Reconstruction at the Si(100)-SiO_2 interface

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We characterize the structure of the Si(100)-SiO_2 interface at the atomic scale by combining Rutherford ion scattering measurements and theoretical modeling. Using varying ion energies in the channeling geometry, we obtain a measure of Si displacements at the interface. To interpret our experimental results, we generate realistic atomic-scale models using a first-principles approach and carry out ion scattering simulations based on classical interatomic potentials. Comparison between experiment and theory provides evidence for a reconstruction involving the upper layer of the silicon substrate.