Molecular Dynamics Simulations on Glass Forming Ability and Mechanical Properties of Both Cu-Zr-(Al, Ti) and Cu-Ni Metallic Glasses

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Computational materials have become an important tool in materials science and play an increasingly important role in modern technology. In this conference, we will present our recent work in atomistic computer simulations by classical molecular dynamics method, in order to understand the structures on short-range order level and the relationships between structure and properties in metallic glass. First, we will show the molecular dynamics simulations to understand the glass forming ability in both Cu-Zr-Al and Cu-Zr-Ti metallic glasses by using the EAM-FS potentials. Despite the wide study on these systems, there are significant challenges in understanding their glass forming ability and thermophysical properties as function of the viscosity evolution. Moreover, obtaining the simulated mechanical properties is also relevant in metallic glass development. Particularly, the effect of cooling rate and system size effects on the glass structure will be addressed here. Secondly, we will present a study related to the GFA in Cu-Ni alloys under different cooling rates and their relationship between the structure and properties such as crystallization and they strain-stress behaviour. These findings show that computational materials methods, when carefully performed and validated by experiments, are very useful to elucidate the complex structure features and structural origin of materials peculiarities and contribute to the research and design of new engineering materials. !