Molecular dynamics simulations of irradiation induced changes in material micro-structure: Defect cluster classification and stability

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Irradiation induced changes in materials are not only an an important aspect of plasma treatment of surfaces but also give insight into the lifetime of various reactor components. The Computational Analysis Division, BARC, have been developing fast computational tools for multi-scale modeling of irradiation induced changes in the micro-structure of materials using MD and Dynamic Monte Carlo methods [1,2]. In this presentation, the following studies to understand and quantify "the change in micro-structure due to irradiation" are described:

1. Development of fast computational tools to identify defects from MD simulations of collision cascades [3,4]. The tools can be used to directly process, analyse and visualise cascades of choice either from the online MD collision cascade database, cascadesdb [5] or from local xyz files.
2. Machine learning (ML) to classify defect clusters [4,6]. The software (Csaransh [6]) also analyses the structural properties of the defect clusters such as alignment of defects, dimensionality, etc.
3. MD simuations to study the stability and sessile / glissile nature of the classified defect clusters.

References

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