Simualtions of structural damage in SiO_2 and Si_3N_4 by Swift Heavy Ions

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We study the formation of structural damage in amorphous silicon dioxide (SiO_2) and silicon nitride (Si_3N_4) under swift heavy ion (SHI) irradiation. SHIs are known to give great amounts of energy to the atoms along the ion trajectory, forming cylindrical nanostructures of damaged material, which are called tracks[1]. We simulate the formation of tracks in SiO_2 and Si_3N_4 using the two-temperature model (TTM) to calculate the energy exchange between the hot electrons and the atoms during the irradiation, together with Molecular Dynamics (MD) simulations[2] to analyze the change in the structure as well as the nature of the chemical bonds in the track. We compare the results from the simulations with small angle X-ray and Fourier transform infrared spectroscopy (SAXS and FTIR) experiments where the density change and the nature of the bonds around the ion track are measured.

The simulations agree closely with the experiments and show similar size of the damaged region and type of structural damage. Both simulations and experiments reveal a core-shell damage structure in the materials, where there is an underdense core and an overdense shell. This structure is produced by the viscous flow due to thermal stress from inwards to outwards in the molten region of the track, and the following quick quenching which causes the freezing of the density profile.

[1] D. Kanjijal, Swift heavy ion-induced modification and track formation in materials, Current Science, 80, 12, (2001) 1560.

[2] A. A. Leino, Pakarinen, F. Djurabekova, K. Nordlund, P. Kluth and M. C. Ridgway, Swift Heavy Ion Shape Transformation of Au Nanocrystals Mediated by Molten Material Flow and Recrystallization, Materials Research Letters, 2, 1, (2014) 37-42.