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Study of diameter-dependent swift heavy ion impacts in Bi nanowires using molecular dynamics simulations

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Due to growing technological and scientific interest in radiation effects on various nanomaterials, this work studies the impact of heavy ions on bismuth nanowires (NWs) using molecular dynamics simulations (MD) with "thermal spike"approximation to emulate the high-temperature zone generated by electronic excitation along the ion track. The diameter of the bismuth nanowires was systematically varied between 15 and 50 nm to investigate the influence of size effects for ions with different electronic stopping powers of between ~2 and ~5 keV/nm. The results clearly demonstrate that the effects induced by thermal spikes vary with NW diameters, ranging from perforations in the smallest NWs to cavities, craters and rims in the larger ones. In all cases, the simulations reveal that the track region fully recrystallizes. We additionally observe formation of point defects, and ejected atoms. These simulations exhibit qualitative similarities with experimental results obtained at higher stopping powers.

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