Molecular dynamics studies of metallic glasses

Thesis by

Hyon-Jee Lee

In Partial Fulfillment of the Requirements

for the Degree of

Doctor of Philosophy

California Institute of Technology

Pasadena, California, USA

2003

(Defended May 21, 2003)

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.

Acknowledgements

I have been fortunate enough to meet many brilliant and warm-hearted people during my time at Caltech. Foremost, I owe a debt of gratitude to my two advisors: Professor William L. Johnson, who first directed my attention to metallic glasses and Professor William A. Goddard, who introduced me to the field of computational chemistry. Working with them was an honor. I also would like to thank Professor Brent Fultz, Professor Ersan Ustundag, and Professor Michael Cross for being in my thesis committee.

I also thank my friends and colleagues in Johnson group and Goddard group who have so freely given me the benefit of their expert knowledge. Unfortunately, they are too numerous for me to mention them all, but I am particularly indebted to Dr. Tahir Cagin, Dr. Alejandro Strachan, Dr. Yue Qi, Dr. Goufeng Wang, Dr. Qing Zhang and Peng Xu for many stimulating discussions.

I also thank my teachers and professors prior to Caltech for advice and for the excellent education they provided. While I was at KAIST, Professor O Ok Park, Professor Seung Bin Park, and Professor Seung-Man Yang encouraged me to continue my studies at Caltech. Especially Professor Seung-Man Yang, who was my advisor in Master's program and with whom I wrote my first scientific paper.

Finally, I would like to thank my family for their love and support throughout graduate school. They were encouraging and truly believed in me. Also, I thank Christopher Voigt for helping me in every aspect of my life at Caltech-both personal and professional.

Table of Contents