Research Highlight

DYNAMICS OF VACANCIES IN TWO-DIMENSIONAL LENNARD-JONES CRYSTALS

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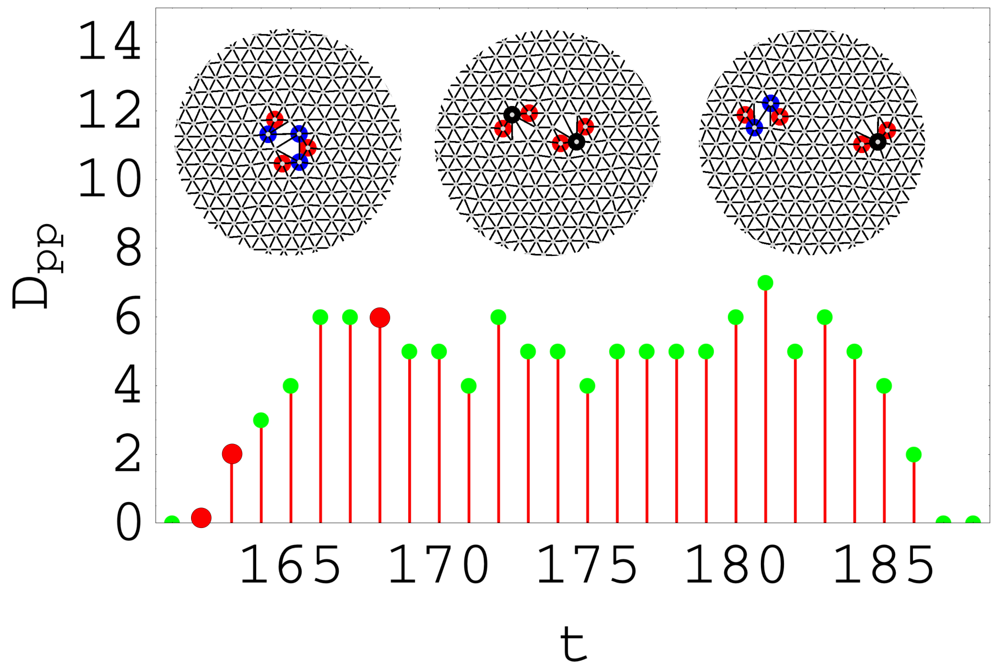

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Scientific Achievement

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 atomic migration. The rich physics of vacancies revealed in this study may have implications in the engineering of defects in extensive crystalline materials for desired properties.

Significance

The dynamics of crystallographic defects influences many aspects of crystalline materials. The two dimensional Lennard-Jones crystal has been extensively used to describe the physical properties of materials such as metals and nanoparticles. This study shows that it also serves to perform fundamental researches on the defect dynamics. Counterintuitive results emerge in the two dimensional Lennard-Jones crystal: two-point vacancies diffuse significantly faster than one-point and three-point vacancies. In addition, rich dynamics of vacancies with different sizes are found in simulations. These results may be useful as well with more complex and realistic three-dimensional structures.

Citation Information

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