

Long range van der Waal epitaxy of Au / MoS₂ moiré superlattices at room temperature

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Abstract

The performance of two-dimensional electronic devices is significantly influenced by the morphology and structural stability of metal/2D semiconductor interfaces. Nevertheless, the structural evolution of these interfaces, particularly at atomic resolution, has not been comprehensively studied. In this work, high-quality Au thin film crystals were epitaxially grown on MoS₂/Sapphire substrates using an E-gun in a high-vacuum environment and at room temperature. The orderly arrangement of atomic structures of Au/MoS₂ and moiré patterns can be observed in HRTEM images. Using the Au/MoS₂ moiré patterns observed in TEM, an atomic model of the interface was constructed with a 11 x 12 unit cell mesh of Au on MoS₂. This structure exhibits a lattice mismatch of 0.63%. The in-plane structural properties were examined using synchrotron-based grazing incidence wide-angle X-ray scattering (GIWAXS), and the Au (111) out-of-plane surface was measured by synchrotron-based high-resolution XRD with an accuracy of one-thousandth of a degree. The epitaxial relationship between Au and MoS₂ was observed through phi scans. Finally, theta-chi scans show that the crystal axis of Au near the MoS₂ surface is tilted by 0.6 degrees during epitaxial growth on MoS₂. This phenomenon reveals that the epitaxial growth of 3D materials on monolayer TMDs can tolerate lattice mismatches through long-range van der Waals epitaxy.

Keywords - *Electron-beam evaporation, Long range van der Waal epitaxy, Metal-semiconductor contact*