Dynamics of vacancies in two-dimensional Lennard-Jones crystals

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Vacancies represent an important class of crystallographic defects, and their behaviors can be strongly coupled with relevant material properties. In this work, we study the dynamics of generic n-point vacancies in two-dimensional Lennard-Jones crystals in several thermodynamic states. Simulations reveal the spectrum of distinct, size-dependent vacancy dynamics, including the nonmonotonously varying diffusive mobilities of one-, two- and three-point vacancies, and several healing routines of linear vacancies. Specifically, we numerically observe significantly faster diffusion of the two-point vacancy that can be attributed to its rotational degree of freedom. The high mobility of the two-point vacancies opens the possibility of doping two-point vacancies into atomic materials to enhance atomicmigration. The rich physics of vacancies revealed in this study may have implications in the engineering of defects in extensive crystalline materials for desired properties.

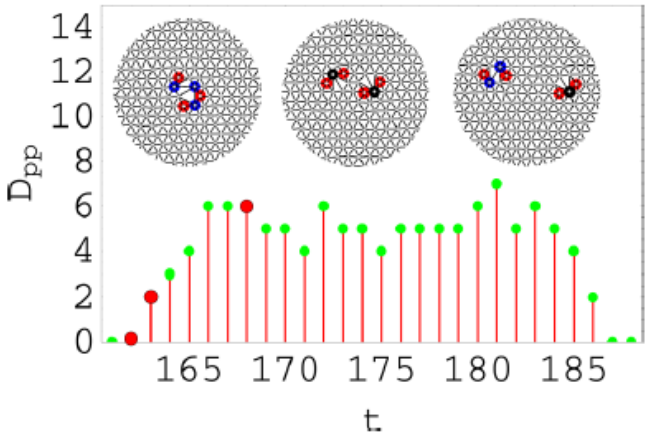

Figure: the distance *Dpp* between two one-point vacancies vs time at T = 0.25. The three configurations in the insets are at t = 162, 163, and 168, in the unit of 25τ0. The red, blue, and black dots represent five-, seven-, and eight-fold disclinations, respectively.

We thank the financial assistance of the U.S. Department of Commerce, National Institute of Standards and Technology as part of the Center for Hierarchical Materials Design (CHiMaD), the Office of the Director of Defense Research and Engineering (DDR&E) and the Air Force Office of Scientific Research (AFOSR).