ABSTRACT

In the present thesis study, we combined molecular dynamics (MD) simulations and experiments to systematically investigate the Debye-Grüneisen thermal expansion effect and configurational potential energy dependence of elastic properties for glassy states of amorphous metals, and utilized the correlation between elastic properties and fragility as a guiding tool to design and to develop novel bulk metallic glasses.

It is extremely important to create appropriate interatomic potentials, generate glassy configurations, and study the local structures of the system before moving to the next step. An effective tight-bonding, RGL-type, n-body force field for the binary Cu-Zr alloy system was constructed and employed in MD simulations. Partial radial distribution functions, coordination numbers, and Honeycutt Andersen (HA) indices have been calculated to analyze the local structures of $Cu_{46}Zr_{54}$ metallic glass.

We report the strong dependence of elastic properties on configurational changes in a Cu-Zr binary metallic glass assessed by molecular dynamics simulations. By directly evaluating the temperature dependence and configurational potential energy dependence of elastic constants, we show that the shear modulus dependence on the specific configurational inherent state of metallic glasses is much stronger than the dependence on Debye-Grüneisen thermal expansion.

We present the isothermal equation of state (EOS) in a wide range of temperatures and pressures by carrying out molecular dynamics simulations on a simple binary model metallic glass. A universal form of EOS proposed by Vinet et al. is utilized to fit the data,

assuming no phase transitions. Pressure-induced cavitation was observed in glassy states and liquids from our simulations. The thermodynamic limit of instability and kinetic limit of instability of the cavitation behavior were analyzed. Negative pressure is critical to trigger the cavitation. The cavitation barrier height was estimated using the classical nucleation theory. The intrinsic origin of why and how Poisson's ratio or the ratio of G/B is involved in the deformation and fracture behavior of glasses is discussed.

The compositional dependence of thermal and elastic properties of Cu-Zr-Be ternary bulk-metallic-glass-forming alloys was systematically studied. There exists a linear relationship between the glass transition temperature, T_g, and the total Zr concentration. Shear modulus G decreases linearly with increasing Zr concentration as well. The results also show that T_g, G, and Poisson's ratio, ν, are very sensitive to changes in compositions. Low T_g, low G, and relatively high ν can be achieved with high Zr and Ti concentration.

Lightweight Ti-based bulk amorphous structural metals with more than double the specific strength of conventional titanium alloys have been discovered. Thermal, elastic, and mechanical properties of these metallic glasses were studied and are presented. These amorphous alloys exhibit good glass-forming ability, exceptional thermal stability, and high strength. The research results have important implications for designing and developing low-density bulk metallic glasses. The technological potential of this class of lightweight Ti-based glassy alloys as structural metals is very promising.

The exceptional processability and large supercooled liquid region of bulk amorphous metals makes them highly promising candidates for thermoplastic processing. We report a lightweight (ρ = 5.4 g/cc) quaternary glass-forming alloy, $Zr_{35}Ti_{30}Cu_{8.25}Be_{26.75}$, having the largest supercooled liquid region, (ΔT = 159 K at 20 K/min heating rate) of any known bulk-glass-forming alloy. The alloy can be cast into fully amorphous rods of diameter ~ 1.5 cm. The undercooled liquid exhibits an unexpectedly high Angell Fragility of m = 65.6. Based on these features, it is demonstrated that this alloy exhibits "benchmark" characteristics for thermoplastic processing. We report results of mechanical, thermal, rheological, and crystallization (TTT-diagrams) studies on this new material. The alloy exhibits high yield strength and excellent fracture toughness, and a relatively high Poisson ratio compared with other Zr- or Ti-based glasses. Simple micro-replication experiments carried out in open air using relatively low applied pressures demonstrate superior thermoplastic processability for engineering applications.

Starting from the two binary bulk-glass formers in the Cu-Zr system, we systematically investigated the compositional dependence of glass formation, and thermal, elastic and mechanical properties in the Cu-Zr-Ag ternary alloys. Both the $Cu_{(50-x)}Zr_{50}Ag_x$ and $Cu_{(64-x)}Zr_{36}Ag_x$ series alloys show a good combination of high glass-forming ability and high Poisson's ratio.

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