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FLOW DEFECTS, SHEAR LOCALIZATION, AND DEFORMATION IN METALLIC GLASSES: ATOMISTIC SIMULATIONS AND A MESOSCOPIC THEORY*

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Shear banding is the primary deformation mode in metallic glasses. It occurs at relatively low temperature and over a wide range of strain rates. Due to the lack of long-range structural order, identification of the defects underlying the shear banding process and understanding of the deformation mechanism itself have not been fully comprehended. We approached this problem with two efforts, (1) Identifying the flow defects using atomistic simulations, and (2) formulating a theory to predict and rationalize the shear localization and general deformation phenomena (shear band multiplication/branching, shear band nucleation and propagation, shear band thickness and shear band spacing, etc.). These efforts allow us, for the first time, to have a glimpse of the microscopic defect process and a coherent understanding of shear banding. Our work from continuum mechanics also indicates that shear band is a unique entity that is fundamentally different from dislocations and cracks.

CONCEPT OF THE CLUSTER OF SHORT RANGE ORDER AND THE GLASS FORMING ABILITY IN MULTICOMPONENT LIQUID

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The paper is composed of three parts: (1) The concept of the cluster of short range order in multicomponent liquid is elucidated. This concept not only describes the neighbor relationship between constituent atoms, but also reflects the bounding abilities between different atomic clusters with the composition similar to corresponding well-defined compounds or intermetallics. A parameter (f) is used to express the cluster of short-range order in composition. (2) A thermodynamic model of mole fraction of the clusters of short-range order is completely established. Corresponding numerical simulation programs are also designed, which is composed of the Fitbin subroutine for the activity coefficient of constituents, multivariant linear adapting and multielement coexisting equilibrium subroutine for the calculation of all short-range orders. The number of every kind cluster can be determined depending on the composition of the alloy, chemical bounding energies of the clusters and temperature. (3) The relationship between the thermodynamic properties and the glass forming ability is investigated. The multicomponent chemical short range order undercooling principle is proposed to predicate the glass forming ability. In this part, The glass forming ability of some typical ternary systems, such as Zr-Ni-Cu, Zr-Al-Cu, Pd-Ni-P, is evaluated. The optimal glass forming compositions of these alloys are predicated. Effects of the fourth constituent on the glass forming ability in quarternary systems are discussed in detail. The correlation between the thermodynamic properties of the fourth constituent and the glass forming ability is investigated.

STRUCTURE-FORMING PRINCIPLES FOR AMORPHOUS METALS

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After extensive experimental and computational research over the past several decades, there is still a poor understanding regarding the structure of metallic glasses. The clearest picture exists for metal-metalloid glasses, where detailed spectroscopic data, coupled with atomic simulations, have identified a specific atomic configuration, a capped trigonal prism atomic cluster, which is responsible for the observed short-range atomic ordering. However, there is still no systematic model which describes the atomic structures which may exist beyond the first coordination shell. Further, the chemical and topological aspects of metal-metalloid glasses differ, sometimes strongly, from many other well-established metallic glass systems, so that the specific atomic configurations which describe the structure of these glasses are not expected to apply broadly to other metallic glass systems. The purpose of this research is to propose specific structure-forming principles which may govern the atomic structures of metallic glasses. Earlier concepts of high atomic packing efficiency will be extended and applied to the topological systems which represent most metallic glass alloys. The concept of high packing efficiency has direct and specific implications regarding the topology, and hence the composition, of metallic glasses. Atomic packing efficiency also governs the short- and medium-range atomic configurations. Each of these concepts will be presented and discussed. Possible atomic configurations will be explored and presented, and consistency with experimental observations will be provided and discussed. Suggestions for experimental and computational studies to explore these concepts will be provided.