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Opinion

Bandgap Modulation Based on II-VI Oxides

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Introduction

Zinc Oxide (ZnO), as a traditional II-VI semiconductor material with direct wide bandgap of 3.37eV and large exciton binding energy of 60meV, has been regarded as a promising candidate for optoelectronic devices including light emitting diodes (LEDs), lasing diodes (LDs), and ultraviolet (UV) photodetector [1-3]. For realizing such high-performance optoelectronic devices, bandgap engineering is extremely important. High quality multiquantum wells (MQWs) are required within a standard LED structure, in which the bandgap of the barrier layer is widened by alloying BeO (or MgO) with ZnO. For UV photodetectors, ZnO-based ternary or quaternary alloys with adjustable bandgaps are demanded to realize different cut-off response wavelengths. In this case, the tunable bandgap plays a key role as an optical filter, intercepting the incident lights with photon energy smaller than the bandgap of the material. Therefore, bandgap modulation based on II-VI Oxides (ZnO, BeO, and MgO) is urgently required, while some key issues are still beyond challenge.

Figure 1 presents the crystal structure and lattice constants of BeO, ZnO, and MgO; and the ion radius of Be^{2+}, Zn^{2+}, and Mg^{2+}. $Mg_xZn_{1-x}O$ is first proposed by doping appropriate amount of Mg into the host lattice of ZnO. The ion radius of Mg^{2+} (0.74Å) is close to that of Zn^{2+} (0.72Å), thus the lattice distortion of $Mg_xZn_{1-x}O$ can be effectively suppressed. However, owing to the crystal structure difference between ZnO (Hexagonal) and MgO (Cubic), phase transition of $Mg_xZn_{1-x}O$ occurs when $x \geq 0.33$, and corresponding bandgap is limited to 3.99eV [4,5]. $Be_xZn_{1-x}O$ also encounters the problem of bandgap limitation, while it reveals quite different physical characteristics. Though both BeO and ZnO belong to hexagonal structure, the lattice mismatch between BeO (a: 2.72Å; c: 4.32Å) and ZnO (a: 3.25Å; c: 5.23Å), and the ion radius difference between Be^{2+} (0.35Å) and Zn^{2+} (0.72Å) are large. Therefore, localized lattice distortion and phase separation are observed in $Be_xZn_{1-x}O$ [6-8]. The bandgap of $Be_xZn_{1-x}O$ is only widened to 3.55eV, and the Be^{2+} with small ion radius also has chances to occupy the interstitial sites. Finally, we introduce a quaternary $Be_xMg_yZn_{1-x-y}O$ alloy with low Be/Mg atom ratio, the bandgap of $Be_xMg_yZn_{1-x-y}O$ can be widened to 5.14eV while the hexagonal structure is still maintained [9]. The success of Be_xMg_yZ O can be ascribed to 1, Be substitution induces tensile strain compensates the compressive strain caused by Mg substitution; 2, tetra-coordination preference of Be atom should suppress the lattice distortion induced by the Mg atom with six-coordination preference .

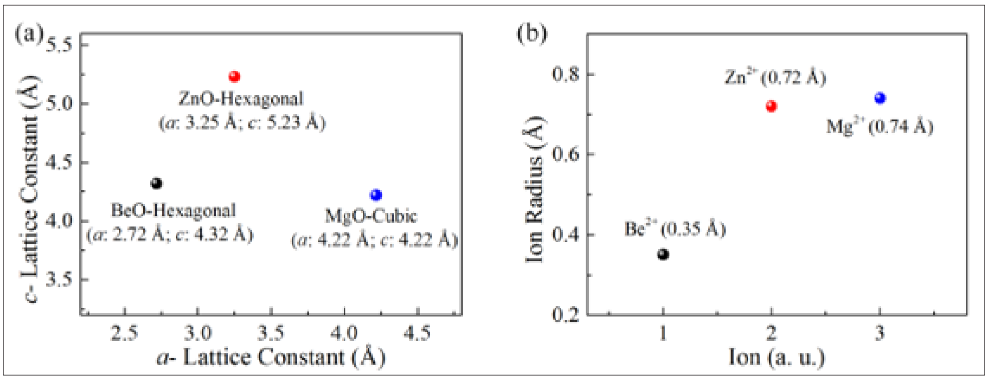

Figure 1: (a) The crystal structure and lattice constants of II-VI Oxides (BeO, ZnO, and MgO); (b) the ion radius of Be^{2+}, Zn^{2+}, and Mg^{2+}.

In conclusion, we have achieved in this effort is demonstrating the wide range bandgap modulation of quaternary $Be_xMg_yZn_{1-x-y}O$ alloy with specific atomic ratio. Our work regarding to the bandgap engineering is an important step towards high performance ZnO based optoelectronic devices.

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Conflict of Interest

The author declares that he has no conflict of interest.

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