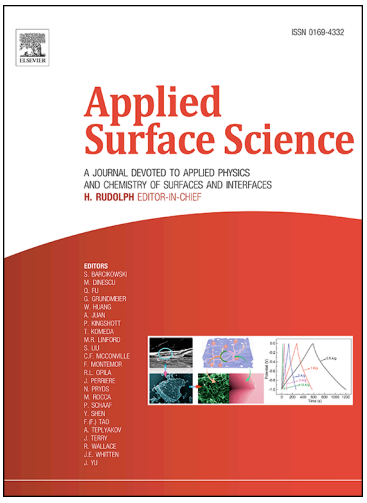

Full Length Article

Epitaxial Growth and Band Alignment of p-NiO/n-Fe_2O_3 Heterojunction on Al_2O_3(0001)

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Epitaxial Growth and Band Alignment of p-NiO/n-Fe_2O_3 Heterojunction on Al_2O_3(0001)

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Abstract

Fe_2O_3 is one of the promising oxide semiconductors as photoanodes for photoelectrochemical water splitting, but its efficiency is still limited by the short diffusion length of photo-excited carriers. Using the internal electric field formed at a p-n heterojunction (HJ) is an efficient strategy to mitigate such limitation. Accordingly, the interfacial atomic structure and band alignment are the most crucial parameters for efficiency optimization. In this work, we report on the epitaxial growth and determination of the band energy alignment of NiO/Fe_2O_3 p-n heterojunction grown on Al_2O_3(0001) substrate by pulsed laser deposition. We show that high crystalline quality NiO(111) thin films can be grown on Fe_2O_3(0001) with epitaxial relationships of $[\bar{1}11]_{NiO}\|[000\bar{1}]_{Fe2O3}$(out-of-plane), $[\bar{1}\bar{1}0]_{NiO}\|[01\bar{1}0]_{Fe2O3}$ and $[\bar{1}1\bar{2}]_{NiO}\|[2\bar{1}\bar{1}0]_{Fe2O3}$(in-plane). The rotation of NiO hexagons by 30° can effectively reduce the lattice mismatch from ~17.4% to ~1.58%. High resolution X-ray photoelectron spectroscopy reveals that valence and conduction band offset of NiO/Fe_2O_3 heterojunction are 0.6 eV and 2.2 eV, respectively. Furthermore, our results also indicate that the energy level of Ni 3d is higher than the valence band maximum of Fe_2O_3. This kind of interfacial electronic structure not only facilitates the charge separation, but lowers the overpotentials for oxygen evolution reaction.

Keywords: Photoelectrochemical Water Splitting; Oxide Semiconductor; Heterojunction; Electronic Structure; Band Offset; Fe_2O_3