

Abstract Submitted
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FEL approach to the crystallization of super-cooled liquids¹

TAKASHI ODAGAKI, ANJU OKADA, Tokyo Denki University — The crystallization time of most super-cooled liquids as a function of temperature (time-temperature-transformation (TTT) diagram) show a nose-shaped form, namely near the melting temperature it is an increasing function of temperature and at much lower temperatures it becomes a decreasing function of temperature. The former behavior is believed to be controlled by the thermodynamics and the latter is governed by the slow dynamics. Exploiting the merit of the free energy landscape (FEL) approach which can handle both thermodynamic and dynamic processes in the same frame work, we investigate the crystallization of super-cooled liquids as the first passage process of a representative point to the crystalline basin in the FEL. We first show that the crystallization time can be related to the eigenvalues of the transition matrix which governs the stochastic dynamics of the representative point in the FEL. We apply this formalism to various structures of the FEL which include the small world and the scale free network. We show that the TTT diagram is sensitive to the structure of the FEL, indicating the possibility of obtaining the structural information from the TTT diagram.

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