別紙第１号様式　　　　　　　　　　　　　No.1

博　士　論　文　の　要　旨

専攻名　システム創成科学専攻
氏　名　JANG HYOCHANG　　　　　　　　印

博士論文題名

Bandgap Engineering and Doping in ZnCdO Thin Films
(ZnCdO 薄膜のバンドギャップエンジニアリングとドーピング)

要旨

Transparent conducting oxides (TCOs) are one of the key components of a solar cell to collect charge carriers from the illuminated side of the cell. In order to achieve high conversion efficiency, TCOs that can transmit light in a wide range of wavelengths is required. However, widely used TCOs such as In_2O_3: Sn (ITO), In_2O_3:Ga (IGO), and ZnO:Al (AZO) have limited transmittance in the IR region (>1000 nm) because of their high electron concentration (> 10^{21} cm^{-3}) and low mobility (< 40 cm^2/Vs) which give rise to strong free carrier absorption (FCA) and plasma reflection. Therefore, the research to find new TCO materials with high transmittance extending into the IR region (> 1500 nm) are essential for full solar spectrum photovoltaics.

Among the various TCO material candidates, CdO has the highest reported mobility values of 200 cm^2/Vs at an electron concentration > 10^{21} cm^{-3}, and thus has been considered as a promising candidate for full spectrum solar cell applications. Because of the high mobility, CdO is expected to realize a low resistive thin film with a low carrier concentration, extending the FCA and a plasma reflection effect to a much longer wavelength region (λ > 2000 nm). Hence it can be used as transparent conductors on devices in which transparency in the long wavelength infrared region is required. Although the band gap (2.3 eV) of CdO is small for a transparent conductor application, it can be increased by alloying with a larger gap oxide such as ZnO which has a band gap of ~ 3.3 eV. However, because ZnO has a wurtzite (WZ) structure (α=3.25 Å, c=5.21 Å) whereas CdO a rocksalt (RS) structure (α=4.70 Å), the crystal structure of $Zn_{1-x}Cd_xO$ (ZnCdO) is expected to change at a certain Cd composition. However, reported ZnCdO thin films shows lower band gap compared to other TCOs materials. Therefore, this research mainly focused on expanding the band gap of ZnCdO thin films to absorb much more sun spectrum, archiving higher conversion efficiency

This dissertation explores the optical, structural, and electrical properties of ZnCdO thin film alloys (0 ≤ x c≤ 1) grown by molecular beam epitaxy under various growth condition.

At the beginning of this research, ZnCdO thin films are grown on sapphire substrate by MBE with various Cd compositions for studying structural, electrical, and optical properties of ZnCdO thin films. The phase transition from WZ to RS is found to take a place at the Cd content x ~ 0.5 to 0.6. Within the composition region of x ~ 0.5 to 0.6, both RS and WZ crystals co-exist. Transmittance above 80 ~ 95 % in the visible range is observed for both the WZ and RS alloys. Optical gap of the WZ alloys decreases from 3.27 eV for ZnO to ~ 2.35 eV (x ~ 0.44). At the phase transition to RS at x ~ 0.55, the optical gap increases drastically to >

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3.0 eV RS-alloys with a large optical gap of 3.0 eV (an intrinsic gap of ~ 2.7 eV) is achieved for x ~ 0.6. RS-ZnCdO thin films exhibit a low resistivity of 5×10^{-4} Ωcm with maximum mobility of ~ 90 cm^2/Vs and a high carrier concentration 4×10^{20} cm^{-3}.

Secondly, the sapphire substrate is replaced with MgO (100) substrate to improve the crystallinity and increase the bandgap of RS-ZnCdO thin films. It is found that the phase transition from WZ to RS occurs at the Cd composition x between 0.51 and 0.59, and RS-ZnCdO is epitaxially grown on MgO (100) at the Cd composition x above 0.59. In the visible range, high transmittance above 85% is observed for RS-ZnCdO films ($0.59 \leq x \leq 1.0$). In the WZ-phase region, the optical band gap energy decreases from 3.25 eV for ZnO to ~ 2.16 eV for WZ-ZnCdO with x ~ 0.51. After the partial phase transition from WZ to RS at $x > 0.51$, the optical band gap energy increases intensely and the largest optical band gap energy of 3.08 eV is obtained for x =0.59 with an intrinsic band gap energy of 2.72 eV. RS-ZnCdO films shows a low resistivity around 2.5×10^{-4} Ωcm with a maximum mobility of ~ 51.7 cm^2/Vs and a high carrier concentration around 5×10^{20} cm^{-3}.

Finally, in order to further increase the band gap energy of ZnCdO, the effects of Al doping on the structural, electrical, and optical properties of RS-ZnCdO thin films on MgO substrates are investigated. The electron concentration increases with increasing Al cell temperature T_{Al}, and is n~1.5×10^{21} cm^{-3} at T_{Al} = 875 °C, which corresponds to an Al-doping concentration of ~7.8%. The corresponding optical band gap energy increases because of free-carrier effects including Burstein-Moss-shift and band-renormalization. Furthermore, Al is an efficient donor dopant in both RS-ZnCdO and WZ-ZnCdO thin films. Electron concentrations $>10^{21}$ cm^{-3} are obtained with Al doping for alloys incorporating Cd content x ranging from 0.27 to 1.0, regardless of the crystal structure. A large optical band gap energy of 3.45 eV is observed in the RS-ZnCdO thin film having $x\approx0.7$, with a resistivity of 1×10^{-4} Ω-cm, and a wide transmission window of up to 2000 nm. These characteristics of RS-ZnCdO are attractive as TCO materials in future full spectrum solar cells.