

Accepted Manuscript

Full Length Article

Epitaxial Growth and Band Alignment of p-NiO/n-Fe₂O₃ Heterojunction on Al₂O₃(0001)

Y.X. Qin, Z.Z. Yang, J.J. Wang, Z.Y. Xie, M.Y. Cui, C.M. Tian, Y.G. Du, K.H.L. Zhang

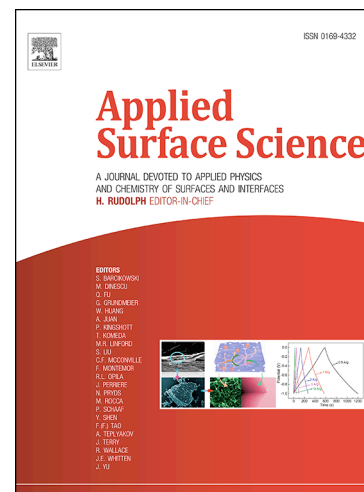
PII: S0169-4332(18)32522-4
DOI: <https://doi.org/10.1016/j.apsusc.2018.09.106>
Reference: APSUSC 40410

To appear in: *Applied Surface Science*

Received Date: 20 August 2018
Accepted Date: 11 September 2018

Please cite this article as: Y.X. Qin, Z.Z. Yang, J.J. Wang, Z.Y. Xie, M.Y. Cui, C.M. Tian, Y.G. Du, K.H.L. Zhang, Epitaxial Growth and Band Alignment of p-NiO/n-Fe₂O₃ Heterojunction on Al₂O₃(0001), *Applied Surface Science* (2018), doi: <https://doi.org/10.1016/j.apsusc.2018.09.106>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Epitaxial Growth and Band Alignment of p-NiO/n-Fe₂O₃ Heterojunction on Al₂O₃(0001)

Y. X. Qin^a, Z. Z. Yang^b, J. J. Wang^a, Z. Y. Xie^a, M. Y. Cui^a, C. M. Tian^a, Y. G. Du^b, K. H. L. Zhang^{a,*}

^aState Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, P.R. China

^bPhysical Sciences Division, Physical & Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, Washington 99352, USA

Email: Kelvinzhang@xmu.edu.cn

Abstract

Fe₂O₃ 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/Fe₂O₃ p-n heterojunction grown on Al₂O₃(0001) substrate by pulsed laser deposition. We show that high crystalline quality NiO(111) thin films can be grown on Fe₂O₃(0001) with epitaxial relationships of $[\bar{1}11]_{\text{NiO}} \parallel [000\bar{1}]_{\text{Fe}_2\text{O}_3}(\text{out-of-plane})$, $[\bar{1}\bar{1}0]_{\text{NiO}} \parallel [01\bar{1}0]_{\text{Fe}_2\text{O}_3}$ and $[\bar{1}1\bar{2}]_{\text{NiO}} \parallel [2\bar{1}\bar{1}0]_{\text{Fe}_2\text{O}_3}(\text{in-plane})$. 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/Fe₂O₃ 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 Fe₂O₃. 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; Fe₂O₃

Download English Version:

<https://daneshyari.com/en/article/9951524>

Download Persian Version:

<https://daneshyari.com/article/9951524>

[Daneshyari.com](https://daneshyari.com)