Accurate determination of optical bandgap and lattice parameters of $Zn_{1-x}Mg_xO$ epitaxial films ($0 \leq x \leq 0.3$)

B. Laumer, M. Eickhoff, Justus–Liebig–Universität Gießen, Germany
F. Schuster, M. Stutzmann, Walter Schottky Institut München, Germany
A. Bergmaier, S. Eschbaumer, G. Dollinger, LRT2, UniBw München, Germany

Although ZnO and its related $Zn_{1-x}Mg_xO$ alloys have been studied intensely in the past years owing to the favorable properties of these materials for the fabrication of optoelectronic devices, the experimental data for the evolution of the $Zn_{1-x}Mg_xO$ bandgap and lattice parameters with the amount of incorporated Mg varies considerably in the literature [1]. Several factors are identified to be responsible for these variations, such as uncertainties due to an inaccurate determination of the Mg concentration x, the formation of a coincidence lattice dependent on the type of substrate used, and the determination of the bandgap from absorption measurements neglecting the strong modification of the spectra due to excitonic contributions.

In this work $Zn_{1-x}Mg_xO$ epitaxial films with Mg concentrations $0 \leq x \leq 0.3$ were grown by plasma–assisted molecular beam epitaxy on a–plane sapphire substrates. Precise determination of the Mg concentration x was performed by elastic recoil detection analysis. The bandgap energy was extracted from absorption measurements with high accuracy taking electron-hole interaction and exciton-phonon complexes into account. From these results a linear relationship between bandgap energy and Mg concentration is established for $x \leq 0.3$. Due to alloy disorder, the increase of the photoluminescence emission energy with Mg concentration is less pronounced. An analysis of the lattice parameters reveals that the epitaxial films grow biaxially strained on a–plane sapphire [2].

The $Zn_{1-x}Mg_xO$ films investigated in this study were grown by plasma–assisted molecular beam epitaxy (PAMBE). For an accurate determination of the sample composition, elastic recoil detection (ERD) measurements were performed using a 170 MeV ^{127}I beam. The scattering angle for the recoil ions was 38°, the incident angle of the projectile ions was 10° with respect to the sample surface, whose size was at least $4\,\mathrm{mm}^2$. The recoil ions were analyzed in a ΔE–E_{res} detector telescope with a solid angle of detection of 3.5 msr [3]. ERD is an inherent quantitative ion beam analysis technique as long as ion beam damage can be avoided and the scattering geometry is exactly controlled. In the present case, differences from one measurement to another or fluctuations in the profiles are just due to statistical uncertainties. As an example Fig. 1 shows the ERD depth profiles of O, Mg and Zn of the analyzed $Zn_{1-x}Mg_xO$ film having a Mg concentration of $x = 0.22$.

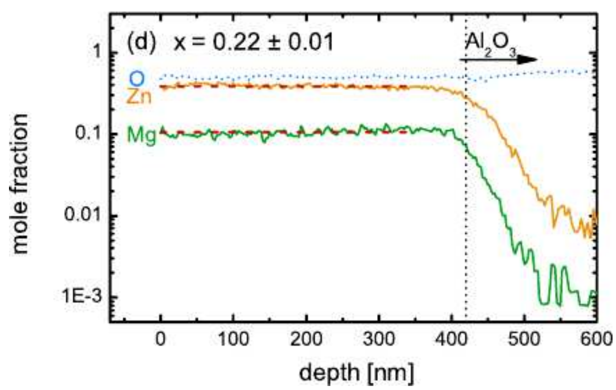

Figure 1: ERD depth profiles of Zn, Mg (continuous lines), and O (short-dashed line) of a $Zn_{1-x}Mg_xO$ films with $x = 0.22$. The long–dashed lines represent linear fits to the Zn and Mg profiles. The vertical short-dashed line marks the interface between epitaxial film and sapphire substrate.

For absorption and photoluminescence (PL) measurements at $T = 4.2\,\mathrm{K}$, the samples were mounted into a contact gas cryostat after backside polishing of the sapphire substrates. From the obtained data the absorption coefficient is calculated. For PL measurements, the 244 nm line of a frequency-doubled Ar laser with a power density of 30 MW/cm^2 was used for excitation. The luminescence signal was collected normal to the sample surface and was spectrally dispersed using a double grating spectrometer with a resolution of 0.1 nm and detected with a photomulti- plier. The lattice parameters were determined by high- resolution X–ray diffraction (HRXRD) [2]. The dependence of the PL energy and bandgap on the Mg content is shown in Fig. 2.

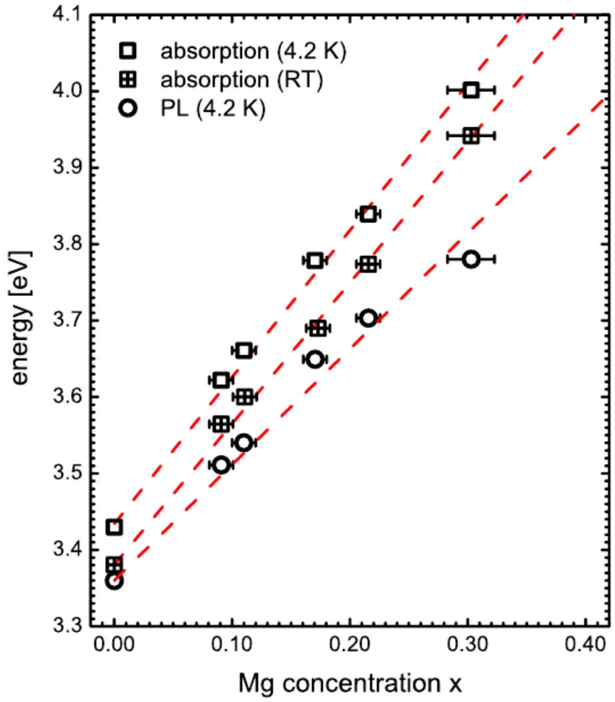

Figure 2: Dependence of the PL peak energy at 4.2 K and bandgap as determined by absorption measurements at 4.2 K and at RT on the Mg content determined by ERD.

In summary, a composition analysis of PAMBE grown $\mathrm{Zn_{1-x}Mg_xO}$ epitaxial films was carried out by elastic recoil detection analysis for a precise determination of the Mg concentration x. In addition, the bandgap energy was extracted from absorption measurements with high accuracy employing an inhomogeneously broadened Elliott model and including the effect of exciton-phonon complexes. From these results a linear relationship between the low– and room temperature bandgap energy and the Mg concentration x is established. The variation of the low–temperature PL emission energy is found to deviate from a linear behavior due to the increase of the disorder–induced Stokes shift for higher Mg concentrations. An analysis of the lattice parameters suggests that epitaxial $\mathrm{Zn_{1-x}Mg_xO}$ films form a coincidence lattice with the a–plane sapphire substrates, and therefore are subject to biaxial compressive strain, which gives rise to a nonlinear variation of the a– and c–lattice parameters for increasing Mg concentration x.

ACKNOWLEDGMENT

Financial support from the European Union via the IP ORAMA (CP–IP 246334–2) and via the Integrating Activity ”Support of Public and Industrial Research Using Ion Beam Technology (SPIRIT)” under EC Contract No. 227012 was gratefully acknowledged.

REFERENCES

[1] see references in [2].

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[3] A. Bergmaier et al., Nucl. Instrum. Methods B 136–138 (1998) 638.