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Atomistic Modeling of the Detailed Structure of Si/SiO_2 Interfaces Using AIDA-TEM (*A*b-initio *I*nterface *D*efect detection by *A*nalytic *T*ransmission *E*lectron *M*icroscopy)

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The continuous reduction of the MOS channel length requires a concomitant minimization in the thickness of gate dielectric. However, a gate oxide thickness of less than 2 nm results in prohibitively high leakage currents. High-K dielectrics are a promising alternative, but currently cannot match the unparalleled mobility values of Si/SiO_2 systems. A physical insight into the causes of mobility degradation is urgently required for timely realization of the ITRS roadmap. This can only be achieved from an understanding of the atomic interface structure by new analytic techniques and consistent atomic-level models for nano-scale devices.

The literature provides a multitude of (theoretical) structural models for Si/SiO_2 and, more recently, Si/high-k material interfaces (the latter usually also with an amorphous interlayer through aging or intentional growth). However, no method for experimental detection of the exact interfacial structure exists. Using dopants as a probe, we are working on determining the interface structure by AIDA-TEM, a combination of theory and experiment.

The experimental part of AIDA-TEM consists of TEM-based methods, Z-contrast imaging to study the segregation of heavy atoms and EELS for light elements, both with single-atom resolution of ~0.5 Å. Samples with varying processing conditions and thus different interface geometries show different atomistic structures, which we probe through the segregation behavior of dopants. The experimental part of AIDA-TEM is shown schematically in Fig. 1.

The same dopants are tested in theoretical ab-initio calculations for their preferred segregation sites and corresponding energies in different structural models. The identification of key features of the winning structural models (whose dopant segregation patterns match the STEM findings) and their influence on segregation of various dopants enables us to design realistic models of interface structures. The theoretical part of AIDA-TEM is shown schematically in Fig. 2.

In this presentation, we will show first results of this work, where we study the segregation behavior of selected impurity atoms in different atomistic models and compare them to corresponding segregation patterns measured with Z-contrast spectroscopy.

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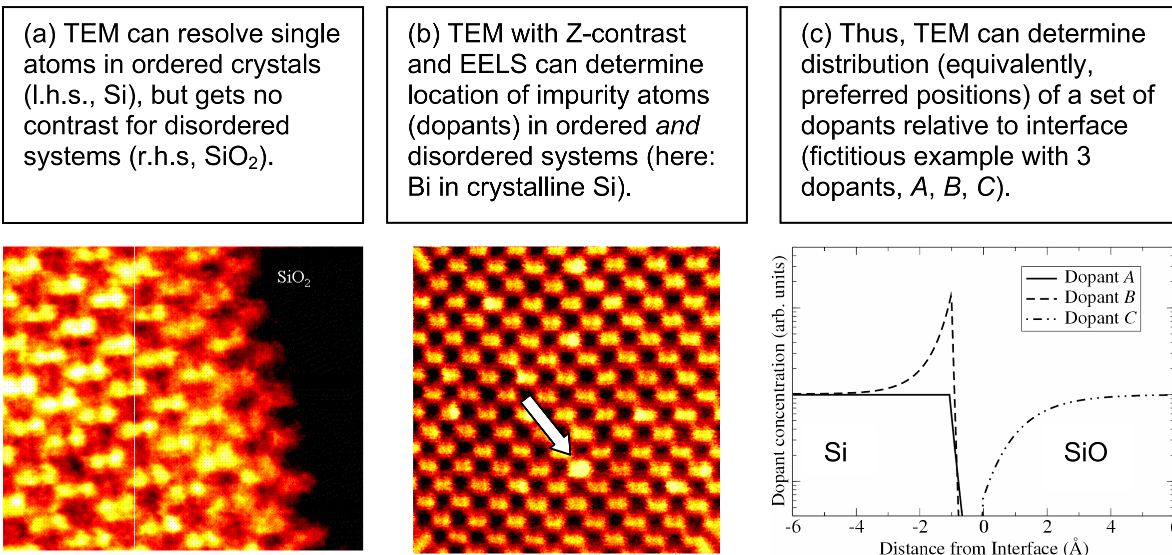

Fig. 1: Experimental part of AIDA-TEM: Atomic-scale distribution of several dopants around Si-ox interface.

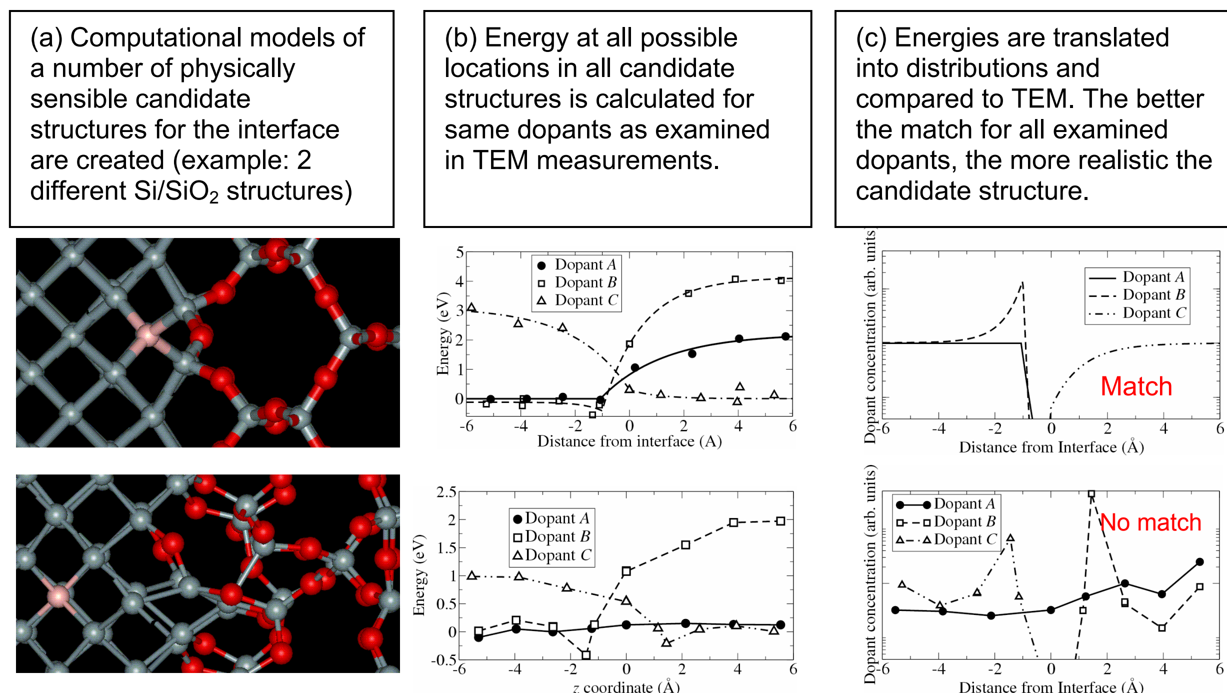

Fig. 2: Theoretical part of AIDA-TEM: Determination of dopant distribution for candidate structures.

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