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STUDIES OF THE SI/SIO_2 INTERFACE BY Z-CONTRAST MICROSCOPY, ELECTRON ENERGY LOSS SPECTROSCOPY AND FIRST-PRINCIPLES THEORY

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STUDIES OF THE SI/SIO$_2$ INTERFACE BY Z-CONTRAST MICROSCOPY, ELECTRON ENERGY LOSS SPECTROSCOPY AND FIRST-PRINCIPLES THEORY

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The combination of atomic-resolution Z-contrast scanning transmission electron microscopy, electron energy loss spectroscopy, and first-principles theory represents a powerful set of tools to link the atomic and electronic structure of the Si/SiO$_2$ interface to macroscopic properties. At a resolution today of 0.13 nm, Z-contrast microscopy can image each atom column in the crystalline Si and distinguish an atomically abrupt interface from a rough interface. Quantitative measurements of the static atomic displacements induced by the interface can also be made. Electron energy loss spectroscopy provides a sensitive means to probe the evolution of the band gap from Si into the oxide, with the same spatial resolution as the Z-contrast image. We have recently developed quantitative theoretical techniques to invert energy loss spectra fine structure to reveal the nature of the bonding. Theory also predicts that abrupt interfaces are energetically preferred, since the pivoting action of the Si-O bond allows more strain relaxation than the stiff Si-Si bond. For this interface, theory predicts that the full SiO$_2$ bandgap is achieved only 0.4 nm within the SiO$_2$.