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Full-band approaches for the quantum treatment of nanometer-scale MOS structures

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Abstract

Using quantum mechanical methods that include the full-band structure, we study two quantum mechanical phenomena that occur in MOS transistors: ultrathin oxide tunneling and inversion layer quantization. We obtain good agreement between calculated and measured tunneling current densities for a n-poly Si/SiO_2/p-Si capacitor under negative gate bias. In addition, we find that for typical inversion layer fields, quantization energies $<0.5\,eV$ can be calculated with extremely high accuracy in the parabolic effective-mass approximation. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Due to the steady progress in Si nanotechnology, prototypes of Si MOSFETs with gate lengths well below 50 nm and only 1–2 nm thin gate oxides have been already successfully fabricated and characterized (see, for example, Refs. [1–3]). Consequently, quantum mechanical effects such as size quantization and gate oxide tunneling have become increasingly important and can affect the device behavior significantly. Usually, these phenomena are either neglected or treated within simplified schemes, for instance the effective-mass approximation (EMA) [4–6]. Ideally, one should try to combine a complete quantum mechanical description of these heterostructures with a full-band approach, avoiding the well-known inherent physical limitations of the EMA [5,6]. In this paper, we present a study of quantum effects in Si/SiO_2 heterostructures within full-band approaches. Two distinct physical problems are considered: first, the calculation of tunneling currents through very thin oxide layers in MOS capacitors, which we address using a state-of-the-art transfer-matrix-type method [7,8] embedded in an accurate semiempirical tight-binding framework [9]. This three-dimensional approach has several advantages compared to conventional quasi-one-

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dimensional effective-mass methods: for example, the experimentally observed violation of parallel momentum conservation during the tunneling process [10] is accounted for, and reflection from the interfaces as well as microscopic features of the oxide such as defects [11] can be included more realistically. Previously, gate currents have only been calculated for MOSFETs [11]. The second phenomenon studied in this paper is the quantization of Si states in the inversion channel of a MOSFET. We have used a recently developed linear combination of bulk Bloch states method [12] based on empirical pseudo-potential band structures. This approach has been already successfully applied to GaAs/AlAs quantum wells [12]. We compare quantization energies and band dispersions obtained with this method with corresponding effective-mass-based results.

2. Full-band approach to oxide tunneling

2.1. Theoretical method

To calculate direct tunneling currents through ultrathin oxide layers in Si/SiO$_2$ MOS structures, we have followed a methodology that has been described in detail in Ref. [8]. Here, we will briefly summarize this approach.

In a first step, we constructed microscopic Si[0 0 1]/β-cristobalite-SiO$_2$/Si[0 0 1] models (see Fig. 1), similar to the ones described in Ref. [13]. The interfaces of these structures do not contain any dangling bonds. The corresponding unit cells have lateral sizes of 0.543×0.543 nm and SiO$_2$ thickness between 0.7 and 3.0 nm, depending on the number of SiO$_2$ units (1–4, a unit consists of 4 Si and 8 O atoms) sandwiched between the Si semibulk regions. All the structures are repeated periodically in a plane parallel to the interfaces.

Then, semiempirical sp^3 tight-binding parameters for the cristobalite SiO$_2$ units were determined that reproduce first-principles Full Potential Linearized Augmented Plane Wave (FLAPW) [18] band dispersions as well as the experimental oxide gap of $\sim$9 eV. The effective mass at the minimum of the lowest conduction band of cristobalite is found to be 0.57 (in units of the free electron mass). For Si, we utilize a recently developed highly accurate sp^{3}s*d^5 parameterization [9], in contrast to previous work that relied on a sp^3 parameter set with second-nearest neighbor interactions [8].

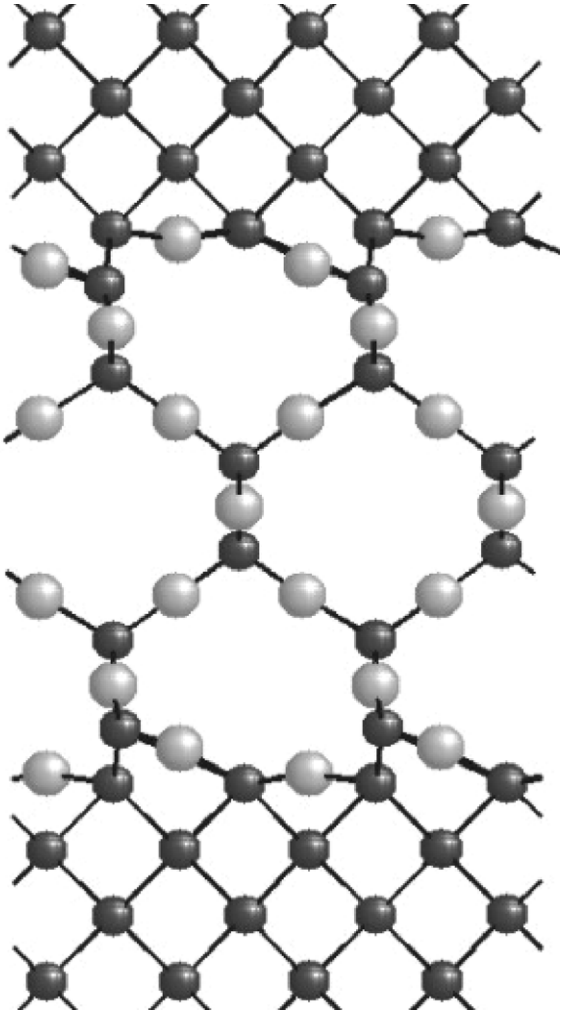

Fig. 1. Ball-and-stick model of a typical 0.8 nm thin Si[1 0 0]-SiO$_2$-Si[1 0 0] model heterojunction based on the cristobalite polytype of SiO$_2$, see Ref. [13].

Energy- and $\mathbf{k}_{\|}$-dependent transmission coefficients $T(E, \mathbf{k}_{\|})$ were determined by applying a transfer-matrix-type scheme. This allows one to calculate the transmission probabilities for propagating states tunneling from one side of an oxide slab to the other. For the calculation of the tunneling currents we considered a n-poly Si/SiO$_2$/

p-Si structure with a negative gate bias V_g. We consider only positive voltage drops $V_{ox} \sim -(V_g - V_{fb})$ across the oxide (i.e., tunneling from the gate into the conduction band of p-Si). Here, V_{fb} denotes the flatband voltage, and the surface potential of the substrate layer was neglected. A n-doped poly Si gate with an impurity concentration of $3 \times 10^{20}\,\mathrm{cm}^{-3}$ is assumed, which results in a Fermi energy $E_f = 160\,\mathrm{meV}$ above the conduction band. For the p-substrate we assumed a background dopant concentration of $10^{15}\,\mathrm{cm}^{-3}$, yielding a Fermi level located 300 meV above the top of the Si valence bands. The currents were obtained through the formula

$$J = \frac{-e}{(2\pi)^2\hbar}\int_{BZ_\parallel} \mathrm{d}\mathbf{k}_\parallel \int T(E,\mathbf{k}_\parallel)[f_R(E,E_{FR}) - f_L(E,E_{FL})]\mathrm{d}E,$$

where $T(E,\mathbf{k}_\parallel)$ is the transmission coefficient, $BZ_\parallel$ is the two dimensional Brillouin zone, E_{FL} the quasi-Fermi level in poly Si and E_{FR} the quasi-Fermi level in p-Si. Here we perform a full numerical $\mathbf{k}_\parallel$ integration in the irreducible region of the $BZ_\parallel$.

2.2. Results

Fig. 2 shows the calculated transmission coefficients of the described structure for 1–4 units of oxide, in the case of $\mathbf{k}_\parallel = 0$. It can be seen, as expected, that the magnitude of the tunnel probability is strongly dependent on the oxide thickness. We should point out that the energy dependence of the transmission coefficient is related to the (folded) band structure of silicon determined by the chosen unit cell.

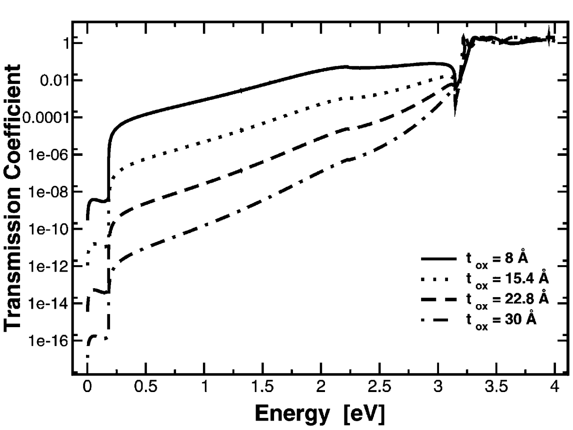

Fig. 2. Transmission coefficients for 1–4 units of oxide, in the case of $\mathbf{k}_\parallel = 0$.

Fig. 3 compares the oxide currents calculated using the present microscopic formalism with experimental data taken from Ref. [14]. Note that due to the construction of the microscopic unit cells considered in the present calculations, the theoretical results refer to other oxide thicknesses than the experimental ones. Experiment and theory agree fairly well, given a typical uncertainty of 0.2 nm in the experimental measurement and the theoretical definition of oxide thickness.

3. Full-band approach to inversion layer quantization

3.1. Theoretical method

A linear combination of bulk Bloch states formalism [12] is used for the calculation of the single-particle electronic states of an inversion channel in Si/SiO$_2$ MOS, approximated here by a triangular potential well, corresponding to a

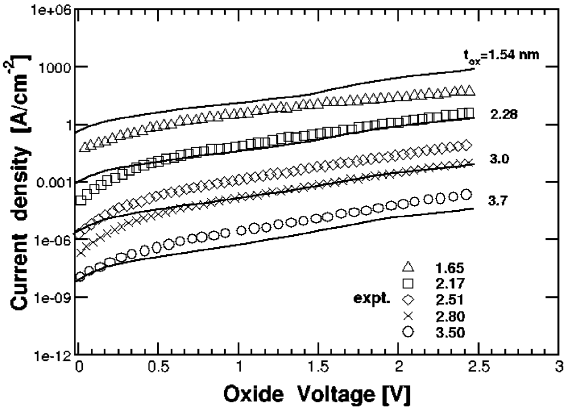

Fig. 3. Comparison of calculated tight-binding (lines) and experimental (symbols) gate current densities for the n-poly Si/SiO$_2$/p-Si MOS structure described in the text, for one set of oxide thickness [nm] each. The experimental data have been taken from Ref. [14].

perpendicular field of 200 kV/cm. The bulk Bloch states were obtained by diagonalization of the empirical pseudo-potential Hamiltonian [15]. As discussed elsewhere [12] the key point of our method is the separation between structure- and material-dependent contributions to the system Hamiltonian. Within this scheme, we find that an efficient implementation of the full-band approach, even if coupled self-consistently with the Poisson equation, is possible with a rather small number of Bloch functions included in the basis. In the following calculation we will use, for example, 200 Bloch function to describe a MOS system of 56 nm.

3.2. Results

Fig. 4 compares the $E(\mathbf{k}_\parallel)$ band dispersion of the five lowest inversion layer states obtained with the present full-band method and with the EMA for two different directions in reciprocal space ([1 0 0] and [1 1 0]). Interestingly, the quantization energies agree extremely well in both approaches, especially in [1 0 0] direction. Here, the energy differences at fixed $\mathbf{k}_\parallel$ are smaller than 30 meV even 0.4 eV above the band minima. Note that in the figure, the levels at $\mathbf{k}_\parallel = 0$ appear to be degenerate (there is a tiny O(meV) splitting [16], however). Along the [1 1 0] direction, this degeneracy is lifted due to nonparabolicity effects that the EMA cannot account for. Our results differ from those obtained in Ref. [17] where a larger difference between EMA and full band were observed. However, in Ref. [17] the approximation made to construct the pseudo-potential Hamiltonian of the MOS structure led to an overestimation of the full-band effects. As we have shown, as soon as this approximation is removed we obtain a close agreement of EMA with full-band approaches. We should point out, however, that such agreement becomes less and less good as soon as the dimension of the nanostructure reduces.

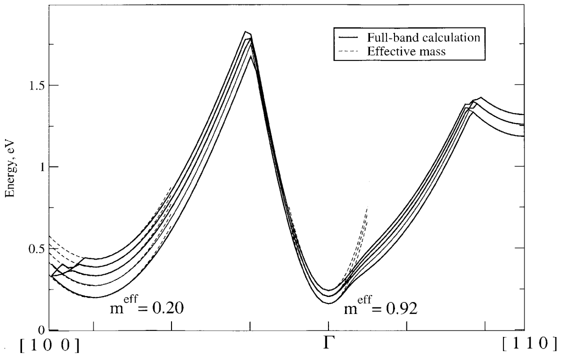

Fig. 4. Band dispersion of the five lowest states in a typical triangular Si inversion layer between Gamma ($\mathbf{k}_\parallel = 0$) and the Brillouin zone boundaries in the [1 0 0] and [1 1 0] directions, in a plane parallel to the Si/SiO$_2$ interface. The normal field was taken to be 200 kV/cm. Solid lines: full-band results based on empirical pseudo-potentials, dotted lines: standard effective-mass approximation.

4. Summary

We have presented results of two quantum mechanical approaches that include band structure effects beyond the EMA. Tunneling currents in MOS structures can be obtained by microscopic calculations based on empirical tight-binding without any fitting parameter (beside those of TB parameterization). The results are in good agreement with published data and confirm the presence of a low- and high-voltage regimes in the tunneling current. A full-band pseudo-potential approach has also been applied to calculate band dispersion in the quantized channel of the MOS. We found that full-band corrections are rather small for typical Si inversion layers at low energies while they become much more important at higher energies and for smaller dimensions of the inversion channel.

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