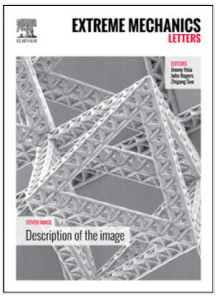
Accepted Manuscript



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PII: S2352-4316(16)30035-9
DOI: http://dx.doi.org/10.1016/j.eml.2016.07.009
Reference: EML 203

To appear in: *Extreme Mechanics Letters*

Received date: 13 February 2016
Revised date: 23 June 2016
Accepted date: 26 July 2016

Please cite this article as: M. Jafary-Zadeh, R. Tavakoli, D.J. Srolovitz, Y.-W. Zhang, Thermally induced failure mechanism transition and its correlation with short-range order evolution in metallic glasses, *Extreme Mechanics Letters* (2016), http://dx.doi.org/10.1016/j.eml.2016.07.009

Thermally induced failure mechanism transition and its correlation with short-range order evolution in metallic glasses

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Abstract

The effect of temperature on the short-range order (SRO) structures, deformation mechanisms and failure modes of metallic glasses (MGs) is of fundamental importance for their practical applications. However, due to lack of direct structural information at the atomistic level from experiments and the absence of previous molecular dynamics (MD) simulations to reproduce experimental observations over a wide range of temperature, this issue has not been well understood. Here, by carefully constructing the atomistic models of $Cu_{64}Zr_{36}$ and $Fe_{80}W_{20}$ MGs, we are able to reproduce the major deformation modes observed experimentally, *i.e.* single shear banding (SB) at low temperatures, multiple shear-bandings at intermediate temperatures and homogeneous plastic flow at elevated temperatures. By examining the evolution of SRO, we find that the different failure modes exhibit distinctively different full-icosahedron (FI) evolution pathways at different temperatures. Specifically, at low temperatures, the FI concentration first deceases to a minimum, then recovers slightly, and finally comes to a plateau; at intermediate temperatures, it first decreases and then reaches a plateau; while at elevated temperatures, it decreases simply monotonically. These different pathways arise from the dynamic competition between the destruction and recovering of FI clusters. We further show that the local softening caused by the destructions of FI clusters is crucial for the formation of localized shear planes and further shear bands. Since our simulations exhibit the same trend for both MG systems, it is expected that these findings may be generic for a wide range of MGs.

Keywords: Metallic glasses; failure mechanisms; temperature effect; molecular dynamics; atomistic structure; mechanical properties; brittle; ductile; plastic flow.