Abstract

In this thesis the growth-pattern of free silicon clusters and vacancy clusters in bulk silicon is investigated. The aim is to describe and to better understand the cluster to bulk transition. Silicon structures in between clusters and solids feature new interesting physical properties. The structure and physical properties of silicon clusters can be revealed by a combination of theory and experiment, only. Low-energy clusters are determined with different optimization techniques and a density-functional based tight-binding method. Additionally, infrared and Raman spectra, and polarizabilities calculated within self-consistent field density-functional theory are provided for the smaller clusters. For clusters with 25 to 35 atoms an analysis of the shape of the clusters and the related mobilities in a buffer gas is given. Finally, the clusters observed in low-temperature experiments are identified via the best match between calculated properties and experimental data. Silicon clusters with 10 to 15 atoms have a tricapped trigonal prism as a common subunit. Clusters with up to about 25 atoms follow a prolate growth-path. In the range from 24 to 30 atoms the geometry of the clusters undergoes a transition towards compact spherical structures. Low-energy clusters with up to 240 atoms feature a bonding pattern strikingly different from the tetrahedral bonding in the solid. It follows that structures with dimensions of several Angström have electrical and optical properties different from the solid. The calculated stabilities and positron-lifetimes of vacancy clusters in bulk silicon indicate the positron-lifetimes of about 435 ps detected in irradiated silicon to be related to clusters of 9 or 10 vacancies. The vacancies in these clusters form neighboring hexa-rings and, therefore, minimize the number of dangling bonds.

Keywords

silicon clusters, vacancy clusters, density-functional theory, tight-binding, infrared-spectrum, Raman-spectrum, mobilities, positron-lifetimes