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On concentration dependence of arsenic diffusivity in silicon

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An analysis of the equations used for modeling thermal arsenic diffusion in silicon has been carried out. It was shown that for arsenic diffusion governed by the vacancy-impurity pairs and the pairs formed due to interaction of impurity atoms with silicon self-interstitials in a neutral charge state, the doping process can be described by the Fick's second law equation with a single effective diffusion coefficient which takes into account two impurity flows arising due to interaction of arsenic atoms with vacancies and silicon self-interstitials, respectively. Arsenic concentration profiles calculated with the use of the effective diffusivity agree well with experimental data if the maximal impurity concentration is near the intrinsic carrier concentration. On the other hand, for higher impurity concentrations a certain deviation in the local regions of arsenic distribution is observed. The difference from the experiment can occur due to the incorrect use of effective diffusivity for the description of two different impurity flows or due to the formation of nonuniform distributions of neutral vacancies and neutral self-interstitials in heavily doped silicon layers. We also suppose that the migration of nonequilibrium arsenic interstitial atoms makes a significant contribution to the formation of a low concentration region on thermal arsenic diffusion.

Keywords: Silicon; arsenic; diffusion; diffusivity; modeling

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