Atomic-scale compensation phenomena at ferroelectric interfaces
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The electrical polarization in ferroelectrics induces electrical charges at the surfaces or interfaces of ferroelectric films. The interfacial screening charge at the ferroelectric/electrode interface is now recognized as the most important factor in determining the stability of ferroelectricity in thin films. By combination of first-principles density-functional theory (DFT) calculations and electron microscopy imaging techniques, we investigate the atomic-scale compensation mechanism at the PbTiO$_3$/SrRuO$_3$ (PTO/SRO) and the PbTiO$_3$/SrTiO$_3$ (PTO/STO) interfaces. Two very different interfacial reactions to screen the depolarization field are identified. In the case of PTO/SRO, screening by ionic displacement is observed, in addition to electronic screening in the metallic SRO. In the case of PTO/STO, a compensation mechanism by oxygen vacancies is identified. This mechanism is an important option for the design and growth of ferroelectric thin films.

This research was sponsored by the DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. Computations were performed at the National Energy Research Scientific Computing Center.

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Date submitted: 20 Nov 2009