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Effects of Applied Strain on Nanoscale Self-Interstitial Cluster Formation in BCC Iron

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Abstract

The effect of applied strains on the configurational evolution of self-interstitial clusters in BCC iron (Fe) is explored with atomistic simulations. A novel cluster configuration is discovered at low temperatures (< 600 K), which consists of $\langle 110 \rangle$ dumbbells and $\langle 111 \rangle$ crowdions in a specific configuration, resulting in an immobile defect. The stability and diffusion of this cluster at higher temperatures is explored. In addition, an anisotropy distribution factor of a particular $[hkl]$ interstitial loop within the family of $\langle hkl \rangle$ loops is calculated as a function of strain. The results show that loop anisotropy is governed by the angle between the stress direction and the orientation of the $\langle 111 \rangle$ crowdions in the loop, and directly linked to the stress induced preferred nucleation of self-interstitial atoms.

Keywords: `self-interstitial cluster, strain effect, anisotropy distribution factor, dislocation loop, molecular dynamics (MD)`

1. Introduction

The formation of point defects, such as self-interstitial atoms (SIAs), vacancies and clusters of these species, through the interaction between energetic particles and atoms in materials, has been studied for decades [1]. In body-centered cubic (BCC) iron (Fe), the ground state configuration of an SIA has

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