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Molecular dynamics simulations of swift heavy ion induced damage and recovery processes

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Swift heavy ion (SHI) irradiation leads to formation of narrow ion tracks in many materials, can be used in modifying nanomaterials, and in some materials with existing damage induces defect recovery. Molecular Dynamics (MD) simulations, which include the energy deposition from electronic stopping following the inelastic thermal spike calculation input, can show the time evolution of these processes, and reveal how differences in solid –liquid phase transitions and recrystallization lead to very different behavior in damage formation and recovery in different insulator and semiconductor materials, subjected to similar initial electronic excitation.

In silicon carbide (3C-SiC), MD simulations complement our recent ion-beam experiments and clearly show that the irradiation-induced defect recovery process in SiC is active from swift heavy ions to low values of electronic stopping, in a regime where electronic stopping is often considered negligible. In other materials like zircon, an opposite co-operative effect of nuclear and electronic stopping is observed. The competitive processes of damage production and defect recovery are relevant for understanding radiation damage production for many materials in nuclear energy applications and for investigating radiation damage in materials using ion irradiation methods.

In a-Ge, a-Si and their alloys, local melting around the swift heavy ion path leads to formation of nanometer scale voids and/or ion tracks, the latter observable in these amorphous materials only indirectly as localized density changes in SAXS experiments. MD simulations explain the formation of the density variations and the shape of voids, due to the volume contraction associated with the molten phase and the following radially progressing expansion of the resolidifying ion track.

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