

Defect Cluster Classification, Morphology and Stability Studies from Molecular Dynamics Simulations of Collision Cascades

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A brief introduction to the earlier classification of defect clusters using artificial Intelligence techniques is presented [1]. A new method of classifying defects using a graph data structure has been developed [2]. The advantages of the new method, viz. (i) obtaining the internal morphology of the defect cluster (ii) orientation of its homologous components, etc., will be discussed. We apply the new method to analyze collision cascades in W at 100 - 200 keV primary knock-on atoms (PKA) using three different interaction potentials [3]. Results of the distribution of different defect clusters for the three potentials show that there exist a basic set of six defect morphologies in W. The fraction of the different morphologies vary based on the potential used.

Preliminary results of the stability of the $\langle 100 \rangle$ defect clusters of varying sizes using the three interatomic potentials are then presented.

References

1. Classification of clusters in collision cascades, U Bhardwaj, AE Sand, M Warriar, Computational Materials Science 172 (2020) 109364.
2. Graph theory based approach to characterize self interstitial defect morphology, Utkarsh Bhardwaj, Andrea Sand, M Warriar, Computational Materials Science 195 (2021) 110474.
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