MAR05-2004-000118

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

Atomic structure of novel epitaxial oxide/semiconductor interfaces

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Further scaling of complementary metal-oxide-silicon field-effect transistors may require alternative gate dielectrics. Ultimately, interfaces between Si and these new gate dielectrics need to be atomically abrupt, which may require epitaxial interfaces. In this presentation, we identify the interfacial atomic structure of novel epitaxial Si/oxide interfaces and address some of the challenges in obtaining high-quality heterostructures. We report atomic resolution observations of epitaxial Si/$LaAlO_3$ and Si/Sc_2O_3 interfaces using scanning transmission electron microscopy. An unusual interface reconstruction of the (001) $LaAlO_3$/Si epitaxial interface is observed, with every third La column removed from the interface plane. The interface atomic structure is discussed in the context of electrically favorable interfacial bonding between the ionic oxide and Si. Ideally, bonding at the $LaAlO_3$/Si interface satisfies the valence requirements of the oxide and produces no dangling Si bonds for an insulating interface. We show that electrically favorable $LaAlO_3$/Si interfaces may be difficult to obtain unless processing or growth provide for additional passivation. Epitaxial Sc_2O_3 with the cubic bixbyite structure on (111) Si show a high density of misfit dislocations, which relieve the lattice mismatch by forming a hexagonal network. A high-density of antiphase boundaries is observed. These defects form because films nucleate with no unique arrangement of the ordered oxygen vacancies of the bixbyite lattice relative to the Si substrate lattice.