Density of States and Group Velocity Calculations for SiO_2

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Abstract

Ab initio calculations of the electron group velocity for SiO_2 are worked out. The conduction bands are calculated by means of two different techniques: Hartree-Fock (HF) and Density-Functional Theory (DFT). Eight energy bands have been used to calculate the density of states and group velocity for the energies of interest. Two different crystal structures of SiO_2, built-up by the same fundamental unit, namely, the SiO_4 tetrahedron, are investigated: they are the α-quartz, and the β-cristobalite.

1 Introduction

The interest in silicon dioxide as material for technological applications in electronic devices is growing steadily. In modern semiconductor technology, SiO_2 films grown on silicon have been employed in the construction of integrated circuits in various devices. Thus, especially in recent years, experimental and theoretical investigations focused on microscopic properties of this material related with reliability problems. Electron transport in silicon dioxide has already been tackled in the frame of the spherical-harmonics expansion (SHE) method applied to the solution of the Boltzmann transport equation (BTE), using the parabolic-band approximation [6]. In particular, the first conduction band was assumed to be a spherical and parabolic function terminating at 6 eV, this limiting the validity of the analysis when high electric fields are considered. A more accurate description of the bands at higher energies has already been achieved by tackling the calculation of the full-band structure of SiO_2. In [5] the solution of the Schrödinger equation has been carried out by means of two different *ab initio* techniques (Hartree-Fock (HF) and Density-Functional Theory (DFT)). In this paper, the same techniques are exploited to determine the coefficients of the SHE method, namely the density of states (DOS) and group velocity (GV) as a function of energy, along the same line already worked out for silicon [7]. As in the SHE scheme the band structure of the material appears through these electronic properties, the calculations reported in this work constitute the basis for an accurate description of the transport properties for SiO_2 at higher energies. In the authors' knowledge, such calculations have not been carried out before.

2 Theory and Implementation

In VLSI-CMOS technology, the gate oxide is grown on a silicon crystal in its amorphous phase. Early investigations [1] showed that the amorphous SiO_2 is constituted by SiO_4 tetrahedra with bond-length and bond-angle distortions; as a consequence, the calculation of the transport properties of the crystalline phases of SiO_2 can be exploited to understand the main aspects of the amorphous phase as well. The analysed systems are polymorphs of silica, characterized by an electron density similar to that of amorphous SiO_2. In this work, the α-quartz and β-cristobalite are addressed.
Although the calculation at hand could in principle be restricted to the irreducible Brillouin zone, for programming simplicity the band structure has been tabulated over the first octant of the Brillouin zone (BZ). The band structure has

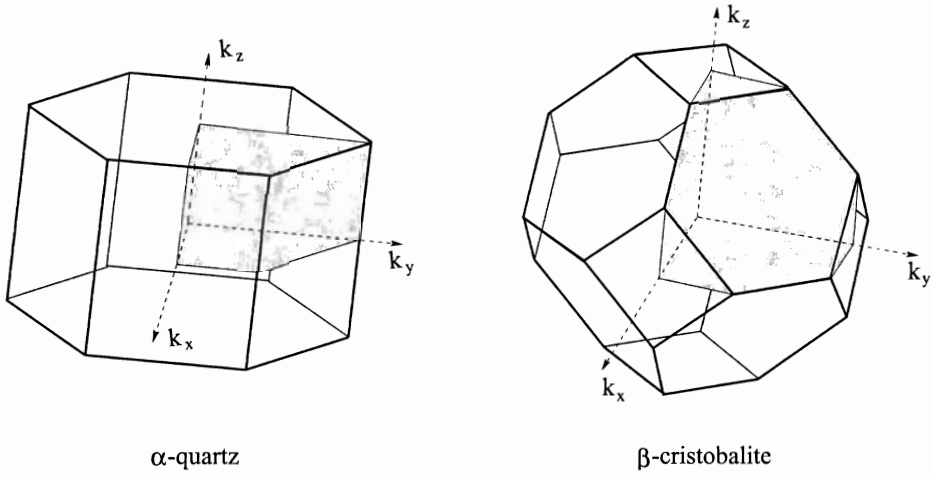

Fig. 1: First Brillouin zone of α-quartz and β-cristobalite.

been calculated in the reciprocal-space domain, by adopting a spatial discretization. More specifically, a $\Delta = 0.05$ mesh step has been adopted to discretize the k_x, k_y and k_z axes with respect to normalized boundaries, this defining an elementary cube associated to each discretization point. According to the crystalline structure, the total number of mesh nodes depends on the shape of the first BZ, shown in gray in Fig. 1. In particular, a mesh tabulation of 5775 and 6951 points has been obtained for the β-cristobalite and α-quartz, respectively. For each point, the eigenvalues of the eight lowest conduction bands have been computed using the CRYSTAL98© code [2]. In order to determine the density of states (DOS) and the group velocity (GV) at a given energy E, and to finally obtain the tabulation of DOS and GV over a wide range of energies, a linearization algorithm has been implemented, based on the Gilat-Raubenheimer method for $\boldsymbol{k}$-space integration [4]. Both DOS and GV have been tabulated on a range of energies up to 6 eV.

3 Results and Conclusions

The numerical accuracy in the description of the DOS and GV functions demanded by the SHE method is very high. Thus, special care has been devoted to the definition of the 3-D mesh in the $\boldsymbol{k}$ space and to the algorithm for calculating the two functions. As consistent data for DOS and GV in SiO_2 are not available elsewhere, the procedure has been validated first by calculating the same functions for Si and comparing the results with available data [3]. Good agreement has been obtained, especially for DFT which is known to provide a more realistic description of the band structure. Then, the procedure has been applied

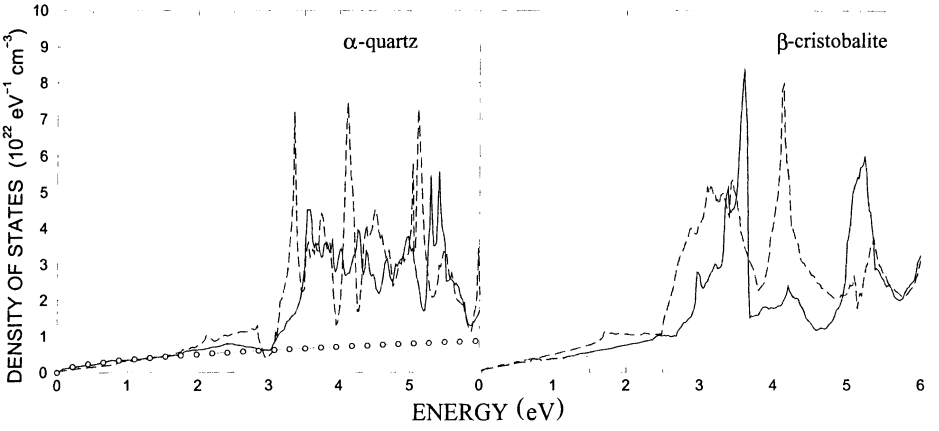

Fig. 2: DOS vs. energy for α-quartz and β-cristobalite. Solid lines: HF; dashed lines: DFT; circles: parabolic-band approximation (the effective masses are $m^* = 0.55\,m_0$ and $m^* = 0.68\,m_0$, respectively).

to the full-band structures of the polymorphs under study. In Figs. 2 and 3, the densities of states and group velocities for the two structures are reported. Both the DFT and HF data are shown, along with the parabolic-band approximation. The latter is seen to hold up to about 1 eV only. The difference between HF and DFT results is due to the intrinsic aspects of the calculation methods [5].

Two computational methods have been applied to determine the density of states and group velocity as functions of energy, with the purpose to be used for solving the BTE by the SHE method within the SiO_2 domain. This investigation is part of a larger project aiming at solving the carrier transport in semiconductor devices, in the frame of the semiclassical Boltzmann Transport Equation in real space and energy. Eight energy bands have been used to calculate both the electronic properties, in the energy range of interest for two different polymorphs of SiO_2. Such information, coupled with those already available for silicon, builds up the physical basis for the full-band calculation of the distribution function in the whole MOS structure.

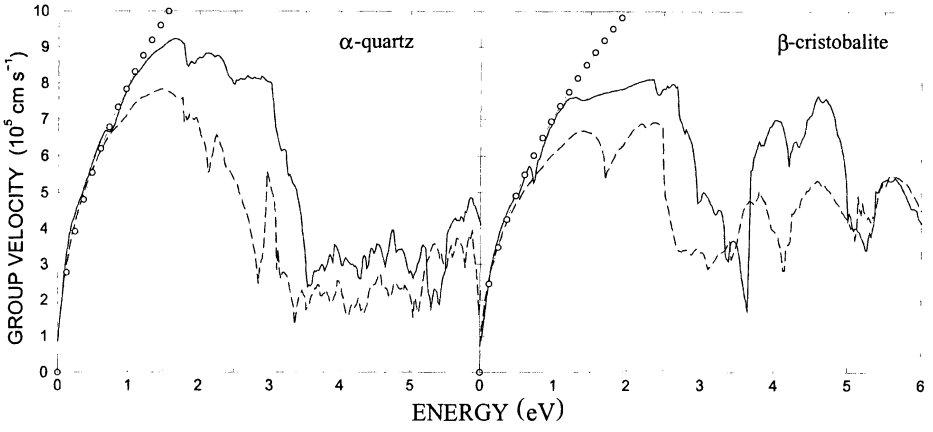

Fig. 3: GV vs. energy for α-quartz and β-cristobalite. Solid lines: HF; dashed lines: DFT; circles: parabolic-band approximation.

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