

Molecular dynamics studies of metallic glasses

Thesis by

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Abstract

The thermodynamic, structural, and mechanical properties of metallic glasses are studied using molecular dynamics simulations. Molecular dynamics provides a computational framework to simulate the movement of interacting atoms in response to external perturbations, such as changes in temperature or pressure. In this thesis, a Sutton-Chen potential was chosen to describe the many-body interactions in metals and alloys. Our first application for this approach is to develop a simple model to derive the thermodynamic properties of metallic alloys (Chapter 2). Based on this model, we demonstrate that the glass transition is thermodynamically sensitive to differences between atomic radii and that there is an optimal difference for glass formation. Next, we extend these simulations to elucidate the details of structural organization in the glass (Chapter 3). We find that the liquid phase is characterized by a local five-fold symmetry, which becomes more prominent as the glass phase forms. This five-fold symmetry is related to the formation of icosahedral structures. The mechanical properties of glasses are also investigated and it is found that shear localization, which accompanies a sharp drop in the stress-strain curve, occurs at 45 degree with respect to the loading axis (Chapter 4). The generation of free volume is found to be the dominant mechanism that leads to shear localization, rather than adiabatic heating. Finally, generic first principle potentials are constructed to guide the experimental development of AlTiNi based metallic glasses (Chapter 5). Together, the results from these simulations improve our understanding of the thermodynamic, structural, and mechanical properties of metallic glasses and will aid computer-driven materials design.

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