Formation and dissociation mechanisms of vacancy-oxygen complex in Si

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Introduction

Process induced point defects become increasingly crucial in the present and future silicon devices with complicated processing steps and a large-sized wafer. The vacancy-oxygen pair (VO) is a precursor of V_XO_Y complex which causes the leakage current of p-n junction [1], the formation and dissociation mechanisms of VO have to be clarified in order to develop a fabrication process of p-n junctions with low leakage current. The aim of this work is to clarify formation, dissociation and diffusion mechanism of VO through first-principles calculations, based on density functional theory (DFT).

Calculation method

DFT calculations were performed using ultrasoft Vanderbilt pseudopotentials, and the generalized gradient approximation for the exchange-correlation potential. Periodically repeated supercells are containing 64 silicon lattice sites with a lattice constant of 10.8 Å. For these cells, we have used a plane wave cutoff energy of 300 eV and a $2 \times 2 \times 2$ Monkhorst-Pack k-point mesh. Atomic positions were allowed to relax fully until all residual forces became smaller than 0.05 eV/Å. We then preformed the synchronous-transit method with a conjugate gradient technique to find the microscopic transition states and activation energies. In transition-state searches, the atoms were relaxed until their residual forces had converged to less than 0.15 eV/Å.

Result and discussion

We calculate the total energies of several microscopic structures, including a vacancy and an interstitial oxygen, in order to elucidate the formation and dissociation of VO. The formation energy of an infinitely separated vacancy from an interstitial oxygen is defined as zero energy and the calculated binding energy of a vacancy and an interstitial oxygen is 1.39 eV.

We investigate two atomic mechanisms involved in the VO diffusion: one is caused by migration of an interstitial oxygen, another by migration of a vacancy along a six-member ring. Diffusion steps of the oxygen migration mechanism are shown in Fig. 1. For VO diffusion in bulk Si, a vacancy of VO separates from the oxygen and forms an atomic structure where the vacancy is adjacent to a Si-O-Si bond (shown as “Bond center” in Fig. 1). This structural change needs an activation energy of 1.22 eV. Subsequently, the oxygen migrates to recombine with the vacancy at a position different to that in the original VO complex. The transition state of the oxygen migration has a energy peak of these structural changes, 2.02 eV. In a diffusion mechanism of VO with a vacancy migration along a six-member ring as shown in Fig. 2., the energies associated with these changes have a peak of 1.98 eV through the transition states shown as Fig. 2(c)→(d). The activation energy of VO diffusion caused by a vacancy migration along a six-member ring is 1.98 eV. The two activation energies agree well with the experimental energy of 2.0 eV [2]. The existence of two activation energies also suggests that two mechanisms occur in a parallel fashion at a similar rate.

In addition, it is clarified that a dissociation of VO has a much higher probability of occurring

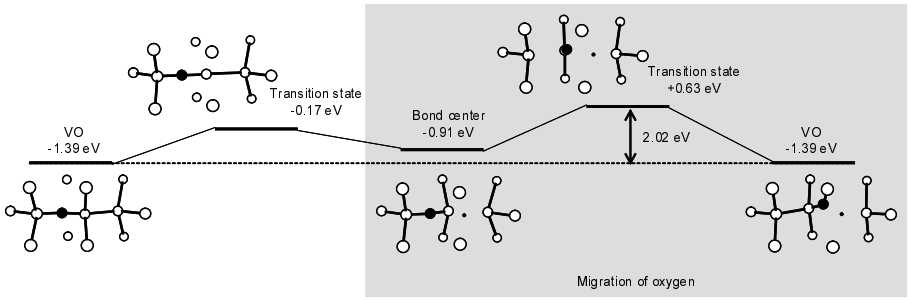

Fig. 1: Diffusion mechanism of vacancy-oxygen pair caused by migration of oxygen. Silicon, oxygen and vacancy are represented as white, black circles and black dot, respectively.

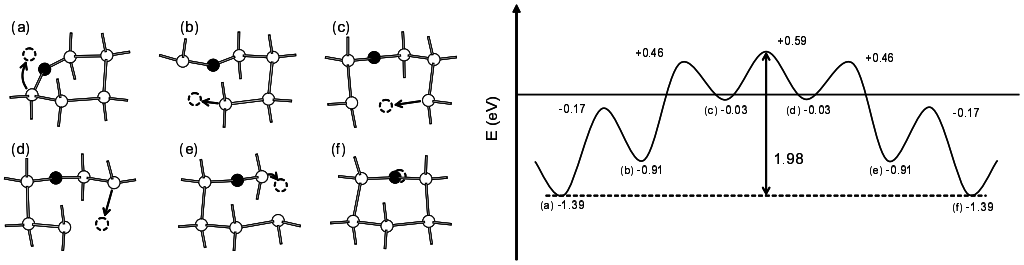

Fig. 2: Structural changes (left) and formation energy diagram (right) of VO diffusion caused by migration of a vacancy along a six-member ring. Silicon, oxygen and vacancy are represented as white, black and dashed circles, respectively.

than a diffusion. Once a vacancy separates from the oxygen, the VO complex generally dissociates unless the vacancy again comes close to the oxygen. This is because the activation energy required for a vacancy to migrate to the outside of a six-member ring (0.45 eV) is lower than that for migrating along a six-member ring (0.62 eV), which means that the dissociation energy 1.85 eV of VO is lower than the diffusion energy.

Summary

We investigated two atomic mechanisms involved in the VO diffusion: one is caused by migration of an interstitial oxygen atom, another by migration of a vacancy along a six-member ring. Calculated activation energies also suggest that two mechanisms occur at a similar rate. In addition, we clarified that the dissociation energy of VO is lower than the diffusion energy.

Reference

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[2] O. O. Awadelkarim, H. Weman, B. G. Svensson, J. L. Lindström, J. Appl. Phys., **60**, 1974 (1986).