Topological Close Packing in Structurally Complex Intermetallics (Crystalline, Quasicrystalline and Noncrystalline)

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14. ABSTRACT

Atomic Cluster Configurations in Metallic Glasses: In connection with the model for metallic glasses proposed by D. B..Miracle [A structural model for metallic glasses. Nature Materials 3 (2004) 697-702], the structures consisting of a single solute atom surrounded by a coordination shell of solvent atoms has been examined. The possible coordination number (CN) depends, of course, on the ratio of radii of the two kinds of atom. Atomic Size Factor Criterion in Designing Bulk Metallic Glasses: In the heuristic formulations for glass forming ability by Inoue, atomic size, negative enthalpy of mixing and multicomponent criteria are used. A study of related crystalline and quasicrystalline intermetallics lends weight to the atomic size being the dominant factor. The largest size atom plays a key role in all topologically close-packed phases, even when it happens to be a minority constituent. The supertetrahedron: The various structures that can arise from supertetrahedral clusters serve to illustrate the interplay between the different approaches to visualising the geometry underlying complex material structures  sphere packing models, clusters describable as sets of nested polyhedra, network structures, and network-type configurations of polyhedra. A concise description and visualization of atomic structures is fundamental to a clear understanding of a broad range of phenomena in the expansive class of intermetallic alloys. Geometrical models based on polytetrahedral units have been adopted in order to rationalize a number of important intermetallic structures: the family of -phases, the Laves phases and the so-called ?anti-Laves? phases. An icosahedral cluster consisting of a 13 equal-sized spheres is a simple polytetrahedral unit of relevance in many crystalline, quasicrystalline and amorphous structures. A more complicated polytetrahedral unit has been emphasized  the supertetrahedron, consisting of four interpenetrating icosahedra, which was first recognised in -brass  to illustrate the complex spatial relationships in these intermetallic structures. Through several geometric models, including clusters, networks and polytetrahedral space tiling, intermetallic structures are described and illustrated using these modular units.

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Research Report

Introduction

It has become apparent in recent years that the relative atomic sizes and the proportions of the various elements have a major role in determining the kind of clustering that will take place in a complex alloy, with a consequent influence on the possibility of forming glassy (amorphous) or quasicrystalline structures. The aim of the project has been to gain insight into the kind of close-packed structures that can be formed by clusters of differently-sized atoms, idealised as ‘hard spheres’ an the influence of relatice sizes on the kinds of structure that can arise.

Atomic Cluster Configurations in Metallic Glasses

In connection with the model for metallic glasses proposed by D. B..Miracle [A structural model for metallic glasses. *Nature Materials* 3 (2004) 697-702], we have examined the structures consisting of a single solute atom surrounded by a coordination shell of solvent atoms. The possible coordination number (CN) depends, of course, on the ratio of radii of the two kinds of atom. A growing body of evidence supports the importance of solute-centered atomic clusters in the structure and stability of metallic glasses. Beyond a few simple cases, a broad account of these clusters had not been provided elsewhere. We have investigated detailed characteristics of a canonical collection of efficiently packed hard sphere clusters, considered as idealized structural elements in metallic glasses. The nomenclature, topology, geometry and packing efficiency of these clusters has been provided, up to CN = 20, and we have emphasised their relevance to the structure of metallic glasses.

Daniel B. Miracle, Eric A. Lord and Srinivasa Ranganathan. Candidate Candidate atomic cluster configurations in metallic glass structures, Materials Transactions , in press

Atomic Size Factor Criterion in Designing Bulk Metallic Glasses

In the heuristic formulations for glass forming ability by Inoue, atomic size, negative enthalpy of mixing and multicomponent criteria are used. A study of related crystalline and quasicrystalline intermetallics lends weight to the atomic size being the dominant factor. The largest size atom plays a key role in all topologically close-packed phases, even when it happens to be a minority constituent.
S Ranganathan, D B Miracle and E A Lord, Atomic Size Factor Criterion in Designing Bulk Metallic Glasses, Proceedings of the International Symposium on Frontiers of Design of Materials, Universities Press, 2006

The supertetrahedron

The various structures that can arise from supertetrahedral clusters serve to illustrate the interplay between the different approaches to visualising the geometry underlying complex material structures – sphere packing models, clusters describable as sets of nested polyhedra, network structures, and network-type configurations of polyhedra.

A concise description and visualization of atomic structures is fundamental to a clear understanding of a broad range of phenomena in the expansive class of intermetallic alloys. We have adopted geometrical models based on polytetrahedral units in order to rationalize a number of important intermetallic structures: the family of γ-phases, the Laves phases and the so-called ‘anti-Laves’ phases. An icosahedral cluster consisting of a 13 equal-sized spheres is a simple polytetrahedral unit of relevance in many crystalline, quasicrystalline and amorphous structures. We have also emphasised a more complicated polytetrahedral unit – the *supertetrahedron*, consisting of four interpenetrating icosahedra, which was first recognised in γ-brass – to illustrate the complex spatial relationships in these intermetallic structures. Through several geometric models, including clusters, networks and polytetrahedral space tiling, intermetallic structures are described and illustrated using these modular units. Geometric frustration is overcome through soft spheres, geometrically specified atom size ratios and varying atomic concentrations. Specific topological parameters that produce efficiently packed atomic structures using supertetrahedra and related polytetrahedral units have been provided.

A study of the geometry underlying the γ-alloys, the Laves phases and the so-called anti-Laves phases reveals the influence of these particular factors. The occurrence of icosahedral coordination is typical of very many complicated intermetallic structures, which may be crystalline, quasicrystalline or amorphous. The simplest possible descriptions of a γ-phase, a Laves phase and a so-called anti-Laves phase involve a 13-atom icosahedron. In the γ-phases these icosahedral clusters combine by *face sharing* and *vertex sharing*. In a Laves phase they are interpenetrating, and in an 'anti-Laves' phase (Ti_2Ni type structure) the icosahedra are *face sharing*. Among the factors that determine the kind of clusters that will form, and the way clusters combine to produce extended structures, are the *ratios of atomic sizes and the relative proportions of the elements involved*. The basic Laves and anti-Laves icosahedra are strikingly similar. Both are oblate, with symmetry $\bar{3}m$; in both cases a central atom is coordinated to a skew hexagonal ring of large atoms and two triangles of small atoms above and below the ring. In one case, the central atom is small, in the other, it is large.

E. A. Lord, S. Ranganathan & D. B. Miracle. The supertetrahedron in complex intermetallic clusters (to be published)