

Deciphering mechanisms of enhanced-retarded oxygen diffusion in doped Si

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Abstract

We study enhanced/retarded diffusion of oxygen in doped silicon by means of first principle calculations. We evidence that the migration energy of oxygen dimers cannot be significantly affected by strain, doping type, or concentration. We attribute the enhanced oxygen diffusion in p-doped silicon to reduced monomer migration energy and the retarded oxygen diffusion in Sb-doped to monomer trapping close to a dopant site. These two mechanisms can appear simultaneously for a given dopant leading to contradictory experimental results. More generally, our findings cast a new light on phenomena involving oxygen diffusion: precipitation, thermal donors formation, and light induced degradation. © 2013 AIP Publishing LLC.

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