ATOMISTIC STUDIES OF GRAIN BOUNDARIES AND HETEROPHASE INTERFACES IN ALLOYS AND COMPOUNDS

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INTRODUCTION

The overarching goal of the research supported by this grant was investigation of the structure and properties of interfaces in multicomponent systems by atomistic modeling. Initially, the research was devoted to studies of segregation to grain boundaries in binary disordered alloys. The next step was then studies of the structure and properties of grain boundaries in ordered compounds, specifically Ni_3Al and NiAl , and grain boundary segregation in these compounds in the case of off-stoichiometry. Finally, the structure of Nb/sapphire interfaces, in particular the core configurations of the misfit dislocations, was studied.

An integral part of this program was development of the description of atomic interactions needed for the above mentioned atomistic studies. In this context we have developed Finnis-Sinclair type central-force many body potentials for a number of alloy systems, advanced tight-binding based approaches for the study of extended crystal defects and developed a simple effective potentials for study of the structure of metal-ceramic interfaces.

Several studies of the structure of grain boundaries as well as the studies of metal/ceramic interfaces were closely linked with experimental observations employing high resolution transmission electron microscopy (HRTEM). This link was very fruitful. Not only the HRTEM served as a test for the validity of the calculations but calculated structures were essential for the correct and physically meaningful interpretation of the corresponding HRTEM observations.

In this report we do not describe details of all the study undertaken during the ten year period. These can be found in thirty seven publications listed at the end of this report. Rather we concentrate on the main highlights of this research which we summarize briefly and details can be found in the appended reprints and preprints.

HIGHLIGHTS OF THE RESEARCH

Structure of grain boundaries in L_{12} alloys: significance of ordering energy

Calculations employing both pair-potentials and central-force many-body potentials revealed that significant structural differences exist between crystallographically identical grain boundaries in Ni_3Al and Cu_3Au . In the case of Cu_3Au (low ordering energy), the relaxation in the boundary is such that the atoms in the boundary region can not be uniquely assigned to either the upper or the lower grain and grain boundary structures in this alloy are topologically similar to those in pure f.c.c. materials. On the other hand, in the case of Ni_3Al (high ordering energy), the atoms in the grain boundary region relax much less and they can be regarded as uniquely attached to either the upper or the lower grain.

Owing to the very small relaxation in grain boundaries in Ni_3Al there are many distinct columnar cavities at these boundaries because of the 'mismatch' arising from the misoriented L_{12} lattices. These columnar cavities may serve as suitable nuclei for the formation of intergranular cracks under external loads and thus render the grain boundary susceptible to cracking. However, the columnar cavities may not be the only and possibly not even the most important factor in the intrinsic brittleness of grain boundaries in Ni_3Al . It has been established recently that the

major reason for the intergranular brittleness of the polycrystalline Ni_3Al is related to the effect of hydrogen on boundary cohesion. The columnar cavities are very suitable channels for the diffusion and collection of hydrogen in the boundaries which are thus embrittled. Since the existence of such cavities is related to the strength of ordering, the same effect can be expected in other strongly ordered L1_2 alloys. In contrast, weakly ordered alloys, such as Cu_3Au , are not susceptible to the same type of embrittlement since the columnar cavities are not present. For more details see references [2, 3, 6, 7, 11, 21, 22, 28, 29, 30] and enclosed reprint (V. Vitek, S. P. Chen, A. F. Voter, J. J. Kruisman and J.Th.M. DeHosson: Grain boundary structure and intergranular fracture in L1_2 ordered alloys, *Mater. Sci. Forum* **46**, 237, 1989.)

Structure of grain boundaries in off-stoichiometric L1_2 alloys at finite temperatures

These studies were carried out by Monte Carlo simulations employing the "modified" grand canonical ensemble; the system studied contains more than one species and the number of atoms for each species is allowed to change but the total number of atoms is fixed. These calculations show that in non-stoichiometric Ni_3Al alloys both Ni and Al segregate to grain boundaries when in surplus in the bulk. However, the impact of the Ni segregation on the boundary structure is very different from that of Al segregation. When nickel segregates, the grain boundary region becomes chemically disordered since additional interchanges of Ni and Al atoms accompany the segregation process and the species 'smear' in the boundary region. In contrast, in the case of aluminum segregation, the Al atoms occupy only certain specific sites in the grain boundary region, and no significant compositional disordering occurs. The selectivity of aluminum segregation is, presumably, related to the fact that Al is a large atom and can only be accommodated at sites associated with a large free volume. Since the segregation of Al is very selective, a two dimensional ordered Ni-Al compound with a high Al content is formed at the grain boundary.

Hence, after nickel segregation the grain boundary region becomes more akin to that found in weakly ordered alloys and the columnar cavities are eliminated. As discussed above, this may render the material more ductile. In contrast, in Al rich Ni_3Al the two dimensional compositionally ordered structure, formed due to the segregation of Al, may render the material even more brittle. This considerable difference between the structural changes invoked by segregation of Ni and Al, respectively, may be the principal reason why only in Ni rich alloys the intergranular brittleness can be inhibited by alloying with boron. For more details see references [11, 21, 23, 24, 30] and enclosed reprint (Min Yan and V. Vitek: Atomistic studies of the structure and composition of boundaries in Cu_3Au and Ni_3Al , *Interface Science* **3**, 17, 1995.)

Central-force many-body potentials of Finnis-Sinclair type for binary alloys

The method of constructing empirical many-body potentials for binary alloy systems in the framework of the Finnis-Sinclair approach has been developed. The most important extension of the model originally developed for elemental metals is a simple incorporation of interspecies interactions which involves fitting certain properties of alloys, such as the alloying energies, elastic moduli and ordering energies. These fitted quantities are either obtained experimentally or as results of ab

initio electronic structure calculations. The importance of properly accounting for the local atomic relaxations when constructing the potentials is emphasized. The observed principal features of phase diagrams of the alloys studies are well reproduced by this scheme and reasonable concentration dependencies of the alloy lattice parameter and elastic constants are obtained. This suggests that fine details of the electronic structure may be less important than are more global parameters such as atomic sizes and binding energies. For more details see references [4, 5, 29] and enclosed reprint (G.J. Ackland and V. Vitek: Many-Body Potentials and Atomic Scale Relaxations in Noble Metal Alloys, *Phys. Rev. B* **41**, 10324 1990.)

Structure of grain boundaries in copper-bismuth alloys

The above mentioned method was used to construct many body potentials for the copper-bismuth system using both experimental data and physical quantities obtained by *ab-initio* full-potential LMTO calculations for a theoretical metastable Cu_3Bi compound. These potentials were then used to model the structure of a $\Sigma=3$ (111)/(11 $\bar{1}$) grain boundary facet containing bismuth that formed as a result of segregation induced faceting. This boundary was at the same time studied by HREM. Excellent agreement between the calculated and observed structures is shown by comparing a through-focal series of observed and calculated images. This study shows, for the first time, that HREM combined with computer modeling employing realistic empirical potentials can decipher with a great accuracy the structure of boundaries containing multiple atomic species. The structure is an ordered Cu-Bi double-layer an *ab initio* FP-LMTO method was then employed to study possible Cu-Bi compounds related to this grain boundary structure. However, this study showed that this double-layer is a unique two-dimensional grain boundary structure. For more details see references [8, 9, 15, 16] and enclosed reprint (Min Yan, M. Sob, D. E. Luzzi, V. Vitek, G. J. Ackland, M. Methfessel and C. O. Rodriguez: Interatomic Forces and Atomic Structure of Grain Boundaries in Copper-Bismuth Alloys, *Phys. Rev. B*, **47**, 5571, 1993.)

Grain boundary segregation in disordered alloys: Cu-Ag

Experimental investigations of grain boundary segregation, for example the Auger electron spectroscopy (AES), as well as the associated thermodynamic analyses, are principally macroscopic. On the other hand, computer modeling of grain boundary segregation provides a very detailed picture of the atomic structures of segregated boundaries. The purpose of this research was to investigate the relationship between macroscopic and microscopic approaches. A Monte Carlo simulations of grain boundaries in Cu-Ag alloys was performed. Ag segregates strongly to grain boundaries and on the atomic level segregation is inhomogeneous, the segregated region extends several lattice spacings away from the boundary and the segregation process cannot be described in the framework of simple thermodynamic analyses. However, on the macroscopic level the picture is much simpler. The average concentration of the segregant in the boundary region follows the McLean's isotherm but no obvious relationship between the 'effective' segregation enthalpy and atomistically determined segregation enthalpies can be established. Furthermore, the Auger analysis assuming a homogeneous distribution of the segregant gives correct average concentrations. Thus this study shows that macroscopic analyses of the segregation are insensitive to complex

atomic level processes and although they give correct average concentrations of the segregant, no conjectures regarding the atomic level processes associated with segregation can be made on the basis of such studies. For more details see references [10, 22] and enclosed reprint (M. Menyhard, Min Yan and V. Vitek: Atomistic Versus Phenomenological Approaches to Grain boundary Segregation: Computer Modeling of Cu-Ag Alloys, *Acta Met. Mater.* **42**, 2783, 1994.)

Grain boundary structure in stoichiometric and non-stoichiometric NiAl

Grain boundaries in NiAl have been studied by computer simulation using empirical many-body central force potentials of the Finnis-Sinclair type which have been constructed for B2 NiAl by fitting a number equilibrium properties of this alloy and reproducing the asymmetric behavior of constitutional point defects in off-stoichiometric NiAl. It was found that in stoichiometric NiAl alloy boundaries with a surplus of aluminum have appreciably lower cohesive strength than the stoichiometric boundaries or boundaries with a surplus of nickel. From the structural point of view, boundaries with a surplus of aluminum possess the largest expansions and large 'holes' usually occur in the boundary regions. On the other hand, boundaries with the stoichiometric configuration or with a surplus of nickel have more compact structures. Thus Al rich boundaries are likely to be the paths of brittle intergranular cracking. At compositions with surplus of Ni, Ni will segregate to layers adjacent to the boundary plane, but not directly to the boundary plane. This was confirmed by HREM observations which are in an excellent agreement with the results of simulations. For more details see references [12, 19, 26, 32] and enclosed reprint (M. Yan, V. Vitek and S. P. Chen: Many-Body Central Force Potentials and Properties of Grain Boundaries in NiAl, *Acta Mater.* **44**, 4351, 1996.)

Structure of lamellar interfaces in TiAl: effect of directional bonding

An ordered twin boundary in the L1₀ TiAl alloy has been investigated by computer modeling and HREM. This combined study demonstrates the significance of directional, covalent type bonding for the interfacial structure. When using the ab-initio full-potential linear muffin-tin orbital method the stable structure exhibits a pronounced asymmetry. This structure is in an excellent agreement with HREM observations. In contrast, calculations employing central-force many-body potentials predict a structure the asymmetry of which is so small that it is not discernible in the HREM image. The preference for the strongly asymmetric structure can be understood in terms of the covalent d-type bonding between Ti atoms in this alloy. For more details see references [14, 17, 25, 26] and enclosed reprint (R. Siegl, V. Vitek, H. Inui, K. Kishida and M. Yamaguchi: Directional Bonding and Asymmetry of Interfacial Structure in Intermetallic TiAl: Combined Theoretical and Electron Microscope Study, *Philos. Mag. A*, **75**, 1447, 1997.)

Structure of misfit dislocations in niobium-sapphire interfaces

Formation of networks of misfit dislocations at the (0001)Al₂O₃ || (111)Nb interface was investigated using an approach which employs a very simple pair-potential to describe interaction between the metal and the substrate that contains the strength of interfacial adhesion as a parameter. These calculations demonstrate how the strength of bonding between the two materials controls both

the form of the network and the atomic structure of the cores of misfit dislocations. The calculated structures are then used to investigate related HREM images using a multislice technique. In these simulations translational symmetry along the electron beam was not assumed but for each slice of material along the beam different sub-structures were used. This is the first time such image modeling was performed. It allows us to investigate fully the effect of the dislocation intersections upon the images of the dislocation cores. Their effect is, indeed, considerable if an intersection is in the region producing the image but if not, the images of the cores of misfit dislocations are affected only marginally and HREM can capture fine details of the core structure. A direct comparison of an experimental observation in with the present simulations demonstrates this ability. For more details see references [18, 20, 33, 37] and enclosed preprint (A. Lévy, G. Möbus, V. Vitek, M. Rühle and G. Tichy: Structure of misfit dislocations in niobium-sapphire interfaces and strength of interfacial bonding: An atomistic study, *Acta Mater.*, to be published, 1999.)

Development of fully quantum mechanics based method

The goal of this research has been to develop descriptions of atomic interactions that can be employed in very large scale real space calculations of extended defects and reflect, at the same time, fully the quantum mechanical nature of bonding. In particular, the development concentrated on metallic systems with significant covalent character of bonding such as transition metals and their alloys. The approaches analyzed are all based on the tight-binding methods and employ results of ab initio calculations as guide lines (Refs. 27, 31, 34). These studies culminated in construction of bond-order potentials that are based on extensive theoretical advances of Prof. Pettifor's group at Oxford with whom an extensive collaboration has been developed (Ref. 36). This approach will be used in our future studies of systems such as transition metal silicides.

PERSONNEL

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