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Extended Abstract

Role of Atomic Bonds on the Structure and Dynamical Properties of Glass-Forming Metallic Alloy Liquids

Gangopadhyay Anup Kumar

Abstract

Bulk metallic glasses have attracted much attention over the last two decades because of their superior physical (mechanical, magnetic, to name a few) properties compared to the crystalline counterparts. Like other glasses (oxides, molecular, and polymers), the dynamical properties (viscosity, diffusion coefficient) of the equilibrium and supercooled (metastable liquid below the melting temperature) metallic liquids change by 12-14 orders of magnitude between the melting and glass-transition temperatures. This talk will focus on the dynamical and structural properties of these equilibrium and supercooled liquids measured by our group. Such measurements have been possible by applying a novel electrostatic levitation (ESL) technique that allows contactless measurements to be made on levitated liquid drops under high-vacuum conditions in contamination-free environments. These measurements reveal a deep connection between chemical bonds, liquid structure, and dynamical properties. A particularly interesting result is that the basic mechanism of glass-transition starts in the liquid at a "crossover" temperature far above the glass transition and equilibrium melting temperatures.

Introduction:

Dr. Gangopadhyay is a senior scientist in the Department of Physics at the Washington University in St. Louis, USA. His primary focus of research is in the field of supercooled liquids and glasses, especially bulk metallic glasses studied under terrestrial and microgravity conditions. Alongside, he has made original contributions in the areas of magnetism, superconductivity, and plasmonics, in bulk and artificial nanostructures. He has published close to one hundred papers with about 3000 citations (h-index: 28) in many high-profile international journals, encompassing the fields of physics, chemistry, materials science, and metallurgy. Several of these publications became news items in the science media, such as in the Physics Today, bulletins of the APS (Argonne) and NASA. He is a member of the American Physical Society, a former Humboldt Fellow, and associated with many international journals. He had his formal education at the Indian Institute of Technologies at Kanpur and Kharagpur in India.

Metallic glass (MGs) has many unique properties like rarity , low Young's modulus , and so on. These unique physical and mechanical properties attract much attention on their application in manufacturing production. While, structural properties like complete absence of the long-range order and most MGs are contains equal or quite ternary constituent which complex factors make that the atomic level structure of metallic glass still haven't documented by researchers. The limited methods and data sets obtained by experiment make the acknowledge in uncovering atomic structure of melt states of alloy, and therefore the supercooled liquid about the alloy is absent as well. These messages are important to enhance and increase the understanding of MGs, as we all know that glasses are essentially frozen liquid made by quenching of their high-temperature melts. Computer simulation method is an useful gizmo to get structure messages of melt and therefore the supercooled liquid. The static, dynamical properties as a function of temperature can also be investigated by ab initio MD simulation. The atomic level rearrangement consists of both local topological structure change and chemical reordering and evolution of electronic properties of the Al87Ni7Nd6 and Ca50Mg20Cu30 alloy during the glass transition process

Atomic packing in metallic glasses is not completely random but displays various degrees of structural ordering. While it is believed that local structures profoundly affect the properties of glasses, a fundamental understanding of the structure–property relationship has been lacking. In this article, we provide a microscopic picture to uncover the intricate interplay between structural defects and dynamic properties of metallic glasses, from the perspective of computational modeling. Computational methodologies for such realistic modeling are introduced. Exploiting the concept of quasi-equivalent cluster packing, we quantify the structural ordering of a prototype metallic glass during its formation process, with a new focus on geometric measures of subatomic "voids." Atomic sites connected with the voids are found to be crucial in terms of understanding the dynamic, including vibrational and atomic transport, properties. Normal mode analysis is

Gangopadhyay Anup Kumar
Department of Physics, Washington University , USA

performed to reveal the structural origin of the anomalous boson peak (BP) in the vibration spectrum of the glass, and its correlation with atomic packing cavities. Through transition-state search on the energy landscape of the system, such structural disorder is found to be a facilitating factor for atomic diffusion, with diffusion energy barriers and diffusion pathways significantly varying with the degree of structural relaxation/ordering.

Discussion and Conclusion :

Metallic liquids, though lacking order, do exhibit interatomic distances within a narrow distribution. As these liquids cool into the glassy state, they tend to form lower-energy local clusters. This has been known as topological short-range ordering (SRO). One typical example is the hypothesis of icosahedral clusters in metallic mercury, as predicted by Frank12 half a century ago. The formation of icosahedral clusters in glasses is called icosahedral short-range order (ISRO). Over the years, much progress has been made in terms of understanding the SRO of MGs. In addition to ISRO, we now know that MGs may exhibit other types of SRO, depending on the chemistry of the system; For instance, in the transition metal–metalloid (TM–M) MG Pd-Si, the tricapped trigonal prism (TTP) type of SRO may be dominant.10,16,19 Knowledge of SRO is fundamental because it can be regarded as the basic building unit for MGs, and larger structural organizations on the medium range (a few atomic shells) are spatial extensions of SRO.16,17,20 Meanwhile, many physical properties are very sensitive to SRO, such as atomic packing density, electron, magnetic, and x-ray spectroscopy, etc. While much recent interest has extended to the structural order beyond the short range, our understanding of the short-range structure of glasses is still far from being complete.