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Configurational Density of States and the Melting of Simple Solids.

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Introduction

Homogeneous melting of crystals is mediated by forming a metastable solid phase, in which complex defects are created. Microcanonical computer simulations have shown this phenomenon during the last two decades despite the difficulty of studying this process. The so-called Z-method [1] is one of the most used computer simulations to determine the melting point of materials and the atomistic behavior of the phase transition. The Z-method is based on the empirical observation that the superheated solids at the limit of superheating temperature have the same internal energy as the liquid at the melting temperature. By combining the Z-method and a recently proposed model for the configurational density of states (CDOS) [2], we can study the melting of simple solids, which is presented here. The CDOS is a function that describes the proportion of states with a specific energy value for a given system.

We analyze the behavior of the microcanonical and canonical caloric curves for the previously mentioned model. Mainly, we explore the configurational density of states of simple solids in the context of melting from the superheated state. The study was realized numerically in the Z-method via atomistic molecular dynamics. The model reproduces a first-order phase transition with metastable regions; therefore beneficial to describe aspects of the melting transition. Within this model, transcendental equations connecting the superheating limit, the melting point, and the specific heat of each phase are presented and numerically solved. The results suggest that the elements of microcanonical Z curves can be extracted from simple modeling of the CDOS.

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