

Atomic Structure Characterization of MgO/SrTiO₃ Heterointerface

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Interface phenomena in oxide-based epitaxial heterostructures have allowed to discover emerging properties not existing in any of their respective bulk constituents. One of the notable characteristics for oxide heterostructures rests with the lattice mismatch between the two components, which can be much larger than in the systems made of semiconductors, yet still permits pseudomorphic growth. Such large inhomogeneous lattice strains in heterointerfaces can further interact with charge (electronic) and orbital (and/or spin) to form multiple coupling states, which are often very sensitive to subtle structural perturbations, thereby stimulating many novel properties.

In this study, we fabricate the MgO film on the (100) SrTiO₃(STO) substrates, and investigate in detail the heterointerfaces by transmission electron microscopy (TEM), atomic-resolution high-angle annular dark-field (HAADF), annular bright-field (ABF) scanning TEM (STEM) and electron energy-loss spectroscopy (EELS).

Figure 1 shows cross-sectional images of the MgO Film on (001) STO. The MgO layers are found to have epitaxial orientation relationships $(001)_{\text{MgO}} // (001)_{\text{STO}}$ and $[100]_{\text{MgO}} // [100]_{\text{STO}}$ with substrate and the XRD analyses also demonstrating strongly (100)-oriented textures for both materials. Figure 2 shows the STEM images of the interface. According to the HAADF-STEM image, TiO₂-MgO chemical bonding was formed at the heterostructure. Moreover, we also find interestingly that the Ti atoms in the STO can diffuse into MgO within one atomic layer. The observed interface configuration are also interpreted in terms of the density-functional-theory (DFT) calculations. The calculated results show an insulating property at the Ti diffused MgO/STO interface, and the energy band gap of the interface is about 1.7 eV.

References

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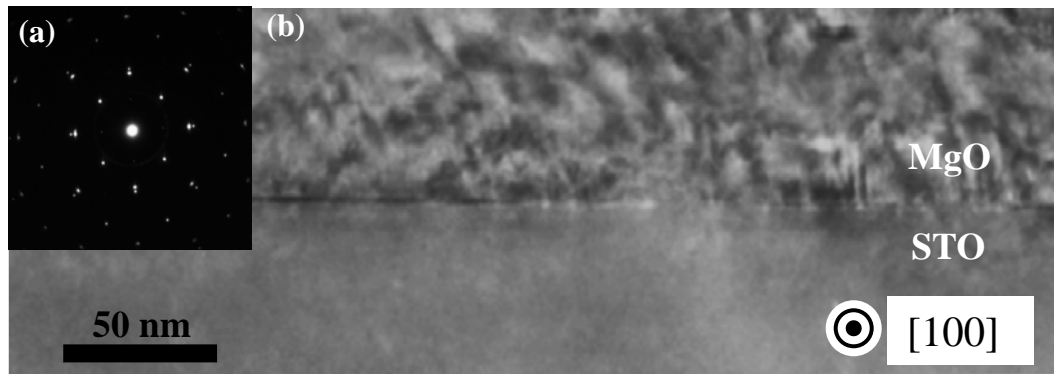


FIG. 1. (a) Diffraction pattern taken from the region including films and substrates, (b) Low magnification TEM image of the MgO/STO interface.

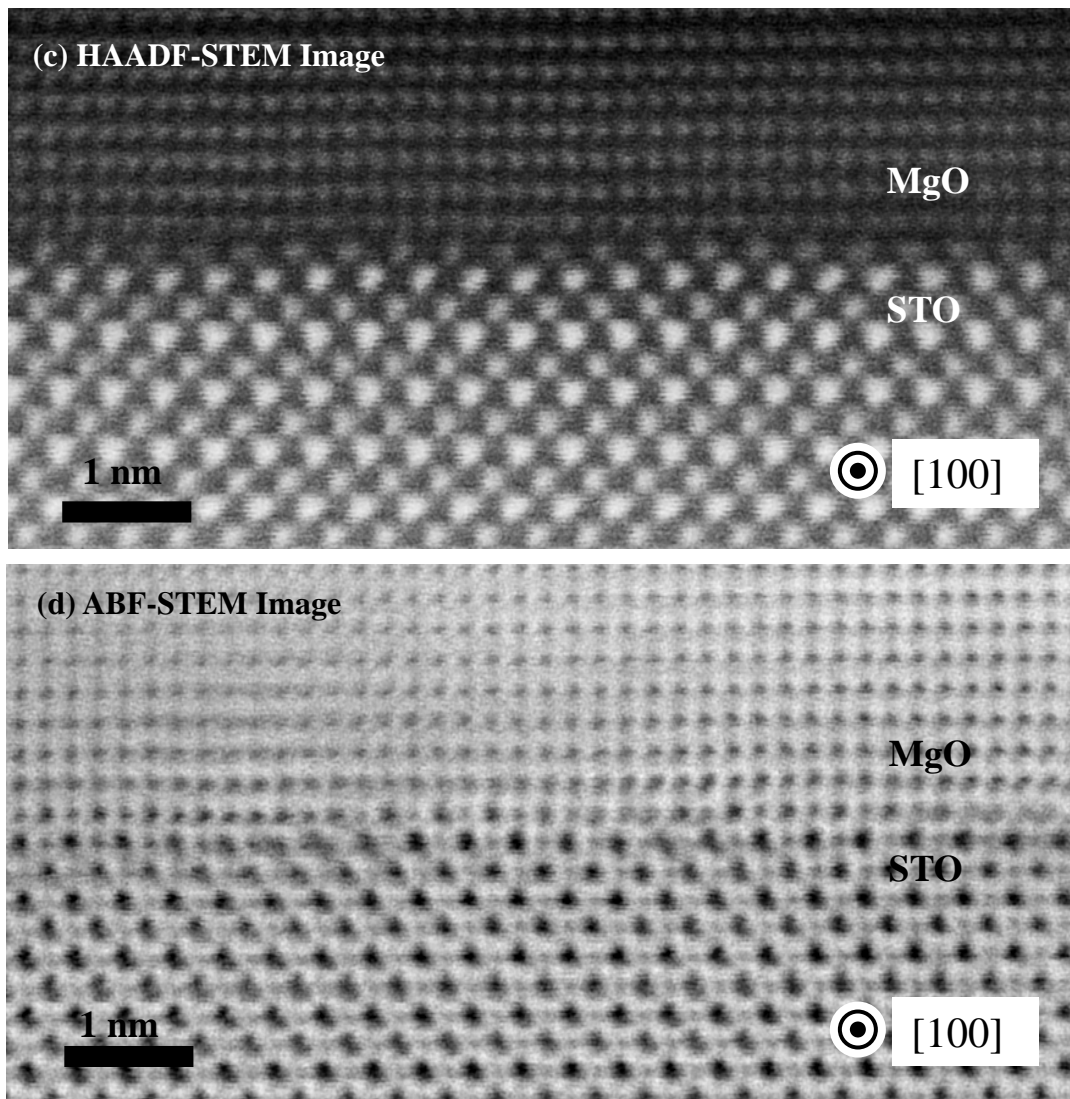


FIG. 2. (c) High-angle annular dark-field and (d) annular bright-field STEM image of MgO/STO interface.