Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Short- and Medium-Range Order in Amorphous Zr_2Ni Metallic Alloy LI HUANG, CAI-ZHUANG WANG, SHAO-GANG HAO, Ames Laboratory, U.S. Department of Energy, MATTHEW J. KRAMER, Department of Materials Science and Engineering; Ames Laboratory, U.S. Department of Energy, KAI-MING HO, Department of Physics, Ames Laboratory, U.S. Department of Energy — Icosahedral clusters are commonly believed to be the key building blocks in many metallic glasses. Here we propose a structural model for Zr_2Ni metallic glass which has a small fraction of icosahedral clusters. By analyzing the correlation between the local structure and dynamics in the undercooled liquid and glass, we show that the formation of metallic glass in this system can be attributed to the slow dynamics of $< 0, 2, 8, 1 >$ and $< 0, 2, 8, 2 >$ Ni-centered Voronoi polyhedra. There is a high proportion of less mobile $< 0, 2, 8, 4 >$, $< 0, 2, 8, 5 >$, $< 0, 1, 10, 4 >$, and $< 0, 1, 10, 3 >$ Zr-centered clusters on the first shell of the two types of Ni-centered clusters. These special Ni- and Zr-centered clusters arrange together to form a string-like backbone network in the metallic glass.

Li Huang
Ames Laboratory, U.S. Department of Energy

Date submitted: 18 Nov 2009 Electronic form version 1.4