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Thermally Induced Deformation in Metallic Glass: the Activations and Relaxations¹ YUE FAN, Oak Ridge National Laboratory, TAKUYA IWASHITA, TAKESHI EGAMI, University of Tennessee — Thermally induced deformation in metallic glasses was investigated by sampling the potential energy landscape (PEL) and probing the changes in the atomic properties (e.g. energy, displacement, stress). The complete deformation processes consist of two stages: the activation (i.e. trigger, from initial minima to nearby saddle states on PEL), and relaxation (i.e. from saddle states to final minima on PEL). We show that the activation stages are triggered by local rearrangements of a small number of atoms, typically 5 atoms in average. Surprisingly, the individual triggers are invariant of the cooling history or elastic structure of the system. However, the organizations between different trigger centers can be varied and are related to the overall stability of the system. On the other hand, relaxation stages consist of two branches, a localized branch, and a cascade branch. While the localized branch is insensitive to the cooling history the system, the cascade branch is highly related with the processing conditions. In particular, for a faster quenched system, the cascade relaxation is found more prominent than in a slowly quenched system.

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