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Nucleation and growth simulation of Si nanocrystals in Si-rich oxide MIHAIL PETKOV, Jet Propulsion Laboratory, L. DOUGLAS BELL, Jet Propulsion Laboratory — Ion implantation profile in SiO2 layers on Si substrate calculated by TRIM was used as initial conditions for a diffusion-driven nucleation and growth model. Nucleation was initiated at randomly chosen seeds satisfying the Poisson distribution, which were used as centers in a Voronoi tessellation of space. The volume fraction of implanted Si ions in each Voronoi polyhedron was calculated based on the polygon volume and the fluence. The nanocrystal growth was considered to occur at the nucleation centers by diffusing of Si ions, which become localized at the seeds. Zero net flux across each of the surfaces of the Voronoi polyhedra was assumed for the diffusing Si species. The calculations were by with periodic boundary conditions in the directions normal to the implantation. We report size and depth distribution of the Si nanocrystals formed under the above conditions.

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