FIRST-PRINCIPLES CALCULATION OF HE-H INTERACTION IN C-SI

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Hydrogen and helium implanted in silicon generate a huge number of point defects and exert influence on different properties of silicon. Hydrogen penetrates into silicon crystals even at room temperatures and reacts with intrinsic lattice defects. Helium, being inert, does not interact chemically with other atoms and evaporates completely at higher temperatures leaving the "empty" voids. According to experimental data the high temperature-high pressure treatment of a Si sample with implanted helium and hydrogen influences strongly hydrogen out-diffusion. In our investigation we used the density functional theory and ab initio pseudopotentials. It was shown that the vacancy and divacancy formation energies are able to decrease by about 2 eV due to the presence of hydrogen. The presence of one or two helium atoms reduces the divacancy formation energy by 0.3 and 0.4 eV, correspondingly. Thus, hydrogen and helium assist the formation of vacancies and their complexes. The pressure also reduces formation energies of vacancy complexes. Leaving silicon interstitial sites for divacancies, H_2 molecules dissociate up and passivate silicon dangling bonds with the energy profit of 1.6 eV. Presence of one or two helium atoms per divacancy reduces this profit by 0.1 eV. At low He concentration (one atom per divacancy) the 5 GPa pressure decreases this energy additionally by 0.2 eV and makes hydrogen less bonded and more mobile in silicon in accordance with experimental data. In the case of high He concentration (two atoms per divacancy) the same pressure increases the H_2 binding energy by 0.2 eV. Thus, high concentrations of He reduce the hydrogen out-diffusion.