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Identifying self-interstitials of bcc and fcc crystals in molecular dynamics

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HIGHLIGHTS

- Max-Space Clustering (MSC) method is developed to identify interstitials in crystals.
- MSC provides a structured way to identify the temperature dependent cut-off radius.
- It is compared with widely used sphere methods and found to be better.
- MSC coupled with graph tree optimization can be used to obtain diffusion trajectory.
- Cascade simulations of Fe, W are carried out and results are compared with various methods.

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ABSTRACT

Identification of self-interstitials in molecular dynamics (MD) simulations is of critical importance. There exist several criteria for identifying the self-interstitial. Most of the existing methods use an assumed cut-off value for the displacement of an atom from its lattice position to identify the self-interstitial. The results obtained are affected by the chosen cut-off value. Moreover, these chosen cut-off values are independent of temperature. We have developed a novel unsupervised learning algorithm called Max-Space Clustering (MSC) to identify an appropriate cut-off value and its dependence on temperature. This method is compared with some widely used methods such as effective sphere (ES) method and nearest neighbor sphere (NNS) method. The cut-off radius obtained using our method shows a linear variation with temperature. The value of cut-off radius and its temperature dependence is derived for five bcc (Cr, Fe, Mo, Nb, W) and six fcc (Ag, Au, Cu, Ni, Pd, Pt) crystals. It is seen that the ratio of the cut-off values "r" to the lattice constant "a" lies between 0.23 and 0.3 at 300 K and this ratio is on an average smaller for the fcc crystals. Collision cascade simulations are carried out for Primary knock-on Atom (PKA) energies of 5 keV in Fe (at 300 K and 1000 K) and W (at 300 K and 2500 K) and the results are compared using the various methods.

1. Introduction

The reactive diffusive transport of radiation-induced point defects (interstitials and vacancies) is widely studied to estimate micro-structural modifications in the structural materials of nuclear reactors. Radiation induced point defects can undergo thermally activated diffusion at reactor operating temperatures. This can lead to either annihilation (recombination of an interstitial with a vacancy) or clustering of defects [1, 2]. Recombination of interstitials with vacancies reduces the radiation damage whereas the further condensation of defect clusters into extended defect clusters such as dislocation loops or voids enhance the material degradation [3]. Hence, it is very important to identify point defects and understand their migration and recombination mechanisms to have a comprehensive knowledge of radiation damage.

Molecular Dynamics (MD) provides valuable insights into the understanding of defect stability, defect recombination and defect migration mechanisms by following the principles of Classical Mechanics as formulated by Newton and Hamilton [4]. There are

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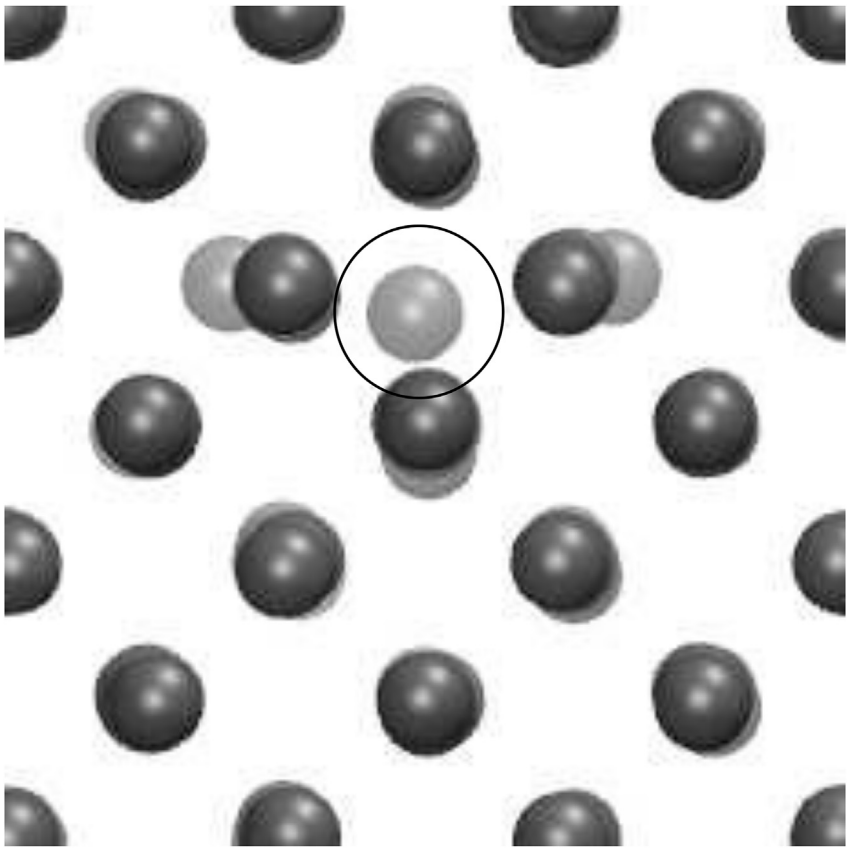

Fig. 1. SIA configuration.

several methods which use different criteria to identify the interstitials in MD. We present a short overview of these methods in Section 2. A similar discussion can also be found in Ref. [5]. Most of these methods are based on some assumed cut-off values which estimate the number of interstitials approximately in cascade simulations at low temperatures and overestimate them at high temperatures [5]. In the interstitialcy diffusion mechanism an interstitial displaces a lattice atom, thereby making the lattice atom an interstitial and hence the identity of interstitial keeps on changing [6]. Moreover there exist crowdion and dumbbell like structures which make it further difficult to identify the true number of interstitials. We have developed a novel unsupervised learning algorithm called Max-Space Clustering (MSC) to (i) identify interstitials and coupled it to a graph-tree data structure to obtain diffusion trajectories from MD simulations [7] and (ii) identify defects in MD simulations of collision cascades.

MD simulations of interstitialcy diffusion for five bcc and six fcc crystals with a single interstitial have been carried out at different temperatures. The MSC method is used to obtain the cut-off value of displacement of an atom from its lattice position so as to classify it as a probable interstitial. We study the temperature dependence of this cut-off value. The cut-off radius obtained by using this method is compared with the cut-off radii of some widely used methods such as the nearest neighbor sphere (NNS) method [8] and the effective sphere (ES) method [9]. We show that the cut-off radius obtained using MSC method shows a linear increase with the temperature. MD simulations of collision cascades in Fe at 300 K and 1000 K and in W at 300 K and 2500 K have been carried out. The results are analyzed using the cut-off radius obtained from the MSC algorithm and compared with the results using the cut-off radii from the ES, NNS and WS methods.

The Max-Space Clustering algorithm is described in Section 3, MD simulations are described in Section 4.1, 4.2 and the results are presented in Section 5.1, 5.2. Though the present work deals with interstitialcy diffusion and cascade simulations, the MSC method can be applied to any phenomenon which involves the identification of point defects in MD simulations.

2. Defect analysis–existing methods

MD has become a primary tool to study the atomistic processes. Though numerous methods are present for identification of interstitials, we perform a comparative study of few commonly used methods.

2.1. Commonly used methods

Several methods have been proposed to identify the interstitials from MD simulations [8-13]. They consider properties of the individual atom like potential energy [12], atomic bonding [13] to identify the interstitial or they use geometric methods like the Wigner-Seitz method and a host of sphere methods. These methods check for atoms within spheres of specified radius centered at ideal lattice positions of the atoms. Some researchers use method of time averaging of atomic coordinates to identify the atom which has the largest average displacement from its lattice site [14–16]. The geometric methods are as follows:

1 Wigner-Seitz (WS) method
2 Lindemann's Sphere (LS)method
3 The Nearest Neighbor Sphere (NNS) method
4 The Effective Sphere (ES) method