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An impasse in molecular dynamics simulations of primary damage in W: which interatomic potential yields the correct defect morphologies?

Five widely used interatomic potentials (IAP) for tungsten were used to simulate collision cascades in crystal tungsten. Three of the IAP were embedded atom model (EAM) based [1,2,3] whilst the other two were machine learning (ML) based [4,5]. The molecular dynamics (MD) simulations were carried out for primary knock-on atoms (PKA) having energies 5, 10, 20, 50, 75, 100 and 150 keV. The PKA were directed along 100 random directions for sufficient statistics at each PKA energy, amounting to a total of 3500 collision cascade simulations. Several terabytes of position data of the atoms were then analyzed using CSaransh [6] to obtain the number of defects, the number of defects in clusters, the defect size distributions, the various classes of defects based on their morphology and orientation using a graph theory based method [7]. It is seen that whilst the number of defects predicted by the IAP compares well with each other and with the arcDPA predictions within statistical errors, other aspects of the defects like the number of defects in clusters, the defect size distributions, the number of defects in various classes, etc., show substantial variation for the various IAP. It is seen that there is no trend for these parameters with traditional properties of the IAP like stiffness/range or their ratio S/R. The main difference is the formation of C15 like rings in two of the IAP, whilst in the other three IAP <111> defect clusters dominate [8]. An experimental and a simulation approach to validate the IAP based on the morphology of the defect it produces will be discussed.

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