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Dynamics of implant damage as a precursor to nanocrystal nucleation MATTHEW J. BECK, SOKRATES T. PANTELIDES, Vanderbilt University — Ion implantation into a -SiO₂ leads to the self-assembly of metal or semiconductor nanocrystal arrays having applications in optical and non-volatile memory devices. The production of uniform arrays of similarly-sized nanocrystals within the a -SiO₂ matrix has been shown to depend strongly on nucleation conditions. Here we report results of quantum mechanical calculations probing the atomic-scale dynamics in the time immediately following ion-induced low-energy recoils. We show that individual low-energy recoils (with KE~100 eV) do not produce individual, isolated defects in the a -SiO₂ structure, but rather produce nanoscale defect pockets. These defect pockets are sources for oxygen out-diffusion, and subsequently represent seed regions for nanocrystal nucleation.

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