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Molecular dynamics analysis of relaxation state control of metallic glasses via thermal and mechanical loadings NARUMASA MIYAZAKI, Osaka Univ, MASATO WAKEDA TEAM, SHIGENOBU OGATA TEAM¹ — Metallic glasses have excellent properties such as high fracture toughness and large elastic strain limit, high corrosion resistance, however they generally exhibit brittle fracture mode at ambient temperature. Since mechanical properties of metallic glasses depend on the degree of relaxation state, it can be tuned by controlling the degree of relaxation state. In this computational study, we focus on a method to control the relaxation state of metallic glasses via thermal and mechanical loadings. Using molecular dynamics, a metallic glass model was applied thermal loading composed of heating, annealing and quenching with external stress. Here, different annealing temperatures ranging from $0.5T_g$ to $1.5T_g$ [K] (T_g : the glass transition temperature), and external stresses ranging from 0 to 10 [GPa] were applied. We found that thermal loading below T_g leads the metallic glasses more relaxed state. On the other hand, the external stress brings metallic glasses less relaxed state, because external stress changes the shape of potential energy surface. These finding allow us to control the relaxation state of metallic glasses.

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