6th RaDIATE Collaboration Meeting



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Computer Simulation of Radiation Damage in Materials

Wednesday, 11 December 2019 11:30 (25 minutes)

We present an overview of computer simulation methods used to study radiation damage from the atomic to the continuum scale. Within the framework of multiscale materials modeling, the study of irradiation damage and associated materials property degradation has required modifications tailored to the application. Particle irradiation damage in accelerator targets begins at the nanometer scale and its effects can be seen at the millimeter scale and beyond. Similarly, the effects of picosecond-scale processes manifest themselves after hours and even months of continued operation. The complex phenomena associated with energetic particle impact include charge transfer, heat transfer, atomic displacement, preferential sputtering, local chemical changes, melting, and phase transformations, such as amorphization and precipitation. Modeling of irradiated materials at different scales to provide a fundamental scientific understanding of radiation-induced changes in microstructure and properties will be discussed.

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