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Abstract

Oxide semiconductors are promising candidates in the semiconductor industry due to their widespread applications, including lasers, light-emitting devices (LEDs), detectors, etc. In recent decades, extensive research has been conducted on ZnO and related alloys (such as ZnO-MgO and ZnO-CdO systems) as potential alternatives to the GaN system (including AlGaN and InGaN). However, despite sharing the same crystal structure as both CdO and MgO (cubic rocksalt structure; $Fm\bar{3}m$), the exploration of CdO-MgO-based alloys remains one of the least studied aspects in the group II-IV oxides system. Notably, the bandgap tunability of CdO, ranging from 2.3 to 7.5 eV through alloying with MgO, enhances the prospective applications of CdO-MgO-based ternary alloys across the visible to deep ultraviolet (UVC) wavelength region. There are two possible approaches to obtaining ternary alloys: random layers and quasi-ternary alloys short period superlattices. Random ternary alloys offer isotropic structural, optical, and electronic properties, whereas quasi-ternary alloys provide tailored physical properties through precise control of the thickness and composition of each sublayer. Furthermore, the growth of alloys on different substrates provides an additional degree of freedom that influences ternary alloys' structural and morphological properties.

This PhD dissertation aims to explore the properties of CdO-MgO-based, both random and quasi-ternary alloys grown using plasma-assisted molecular beam epitaxy (PA-MBE) growth technique. MBE is an advanced epitaxial growth technique that offers sharp interfaces, low levels of impurities, low defect concentration, and precise control of the grown layers. The main key goal is to focus on bandgap tunability in CdO-MgO-based ternary alloys grown on different substrates (including various planes of sapphire, quartz, MgO, and Si). To achieve this objective, a range of characterization techniques are employed in ternary alloys, including XRD, SEM, EDX, AFM, SIMS, TEM, UV-visible spectroscopy, and electrical measurements.

The work of the PhD dissertation is divided into three main parts. In the beginning, I discuss the various physical properties of CdO binary oxide on *m*-plane sapphire, quartz, and Si substrates. The influence of stoichiometry on the structural, morphological, and electrical properties of CdO layers is analyzed. The shifting of bandgap with change in growth conditions is further interpreted using the combining Burstein-Moss, electron-electron, and electron-ion effects. The temperature-dependent bandgap study of CdO/quartz is performed, and the bandgap temperature coefficient is determined. Furthermore, the optical investigations are carried out using reflectance spectra to determine the optical parameters of CdO/Si.

In the second section of my doctoral dissertation, CdMgO random ternary alloys grown on various planes of sapphire, quartz, and Si substrates are studied. The Cd and Mg content in the

CdMgO alloys is controlled by varying the growth conditions. The optical bandgap can be tuned with an increase in Mg content in the alloys from yellow to UVC region. The structural investigations using XRD reveal that different substrates, as well as the growth conditions, influence the orientations of the CdMgO random alloys. However, for higher Mg content, evidence of mixed non-homogeneous crystal starts to appear.

In the last section, I discuss heteroepitaxial and homoepitaxial {CdO/MgO} quasi-ternary alloys short-period superlattice (SL) structures grown on sapphire and MgO substrates, respectively. In the SL structure, the MgO sublayer thickness is fixed at 4 monolayers (MLs), whereas the CdO sublayer thickness is varied from 1 to 10 ML. Structural and morphological investigations reveal that the change in the substrate, as well as the CdO sublayer thickness, influences the physical properties of the SL structure. Furthermore, the bandgap can be tuned by varying the CdO sublayer thickness in the SL structure. The obtained experimental results are well supported by the theoretical calculations. Furthermore, the pressure-dependent bandgap study is performed using a diamond anvil cell (DAC) and it is found that the bandgap can be tuned by applying pressure in the DAC. In the mentioned studies, the band gap pressure coefficient is determined and the obtained experimental results are compared with theoretical results obtained from density functional theory calculations.

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