Supporting Information

Supporting Information for Epitaxial Co on GaN by decomposition of template CoO

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

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Metal/semiconductor heterojunction has attracted interest for many years due to the importance in electronic device applications. Usually, owing to large lattice mismatch between semiconductors and most metals, it is difficult to obtain a high-quality epitaxial interface by direct deposition of metals on semiconductors. In this work, we address this problem by proposing a novel strategy to use metal oxides as templates. Due to the small lattice mismatch between CoO and GaN, it was found that the epitaxial CoO films can be readily formed on GaN. Subsequent decomposition of CoO at high temperature and low oxygen pressure gives rise to an epitaxial metal Co film on GaN, forming Co/GaN interface of good quality, and the inheritance of the orientation relationship between CoO and GaN, i.e., (111)Co//(0001)GaN, $[11\bar{2}]$Co//$[1\bar{1}00]$GaN. Additionally, the atomic structures and electronic properties of the Co(111)/GaN(0001) interface are investigated combining aberration-corrected scanning transmission electron microscopy and first-principles calculations. Utilizing Co/GaN as a model system, this study advances insights into the preparation of high-quality epitaxial metal/semiconductor heterojunctions.

Supporting Information

Fig. S1a and S1b show the projections of the wave function on the Co orbitals.

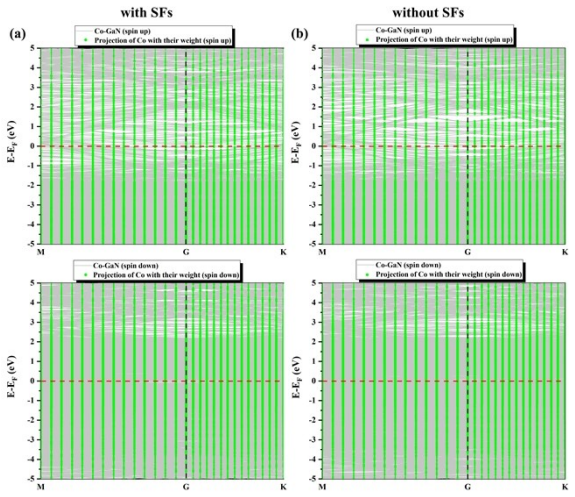

Fig. S1 Projected band structures of Co spin up and spin down in the heterojunction with (a) and without (b) SFs. The black arrows indicate the Schottky barrier height. Gray lines: band structures for the heterojunction system.; green lines: band structures of Co spin up and spin down.

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Fig. S2a and S2b show aberration-corrected HAADF and ABF images, respectively, of the CoO(111)/GaN(0001) interface viewed along $[\bar{1}10]_{CoO}/[11\bar{2}0]_{GaN}$ zone axis. The band structure of the CoO/GaN interface is shown in Fig. S2c.

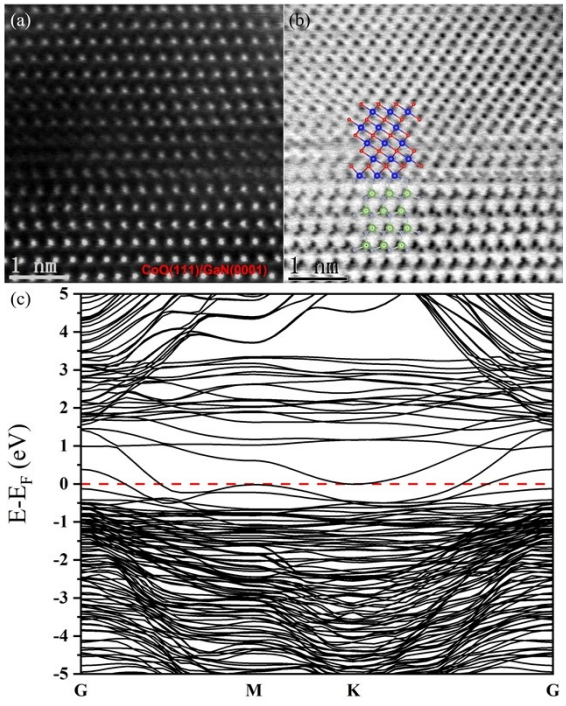

Fig. S2 (a) HAADF-STEM and (b) ABF-STEM images of the CoO(111)/GaN(0001) interface, recorded simultaneously along the $[\bar{1}10]_{CoO}/[11\bar{2}0]_{GaN}$ zone axis. (c) Band structure of the CoO/GaN interface.

The CoO/GaN interface barrier heights have been calculated using the PEB method, as shown in Fig. S3.

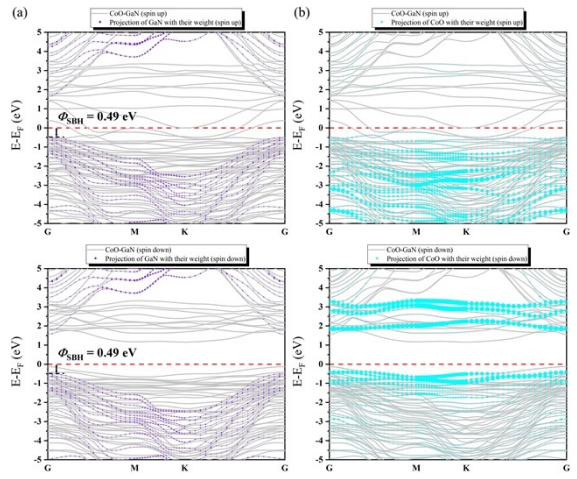

Fig. S3 Spin-resolved projected band structures for (a) GaN and (b) CoO of Co/GaN interfaces. The black arrows indicate the Schottky barrier height.