Variation and uncertainty in cascade damage predictions from simulations

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The first step in modelling radiation damage in materials consists in predicting the primary damage, which forms on picosecond time scales as a direct result of an elastic collision with an impacting particle. The collision cascades caused by the incoming particle, which give rise to structural damage on the nanometer scale, are highly non-equilibrium events, directly involving up to thousands of atoms in a complex non-linear process. Methods based on molecular dynamics have been developed which successfully handle many of the aspects of the dynamics in cascades. However, the predictive capacity of atomistic cascade simulations is still restricted by the level of accuracy of the models used [1,2].

Cascades are highly stochastic in nature, with strong variation between events, which poses a significant challenge for the development of simulation methodology. In addition, the accuracy of predictions is often hard to determine, since the picosecond time scale effects are difficult to capture experimentally. In this presentation, I will describe the inherent variation in cascades and cascade damage in different metals, and outline the main sources of uncertainty in predictions from molecular dynamics simulations. I will present some of the ways in which simulation results can be directly compared to experiment [3,4,5], and discuss the related available experimental data and data needs. Finally, I will consider future directions for developing the simulation methodology and improving the accuracy of predictions from simulations.

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