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Vitrification of a monatomic simple liquid in two dimensions[1]
TAKASHI ODAGAKI, Tokyo Denki University, TOMOKO MIZUGUCHI, Kyushu University — We investigate vitrification and crystallization process of a monatomic system by molecular dynamics simulation, where atoms interact via Lennard-Jones-Gauss potential. We first determine the time-temperature-transformation diagram by observing the crystallization time of the rapidly quenched state from the melt. The crystallization time becomes shortest at a certain temperature T*. The glassy state at low temperatures is shown to be fairly long-lived. In order to examine atomic mechanism of the crystallization, we introduce a modified incoherent intermediate scattering function which measures the structural correlation to a target structure. We show that the crystallization above and below T* take different paths. We also determine the free energy landscape (FEL) and show that the atomic dynamics is consistent with the FEL picture of the glass transition.

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