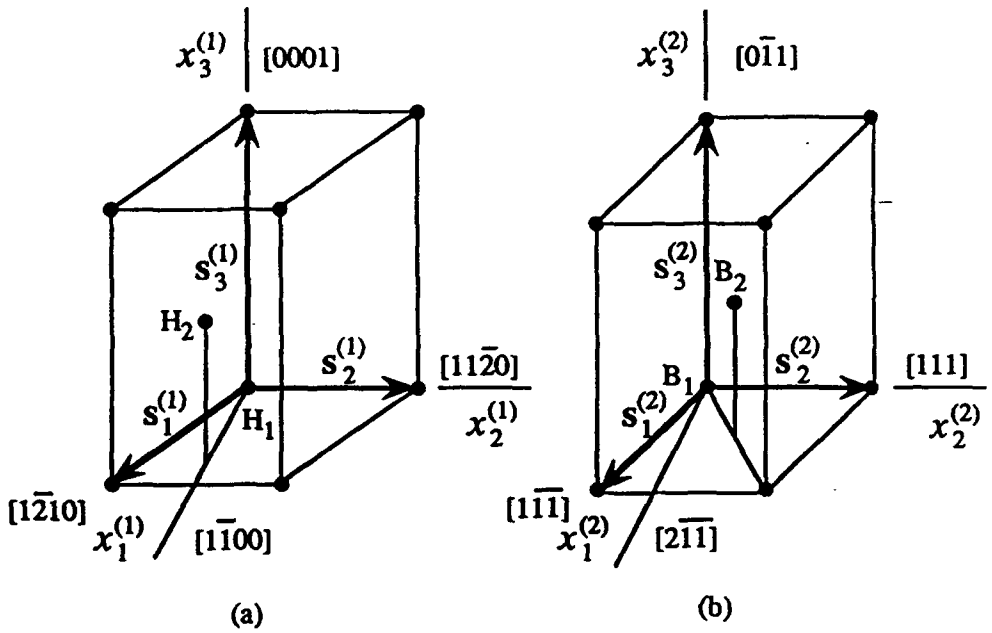


Figure 9: The unit cells of (a) the hcp and (b) bcc phases chosen for the O-lattice construction.

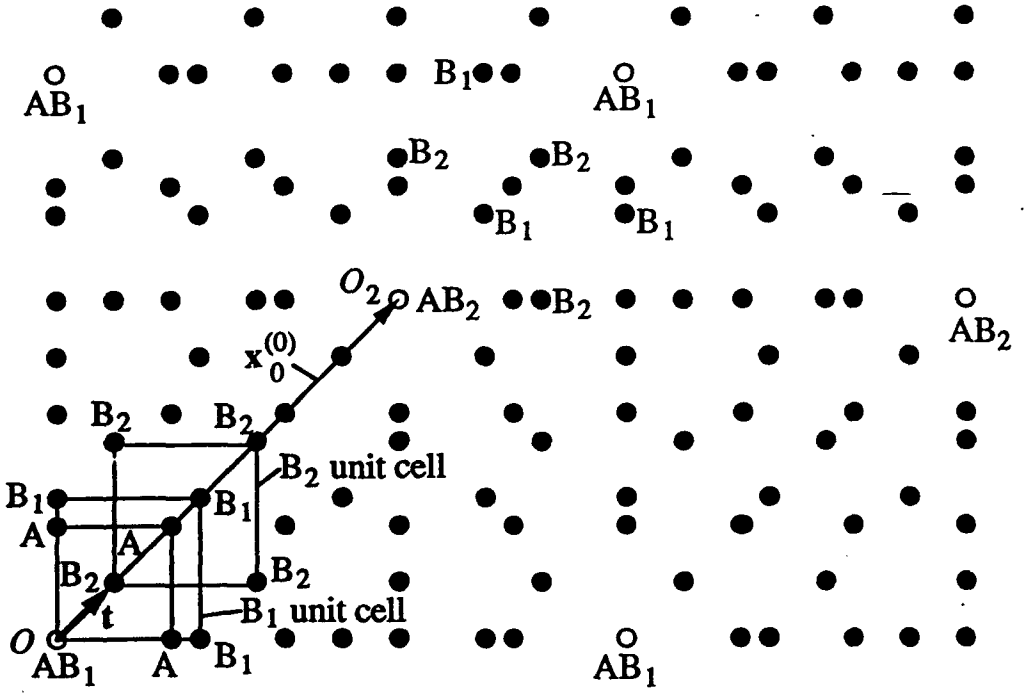


Figure 10: Atom-position matching between structures A and B, with B consisting of two subsets of atom positions, B_1 and B_2.

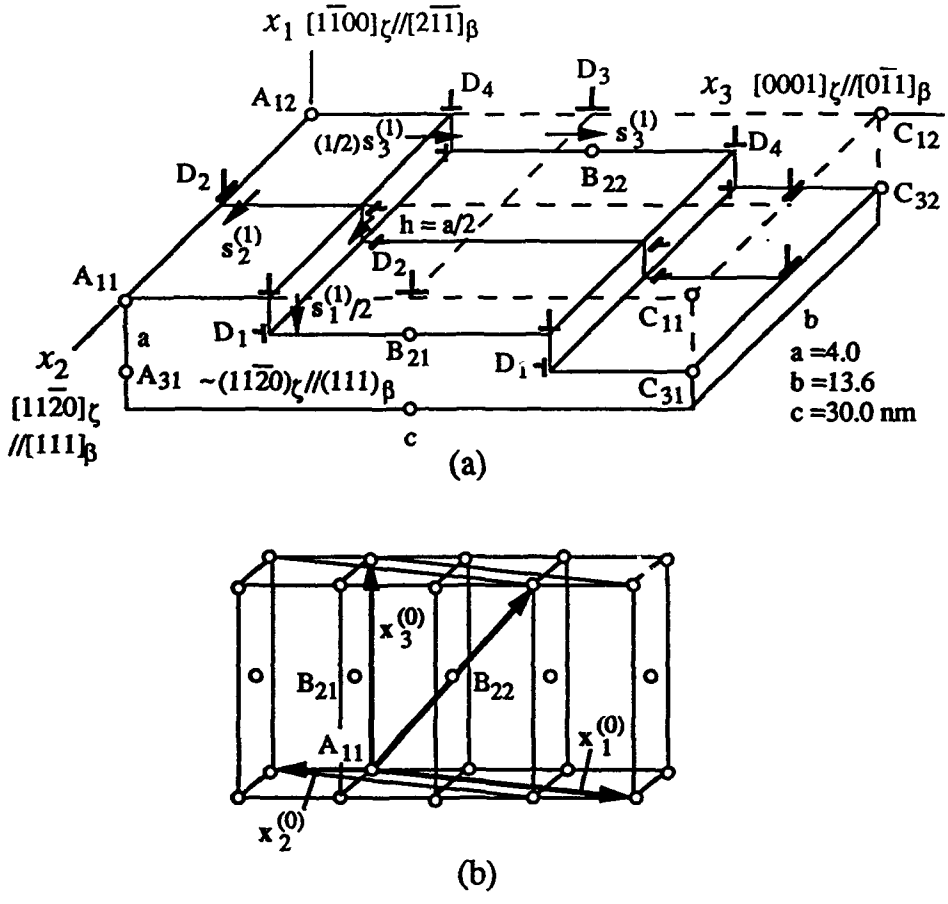


Figure 11: The structure and mismatch accommodation mechanism of misfit-compensating ledges on the Burgers $(1\bar{1}00)_\zeta//(2\bar{1}\bar{1})_\beta$ interface.

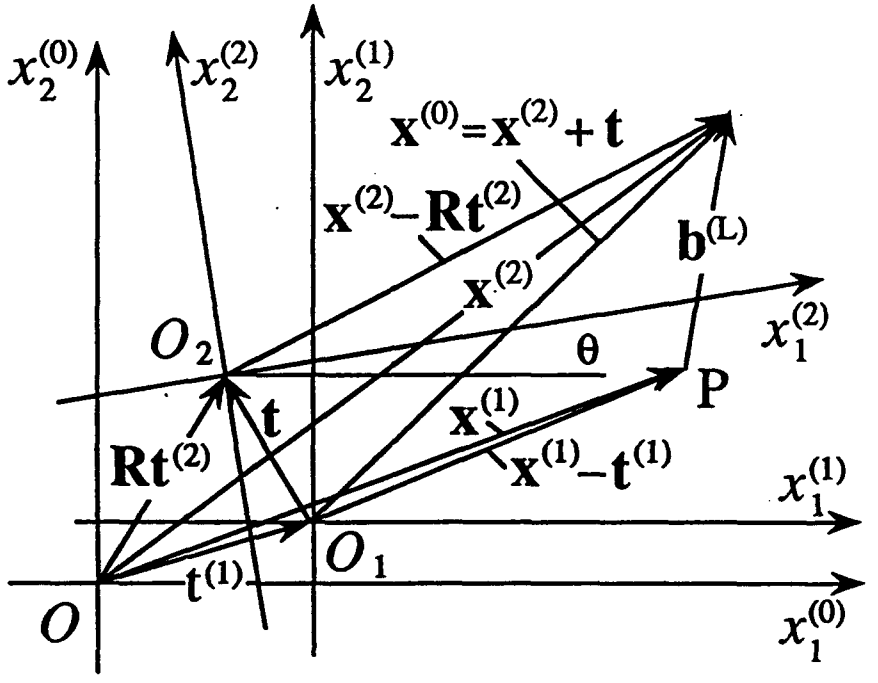


Figure 12: Search for O-points by using a non-homogeneous transformation. Note that when $\mathbf{t}^{(1)}=\mathbf{t}^{(2)}=\mathbf{0}$, the transformation becomes homogeneous.

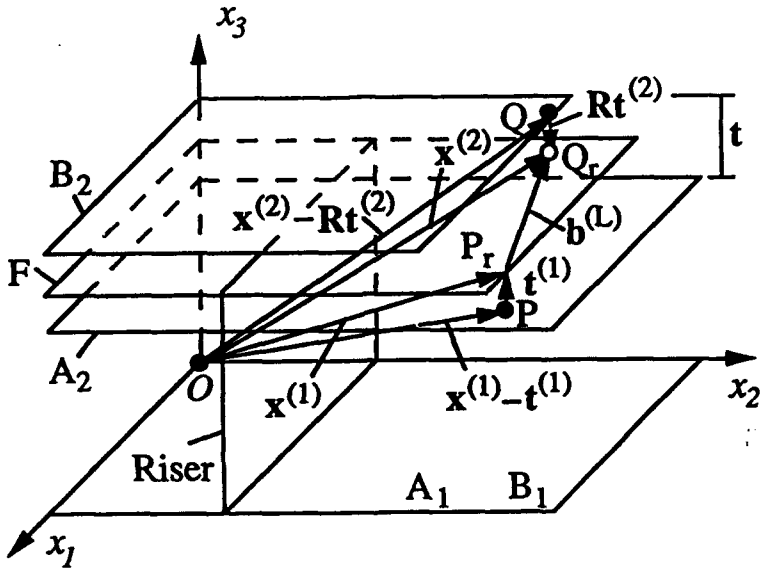
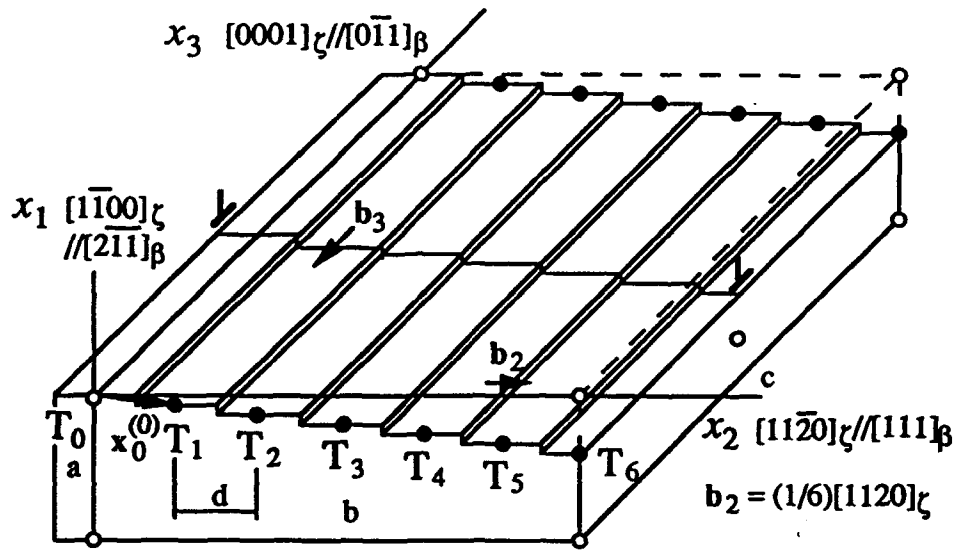


Figure 13: Search for best-matching positions on the terraces of structural ledges by using a non-homogeneous transformation.



a = 4.0, b = 13.6, c = 30.0 (not in scale) nm, d= b/6

Figure 14: Biatomic structural ledges on Burgers-related $(1\bar{1}00)_\zeta//(\bar{2}1\bar{1})_\beta$ interfaces determined by non-homogeneous O-lattice modeling: open circles are O-points, and solid ones best-matching positions with relaxation.

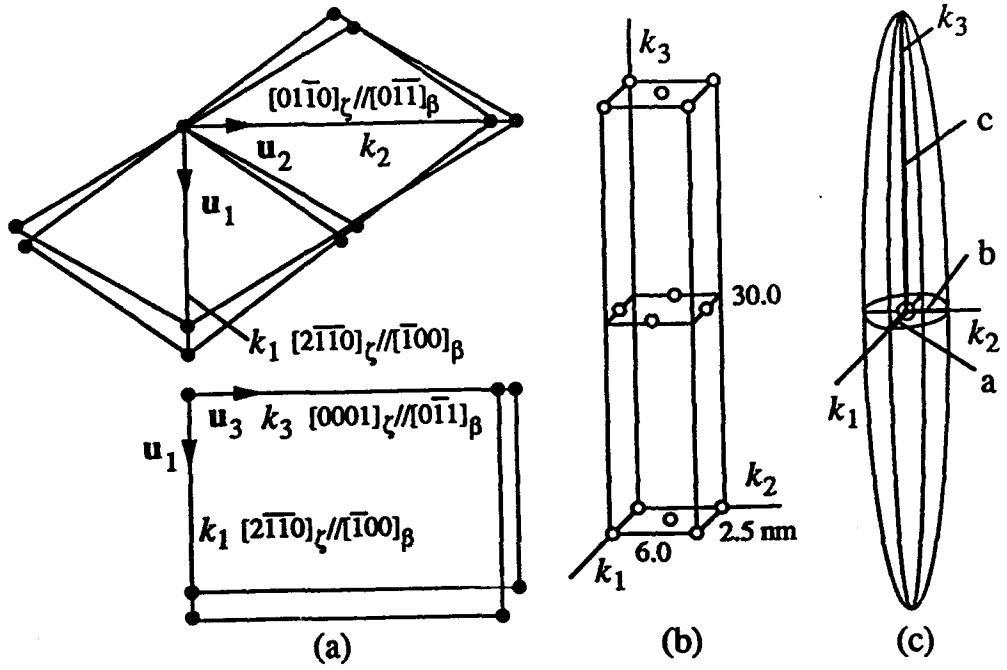


Figure 15: Shape of best-matching regions between bcc and hcp phases in the Pitsch-Schrader orientation relationship: (a) three unrotated lines determined directly from the orientation relationship; (b) corresponding O-lattice [17]; and (c) an ellipsoidal best-matching region around an O-point.

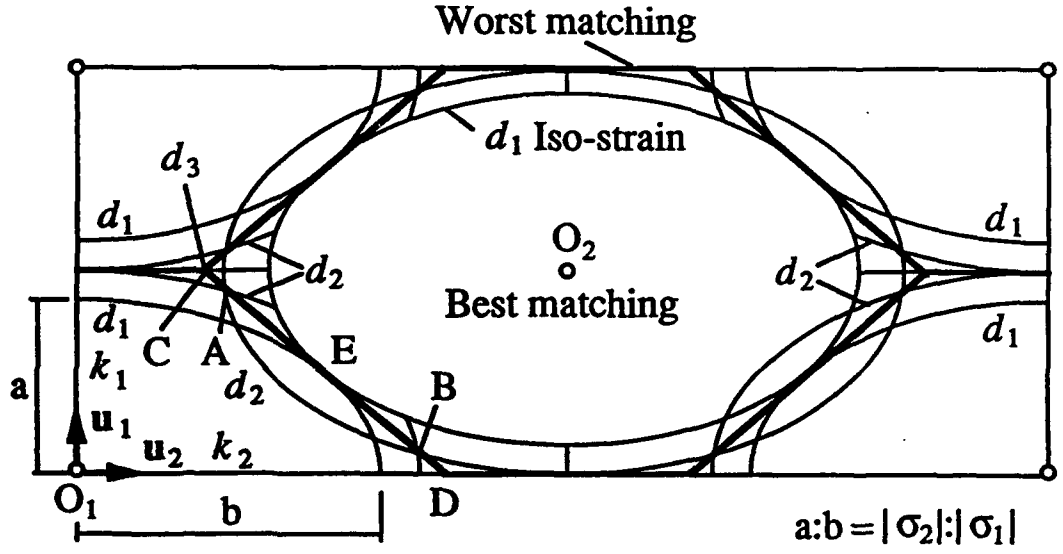


Figure 16: Determination of the worst-matching areas with the ellipses showing the shape of the best-matching areas on a Pitsch-Schrader related $(0001)_{hcp}//(01\bar{1}1)_{bcc}$ interface. Open circles are O-points and misfit dislocation lie along the worst-matching lines (thick lines).

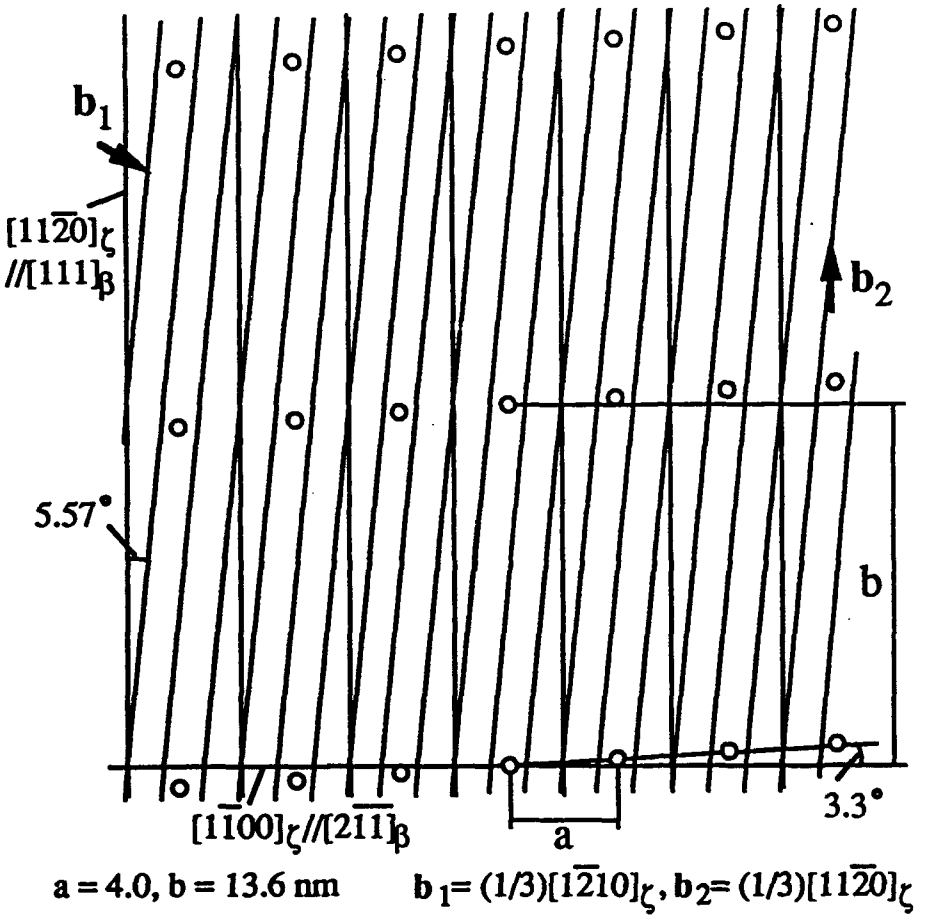
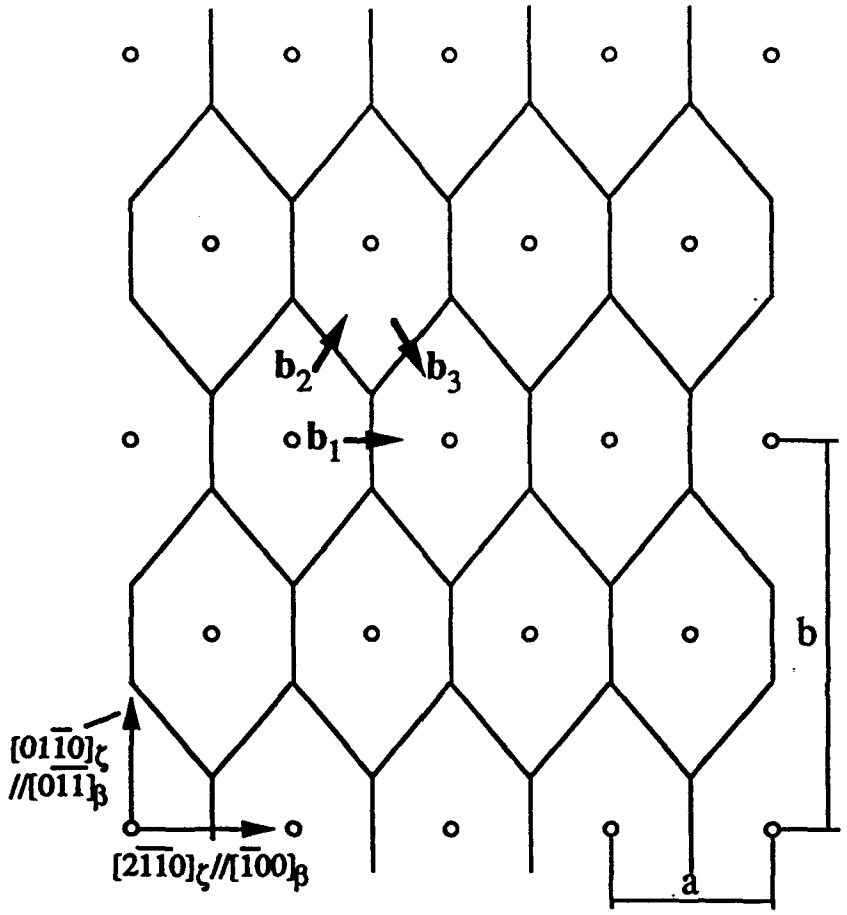


Figure 17: Misfit-dislocation structure on a Burgers-related $(0001)_\zeta//(0\bar{1}\,\bar{1})_\beta$ interface. Open circles are O-points, and thin lines are misfit dislocations. Note that best-matching areas are very much extended in the direction 8.51° away from $[11\bar{2}0]_\zeta//[111]_\beta$.



$b_1 = (1/3)[2\bar{1}\bar{1}0]_\zeta$, $b_2 = (1/3)[11\bar{2}0]_\zeta$, $b_3 = (1/3)[1\bar{2}10]_\zeta$

$a = 2.5$, $b = 6.0$ nm

Figure 18: Misfit-dislocation structure on a Pitsch-Schrader related $(0001)_\zeta//(0\bar{1}\,\bar{1})_\beta$ interface. Open circles are O-points, and thin lines are misfit dislocations forming a hexagonal network.

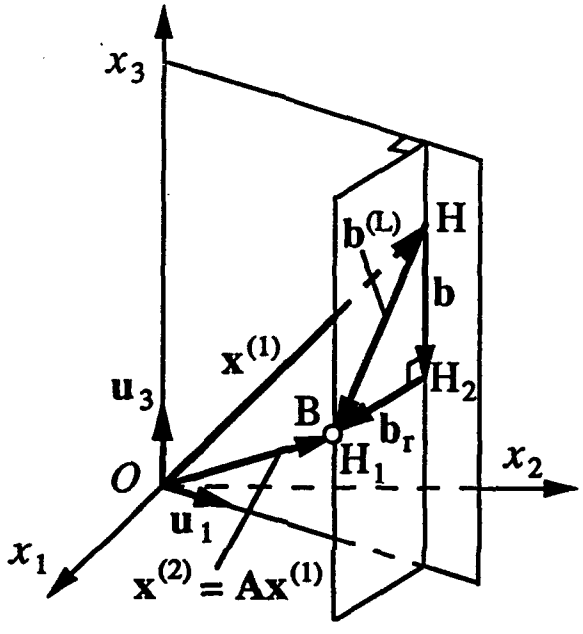


Figure 19: The O-point (or O-line) with near-coincidence of equivalent positions formed by an appropriate relaxation ($\mathbf{b}_r$ is enlarged for clarity).

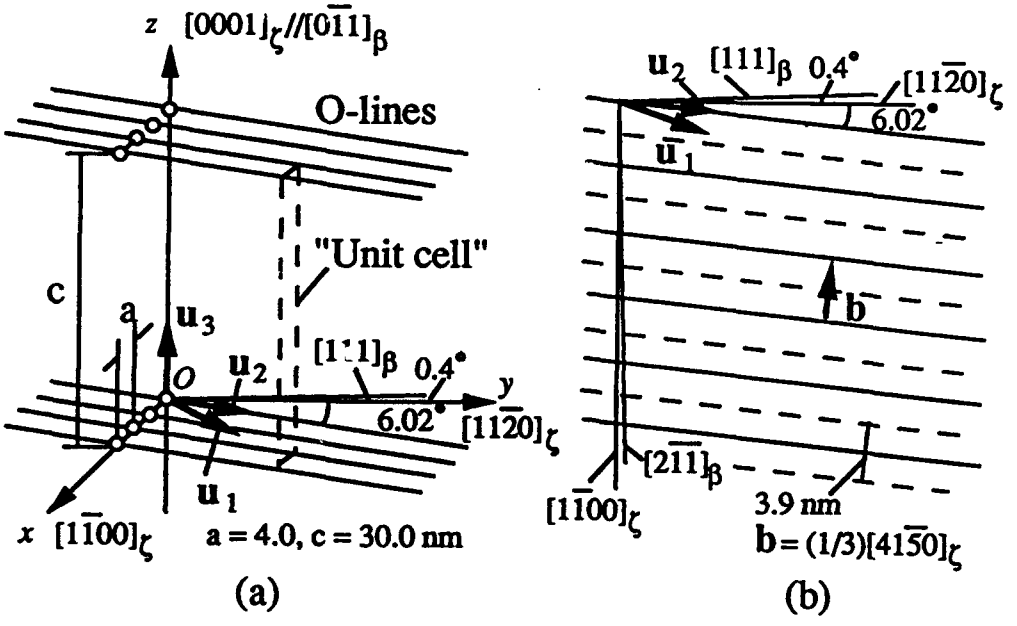


Figure 20: The O-line lattice and misfit-dislocation structure of the β and ζ_m phases at the near-Burgers orientation relationship, *i.e.*, $(0001)_\zeta//(01\bar{1})_\beta$ and $[11\bar{2}0]_\zeta$ 0.3999° away from $[111]_\beta$: (a) the whole O-line lattice; and (b) misfit-dislocation structure at the $(0001)_\zeta//(01)_\beta$ interface.