Efficient Calculation of Quasi-Bound State Tunneling through Stacked Dielectrics

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The continuous progress in the development of MOS field-effect transistors by down-scaling of the device feature size leads to high gate leakage currents. State-of-the-art devices deal with an Equivalent Oxide Thickness (EOT) of 1.5nm and below, and thus high-k dielectrics are a hot research topic[1]. However, quantum mechanical tunneling significantly affects the device characteristics and thus accurate, but still efficient analysis methods are of high interest. This is especially true for material characterization, in order to extract relevant parameters like effective masses of new high-k materials form measurements. Quasi-bound states (QBS) represent the major source of tunneling electrons in the inversion layers of MOS-structures as displayed in Fig. 1. Thus, the estimation of tunneling current is based on the accurate calculation of the QBS, which follows from the SCHRÖDINGER equation. The QBS are determined by the eigenstates of the Hamiltonian where lifetimes are related to the imaginary parts of the eigenvalues: $\tau_i = \hbar/2\mathcal{E}_i$.

However, the major problem is that there is still no generally accepted and efficient algorithm available to determine QBS lifetimes. A widely used approach to determine the lifetime broadening of QBS is based on the quantum-transmitting boundary method (QTBM) [2]. Here, a computational very demanding sampling of the resonance coefficient [3] peaks yields the QBS lifetimes.

Within this work, the determination of QBS is performed by the perfectly matched layers (PML) formalism which is often used in electromagnetic theory [4]. It is based on a complex coordinate stretching to introduce artificial open boundary conditions in the SCHRÖDINGER equation. Inserting the stretched coordinate $\tilde{x} = \int_0^x s_x(\tau)\,\mathrm{d}\tau$ leads to $\partial/\partial\tilde{x} = 1/s_x(x)\partial/\partial x$. Within the PML region the stretching function $s_x(x)$ is given as $s_x(x) = 1 + (\alpha + \imath\beta)x^n$, with $\alpha = 1$, $\beta = 1.4$, and $n = 2$, while it is unity in the physical region. This procedure prevents reflections at the boundary of the physical region and, therefore, the resulting system can be considered as an open-boundary system, although Dirichlet boundary conditions are applied (see Fig. 2). The Hamiltonian becomes non-Hermitian and admits complex eigenvalues $\mathcal{E} = \mathcal{E}_r + \imath\mathcal{E}_i$, where the QBS lifetimes are related to the imaginary parts of the eigenvalues.

Since the Hamiltonian still remains linear, highly efficient algorithms are available. Fig. 3 shows the CPU time necessary to calculate 1, 3, and 30 quasi-bound states with the QTBM and PML methods as a function of the spatial resolution. The PML which delivers all QBS at once, shows a stronger dependence on the spatial resolution. However, the demand on CPU time is always lower compared to the QTBM method, especially for stronger confined states as encountered in MOS structures. Since with PML all QBS are available, the accuracy of tunneling currents analysis in particular for stacked dielectrics including high-k layers, is considerably improved.

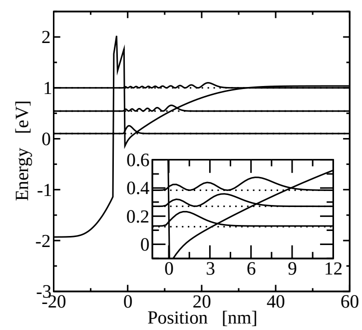

Figure 1: The potential barrier and its eigenstates assuming open boundary conditions. The inset shows the wavefunction of the first QBS at logarithmic scale.

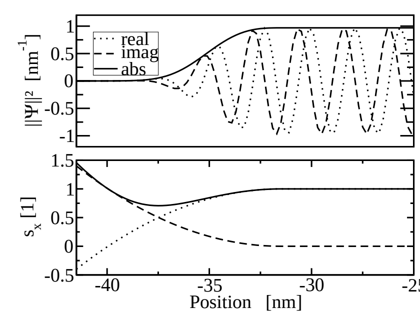

Figure 2: The wavefunction of the first QBS and the complex stretching function are displayed in the perfectly matched layer region as well as its transition to the physical region.

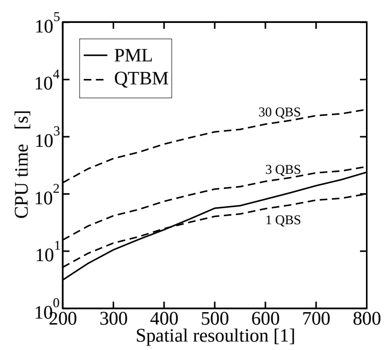

Figure 3: Comparison of the CPU demand for the PML, and QTBM methods with a given set of QBS.

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