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Atomic and electronic structure of the BaTiO3-Ge (001) interface KURT FREDRICKSON, PATRICK PONATH, AGHAM POSADAS, Univ of Texas, Austin, MARTHA MCCARTNEY, TOSHIHIRO AOKI, DAVID SMITH, Arizona State University, ALEXANDER DEMKOV, Univ of Texas, Austin — There is tremendous interest in putting perovskite oxides, such as $SrTiO_3$ (STO) or $BaTiO_3$ (BTO), on semiconductors due to their very high permitivitties. BTO can be grown directly on Ge using an approach similar to the growth of STO in Si. To date, very little is known about the atomic and electronic structure of the BTO-Ge interface. We use molecular beam epitaxy to grow BTO with in-plane polarization directly on Ge(001) using a Sr Zintl buffer layer. This results in an atomically flat, oxygen- and carbon-free Ge surface with very sharp (2x1) reconstruction as observed with reflection high energy electron diffraction. Using scanning transmission electron microscopy, we are able to precisely determine the atomic geometry of the interface, with the exception of the exact positions of the oxygen atoms. *In situ* x-ray photoemission spectroscopy is used to analyze the oxidation state of the interfacial Ge and to determine the valence band offset at the interface. We use density functional theory to determine placement of interfacial O and calculate the valence band offset. The theoretical valence band offset is in good agreement with the photoemission data, strongly suggesting the correctness of the interface geometry. We calculate the effect of O vacancies and ionic substitution at the interface layer on the valence band offsets.

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