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Hydrogen Transport in Doped and Undoped Disordered Silicon

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Hydrogen transport in amorphous, microcrystalline, and polycrystalline silicon has been studied intensively in the past due to its importance for understanding structure, growth, metastability, and defect passivation. Further substantial insight in the microscopic mechanism governing hydrogen diffusion can be obtained by comparing diffusion in doped material with H diffusion in undoped disordered silicon. Hydrogen migration was investigated by deuterium diffusion-experiments as a function of temperature, deuterium, phosphorous, and boron concentrations. At high D concentrations the diffusion is dispersive depending on the plasma exposure time. With increasing doping concentration the effective diffusion-coefficient, D_{eff}, increases. Poly-Si doped with a boron concentration of 10^{18} cm^{-3} exhibits an increase of D_{eff} by one order of magnitude compared to undoped poly-Si. On the other hand, phosphorous doped poly-Si shows only a 40% increase of D_{eff}. The diffusion activation energy, EA, depends significantly on the Fermi energy E_F and the hydrogen concentration. In polycrystalline silicon EA varies between 0.1 and 1.69 eV while in microcrystalline silicon the diffusion activation energy varies between 0.01 and 0.4 eV. This is accompanied by a variation of the diffusion prefactor by 15 orders of magnitude and is even consistent with results reported on H diffusion in hydrogenated amorphous silicon. Using the theoretical diffusion prefactor the energy EA required to yield the diffusion coefficient was calculated. EA reveals a Fermi energy dependence similar to that of the formation energy of H^+ and H^- in c-Si. Based upon the experimental data a unified microscopic model for H diffusion in silicon is proposed.

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