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Band offset measurement of oxygen annealed $SrTiO_3$/Si ERIC JIN, LIOR KORNBLUM, CHARLES AHN, FRED WALKER, Yale Univ — Integration of the perovskite oxide $SrTiO_3$ (STO) with silicon by molecular beam epitaxy (MBE) was initially developed for new high-K gate dielectrics, and more recently as a means to combine the multifunctional properties of oxide heterostructures with the well-established silicon platform. The band alignment at an oxide-semiconductor junction is critical in determining its electrical properties, and control over the conduction band offset is a fundamental goal of materials science. Density functional theory calculations have shown that an interface dipole forms at the STO-Si interface, with the magnitude of this dipole determined by the exact composition of the interface. If the interface is oxygen deficient, the band alignment is type II. If the interface is modified via the addition of a monolayer of oxygen atoms, the predicted heterojunction becomes type-I. We characterize the band alignment of MBE-grown STO-Si films by x-ray photoemission spectroscopy and show that the conduction band offset is negative between STO and Si. We demonstrate an experimental ˜0.5 eV increase in the conduction band offset for in-situ oxygen-annealed films, in close agreement with theoretical predictions. By careful control of the interface atomic structure, we show an approach toward tuning the band offset of the STO-Si system to modify electronic transport for a variety of device applications.

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