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Neutral and Negatively Charged Interstitial Oxygen in Silicon

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INTRODUCTION

Being the predominant impurity in Czochralski-grown silicon, oxygen has been extensively studied since the early years of semiconductor research by a multitude of experimental [1] and theoretical [2] techniques. The generally accepted model shows the oxygen atom 'squeezed' between two neighboring lattice atoms. It is believed that oxygen breaks the silicon-silicon bond and forms a Si-O-Si bridge. The interaction between the neighbors forms a Si-O-Si virtual molecule with C_{2v} symmetry. The defect is electrically neutral and induces a shallow donor level at E_v+0.07 eV. Advent of highly powerful computers offers a chance to shed light on the essential features of the physics behind the charge distribution during the filling period. The problem of the charge distribution has been solved using the translational symmetry of the system [3]. It appeared to be more than a good idea. Using this technique, the equilibrium structure of the oxygen defect in silicon has been extensively studied. Cluster approach with the hydrogen-saturated surface coupled with the Hartree-Fock (HF) techniques [4] developed mostly for quantum chemistry could give advantages in the simulation. Methods based on HF technique usually reduce the time of computation and neglect some computationally expensive procedures but the performance in silicon–oxygen systems is less convicting giving very poor results for Si-O-Si geometry. To solve this problem, we optimized the adjustable parameters for oxygen by fitting the geometrical data to the *ab initio* values. The set of parameters, which is refer to as "new oxygen parametrization" (NOP), was presented recently [5]. The aim of this paper is to report a study on the oxygen defect in various charge states using NOP combined with cluster approach.

METODOLOGY

In our study, we use a cluster of 66 silicon atoms. The lattice constant is set to the experimental value of 5.43 Å [6]. The disconnected bonds to the remaining crystal are terminated with hydrogen. The optimized Si-H bond distance corresponding with the total energy minimum was found to be 1.48 Å. The interstitial oxygen was positioned at the center of Si-Si bond. The final cluster configuration is $Si_{66}H_{58}O$. The Si-O-Si complex was positioned in the cluster center, surrounded by five shells of silicon atoms. All atoms positioned in first two shells around the oxygen were relaxed by Broyden-Fletcher-Goldfarb-Shanno (BFGS) technique. This corresponds to a fixed lattice outside a flexible core region. In Fig. 1 is shown the Si-O-Si complex after relaxation. To simulate the negative charge state either one or two extra electrons were introduced in the Si-O-Si system. The broadened eigenvalue spectrum (DOS function) for the oxygen defect in various charge states is shown in Fig.4.

CONCLUSIONS

The calculations performed in combination with the cluster technique and NOP model have proved to be successful. The main structural features of the oxygen defect in silicon are found in good agreement with the experiment. We confirmed that

the large lattice relaxation is provided by the bridging oxygen atom. The neutral oxygen produces two resonance states in the valence band and a shallow donor level positioned in the gap. Application of HF technique to a charged cluster allows calculate the charge distribution for one or two extra electrons.

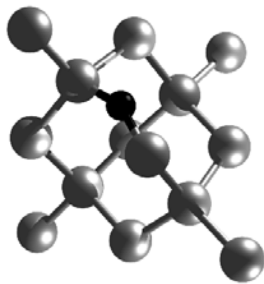

Fig.1. Structure of the oxygen defect in silicon after relaxation. The relaxed structure shows on C_{2v} symmetry. Light gray spheres represent silicon atoms, black sphere interstitial oxygen atom.

Our calculations show that an extra electron trapped on the oxygen defect induces a small change in lattice distortion and push up the donor level in the gap. This state is unstable with a high emission rate of extra electron. DLTS transient controlled by this emission gives the right position of the donor level at E_v+0.07eV. The emission rate of the second extra electron is low in comparison with the previous charge state. A lesson from the present study is that MNDO technique in combination with the NOP is accurate enough to have, at least, predictive power and is fast enough to allow to study large systems.

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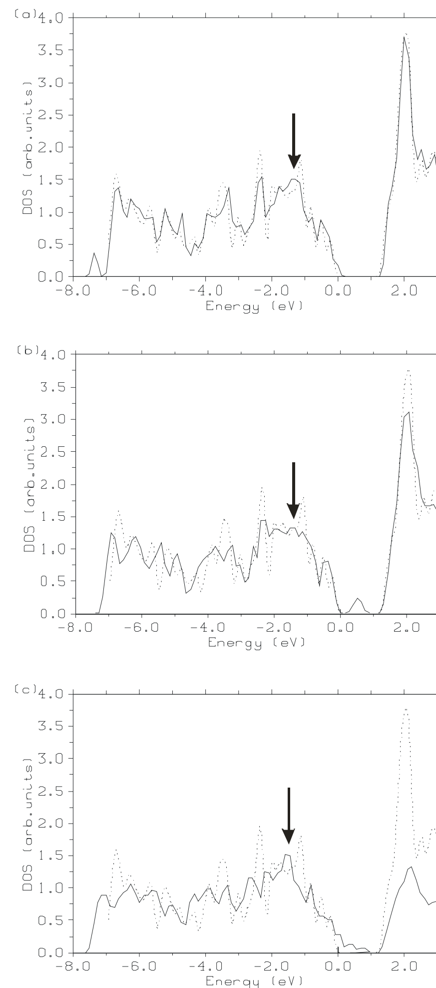

Fig. 2: Computed electronic density of states (DOS) of an interstitial oxygen defect in silicon in various charge states: (a) neutral; (b) negatively charged; (c) double negatively charged . Solid line represents silicon crystal with the oxygen; dashed line represents a perfect silicon crystal. The eigenvalue spectra were broadened by convolution with a Gaussian function. E=0 corresponds to the top of the valence band. The arrows point at the resonance induced by $sp^3 2p$ bond