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First-Principles Calculations of Mobilities in Ultrathin Double-Gate MOSFETs

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Methods for modeling mobilities in MOSFETs rely on empirical models for various scattering mechanisms and generally treat the Si-SiO_2 interface as an infinite potential barrier, confining electrons in the Si channel. The underlying atomic structure in the channel is supressed and its effects are captured either in effective masses or via the energy bands of the bulk crystal. Despite their success in modeling the "universal mobility curve" and other cases, the models are reaching their limits as new materials are being introduced (e.g., strained Si, alternate dielectrics) and devices have nanoscale dimensions (ultrathin double-gate devices have been fabricated with channels only ~2 nm thick[1]).

We recently published a first-principles, quantum-mechanical) method for calculating mobilities in double-gate devices using atomic-scale models with no empirical parameters. Scattering potentials are extracted from the calculations and include all atomic relaxations and self-consistent electrostatic screening. Wave function penetration into the gate dielectric is automatically included (Fig. 1). The initial applications examined the effect of atomic-scale interface roughness[2] in the form of suboxide bonds (Si-Si bonds on the SiO_2 side of the interface) and O protrusion (Si-O-Si bonds on the Si side of the interface). Here we will present our latest applications, including the following:

Calculations of mobilities in ultrathin double-gate devices with a strained-Si channel: Experiments using strained-Si channels in conventional MOSFETs found significantly enhanced mobilities.[3] Fischetti et al.[4] were able to reproduce the data only by introducing an *ad hoc* large reduction of interface roughness. Here we show that enhanced mobility arises from the fact that, in strained Si, the strain fields produced by atomic-scale roughness are reduced significantly (Fig. 2).

Atomically-resolved images of Si-SiO_2-HfO_2 alternate-dielectric structures recently obtained by van Benthem and Pennycook (Fig. 3) revealed the presence of "stray" individual Hf atoms in the thin SiO_2 interlayer. Density-functional calculations were used to obtain relaxed strcutures of such Hf atoms near the interface. Mobility calculations find a significant reduction caused by scattering from neutral Hf atoms, in agreement with measured mobilities in such structures.

Applications to other scattering mechanisms are in progress and available results will be reported at the conference.

Finally, we compare our first-principles method with the Density-Gradient (DG) method,[5] which includes quantum mechanical effects in an approximate way in device modeling (Fig. 4). The DG method reproduces the overall shape of the electron-density spatial distribution, but underestimates carrier penetration into the oxide. The results of first-principles calculations can be used to optimize the range of applicability and accuracy of the DG method for device modeling.

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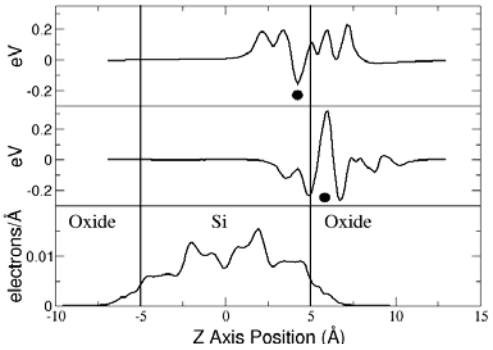

Fig. 1 Scattering potentials and carrier electron density (bottom) for oxygen protrusion (top) and suboxide bond (middle) defects. Black dots indicate defect centers. Penetration of the cannel electron density is evident.

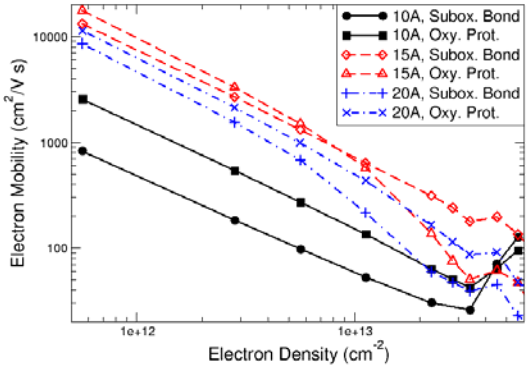

Fig. 2 Calculated mobilities for oxygen protrusions and suboxide bonds in 10Å-20Å channels. Defect density is $5.6x10^{11}$ cm^{-2}. No other scattering mechanisms are included.

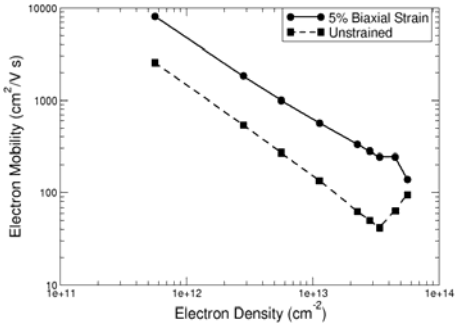

Fig. 3 Calculated mobilities for oxygen protrusions in unstrained and 5% biaxially-strained (001) channels in double-gate channels. Defect density is $5.6x10^{11}$ cm^{-2}. No other scattering mechanisms are included.

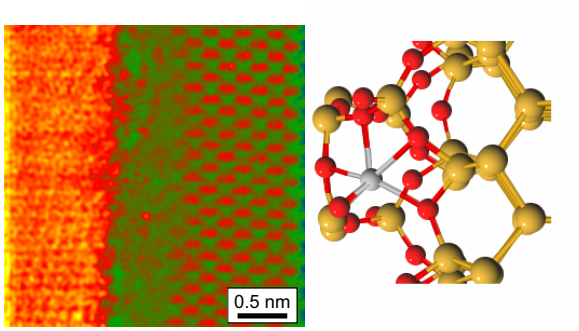

Fig. 4 Left: Z-contrast STEM image of Si-SiO_2/HfO_2 interface. The arrow highlights a stray Hf atom in the SiO_2 interlayer (K. Van Benthem and S. J. Pennycook, unpublished); right: schematic of the stray Hf atom and its neighbors

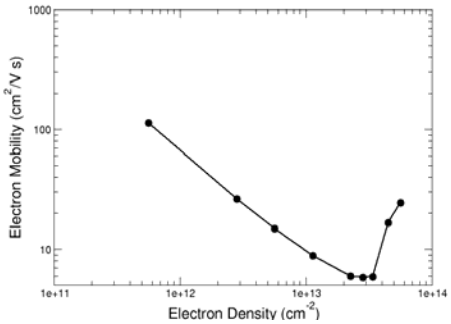

Fig. 5 Calculated mobility due to a neutral Hf defect as shown in Fig. 4. Hf sheet density is 10^{12} cm^{-2}. No other scattering mechanisms are included.

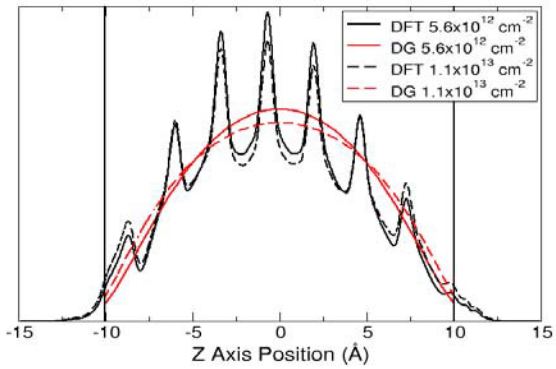

Fig. 6 Conduction electron densities in a 20Å-thick UTSOI channel, calculated from first-principles and the Density Gradient model (DG). Densities are scaled to common, arbitrary units. As carrier density increases (black to red), charge shifts from the center of the channel to the interfaces.