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Homogeneous melting in the microcanonical ensemble

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Introduction

Melting is a common phenomenon in our daily life, and although it is understood in thermodynamic (macro-scopic) terms, the transition itself has eluded a complete description from the point of view of microscopic dynamics. While there are studies of metastable states in classical, glassy systems and other models.

Our work is oriented to the study of the melting process of superheated solids, which is believed to be caused by thermal vacancies in the crystal or by the occupation of interstitial sites [1]. When the crystal reaches a critical temperature T_{LS} above the melting point T_m, it becomes unstable and a collective self-diffusion process is triggered. These studies are often observed in a microcanonical environment, revealing long-range correlations due to collective effects, and from theoretical models using random walks over periodic lattices. Our results suggest that the cooperative motion made possible by the presence of vacancy-interstitial pairs (Frenkel pairs) [2] above the melting temperature induces long-range effective interatomic forces even beyond the neighboring fourth layer [3]. From microcanonical simulations it is also known that an ideal crystal needs a random waiting time until the solid phase collapses [4]. Our results also point towards a description of these waiting times using a model in which there is a positive, unspecified quantity X that accumulates from zero in incremental steps, until X exceeds a threshold value X^* that triggers collapse [5].

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