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Atomic Resolution Study of the Bonding between ZnO Nanowires

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One-dimensional nanostructures have been intensively investigated due to their unique properties and widespread applications [1]. Semiconducting ZnO nanostructures, with a band gap of about 3.4 eV, have broad applications in energy harvesting and storage, catalysis, and optoelectronics [2]. To fully realize the potential of ZnO nanostructure it is important to understand the interfacial properties of ZnO-based devices or systems since these interfaces can significantly affect their physical properties. We report here our recent study of the interfacial atomic structures formed among ZnO nanowires (NWs).

The ZnO NWs were fabricated via a vapor transport and condensation process inside a horizontal tube furnace. The source materials consisted of ZnO and carbon powders. When the mixed powders were heated to about 1100°C, carbothermal decomposition of ZnO occurred and vaporized Zn and oxygen molecules were transported to the low temperature zone by the Ar or N_2 carrier gas. At the low temperature zone ZnO NWs were formed. When the partial vapor pressure of Zn was high, some of the ZnO NWs were bonded together to form coherent or other types of interfaces. Aberration-corrected scanning transmission electron microscope (STEM), with a nominal image resolution of 0.08 nm in the high-angle annular dark-field (HAADF) imaging mode, was used to investigate the atomic structures of the interfaces formed among the ZnO NWs.

Figure1a shows low magnification HAADF image of two ZnO NWs attached to each other. Detailed examinations of the contact regions revealed that the two ZnO NWs formed a strong bond and that atomic diffusion had occurred so that the two NWs bonded strongly to each other. The atomic resolution HAADF image (1b) clearly shows the positions of the Zn columns of both the ZnO NWs and the interfacial region. Both NWs possess the ZnO wurtzite structure. The theoretical unit cell of ZnO wurtzite structure is identified in Fig. 1b (indicated by the yellow parallelogram) for both ZnO NWs. It appears that the two NWs shifted by about 0.11 nm along the [0001] direction. The interface structure is identified by the red squares in Fig. 1b. The interfacial Zn-Zn bonding was measured to be 0.31nm, 7% longer than the Zn-Zn bonding in the NWs. Fig.1c shows a schematic diagram illustrating the interfacial atomic arrangement viewed along the [11-20] zone axis. Fig. 2a shows another atomic resolution HAADF image of a different interface formed between two ZnO NWs, clearly revealing arrays of interfacial misfit dislocations with a periodicity of about 2.5 nm. Fig. 2b shows magnified image illustrating the details of the atomic arrangement near the dislocation core and Fig. 2c is a schematic diagram derived from Fig. 2b. Detailed analyses of the interfacial structures and the growth mechanisms will be discussed [3].

References:
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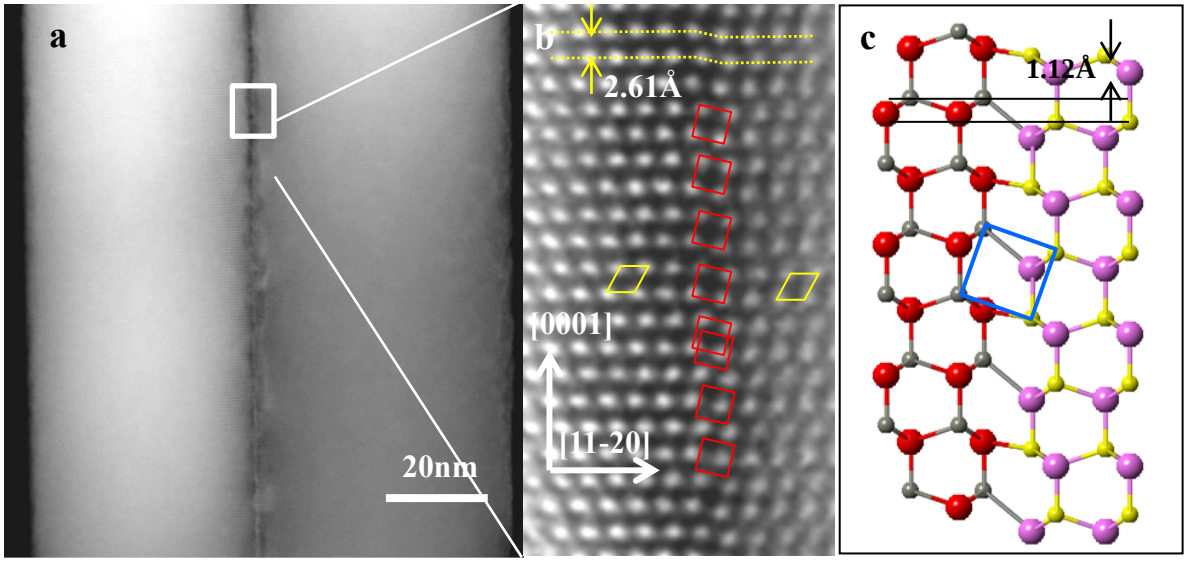

Figure 1. Low (a) and high (b) magnification HAADF images of a typical bonded ZnO NWs, revealing the atomic arrangement of the Zn columns at the interface region. The interface is marked by the red squares. The unit cell of the ZnO wurzite structure is indicated by the yellow paralleograms. Fig. 1c is the schematic diagram illustrating the interfacial atomic arrangement viewed along the ZnO [11-20] zone axis.

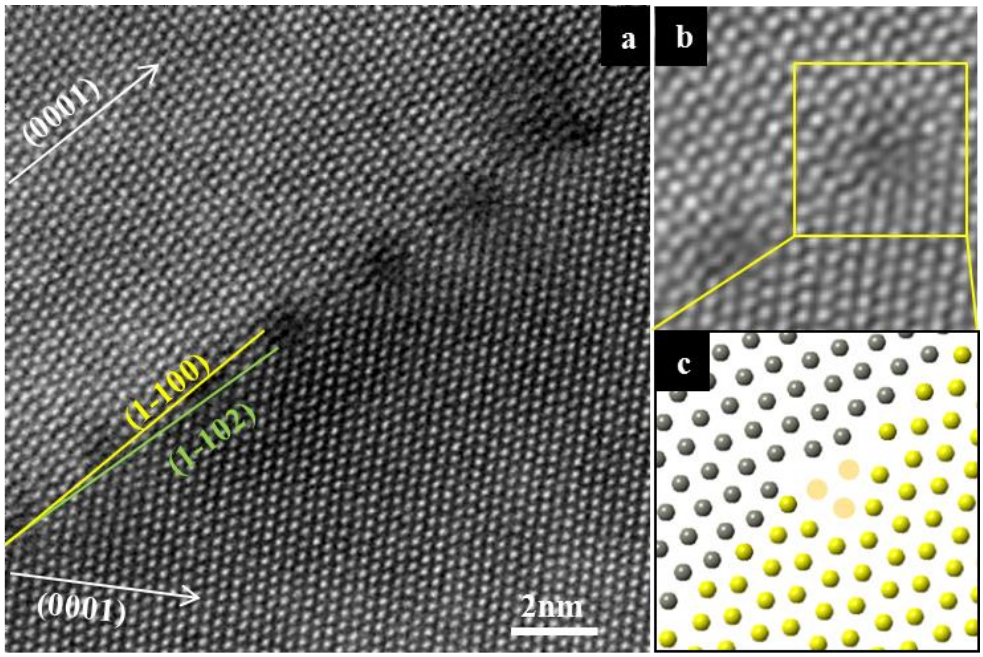

Figure 2. Low (a) and high (b) magnification HAADF images of a typical interface formed by bonding two ZnO NWs, clearly revealing the arrays of interfacial misfit dislocations and the atomic arrangement of the Zn columns near the dislocation cores. Fig. 2c is the schematic diagram illustrating the arrangement of Zn columns shown in Fig. 2b.

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