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Ab Initio Calculations and Rate Equation Simulations for Vacancy and Vacancy-Oxygen Clustering in Silicon

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Abstract

Formation energies of vacancy clusters V_n with ($1 \leq n \leq 11$) in crystalline Si and of their complexes V_nO_m ($1 \leq m \leq 14$) with oxygen were computed by ab initio density functional theory (DFT) within the generalized gradient approximation (GGA) and used to simulate the process of vacancy agglomeration after rapid thermal annealing (RTA) and also the formation of bulk microdefects (BMDs) in Si. Rate equation modeling of vacancy agglomeration after RTA and subsequent annealing below 1000 °C was carried out and the results were compared for binding energies obtained with different cell size. In Czochralski silicon, the interaction between vacancies and interstitial oxygen has to be taken into account. The BMD formation in Czochralski silicon was modeled by a continuum model comprised of a large system of rate equations, which accounts for the free energy of BMDs as a function of BMD size and shape, temperature and point defect concentrations.

Keywords

A1. Defects; B2. Semiconducting Silicon; A1. Point defects; A2. Czochralski method

1. Introduction

Vacancies are well known to enhance the precipitation of supersaturated interstitial oxygen in Czochralski silicon [1]. Meanwhile, rapid thermal annealing (RTA) at temperatures of at least 1200 °C is a well-established technique to generate profiles of supersaturated vacancies in silicon wafers [2]. In this way, the oxygen precipitation is enhanced in the bulk of the silicon wafers, where the precipitates serve as gettering sinks for metal impurities. The near-surface device-active region remains free of oxide precipitates which can degrade or destroy the device function. This effect, called internal gettering [3], is widely used in the microelectronic industry.