G/PII.25

UNIVERSITÄT LEIPZIG

Ellipsometry Workgroup

Phonon and plasmon properties in (Mg,Mn,Ni,Co,Fe,Cu)ZnO alloy and (N,Li,P,Sb,Ga,Al)-doped ZnO and thin films

C. Bundesmann#, M. Schubert, U. Teschner, D. Spemann, H. v. Wenckstern, M. Lorenz, M. Grundmann

Institut für Experimentelle Physik II, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

bundesm@physik.uni-leipzig.de http:\\www.uni-leipzig.de\ellipsometrie

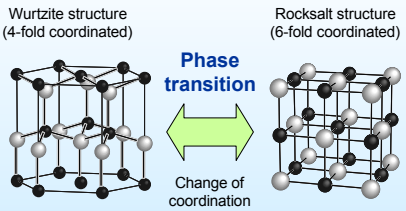
Our Message

- Investigation of lattice (phonons) and free charge carrier properties (plasmons) of ZnO-based alloy and doped ZnO thin films by combination of infrared spectroscopic ellipsometry and Raman scattering
- $Mg_xZn_{1-x}O$ exhibits phase transition from wurtzite to rocksalt crystal structure with change of coordination number

Introduction

Motivation for alloying and doping of ZnO

- Band gap engineering (Mg,Cd)ZnO
- n-type conductivity (Al,Ga)-doped ZnO
- p-type conductivity (Li,N,P,Sb)-doped ZnO
- Ferromagnetism (Mn,Fe,Co,Ni,Cu)ZnO



Growth
PLD technique
Sapphire substrates
(*c*-, *a*-, *r*-plane α-Al_2O_3)

X-ray diffraction
Crystal structure
Lattice constants

Rutherford backscattering
Composition

$Mg_xZn_{1-x}O$ thin films ($0 \le x \le 1$)

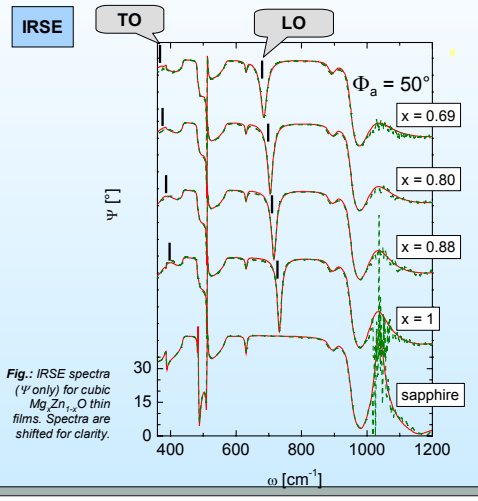
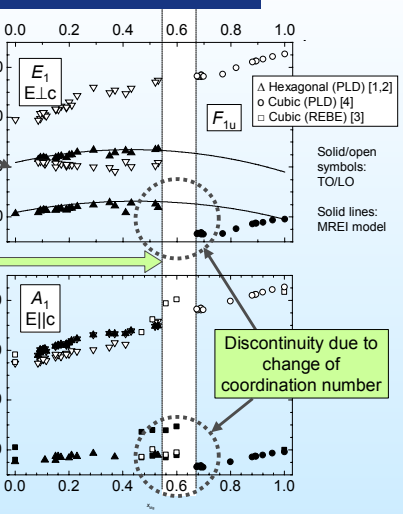


Fig.: IRSE spectra (Ψ only) for cubic $Mg_xZn_{1-x}O$ thin films. Spectra are shifted for clarity.

Local mode
Mg replaces Zn
509 cm^{-1} (Exp.)
518 cm^{-1} (Model)



Phase transition of PLD-grown thin films

Extrapolation to x=0
"Cubic ZnO"
$\varepsilon_\infty \sim 4.15$
$\omega_{TO} \sim 300$ cm^{-1}
$\omega_{LO} \sim 580$ cm^{-1}

Agrees qualitatively with calculated data [5].

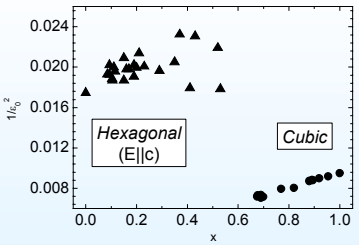


Fig.: From experimental data calculated $1/\varepsilon_0^2$ values for E||c.

Change of reduced exciton mass μ_{ex} upon phase transition, according to

$$E_{ex}^b \sim \frac{\mu_{ex}}{\varepsilon_0^2}$$

(E_{ex}^b changes continiously)

[1] C. Bundesmann et al., APL 81, 2376 (2002).
[2] R. Schmidt et al., Proceedings ICPS 26 (20029.
[3] J. Chen and W. Z. Shen, APL 83, 2154 (2003).
[4] C. Bundesmann et al., APL 85, 905 (2004).
[5] J. Serrano et al., Phys. Rev. B 69, 094306 (2004).

(Li,N,Al,P,Ga,Sb)-doped ZnO thin films

Raman scattering

Phonon modes

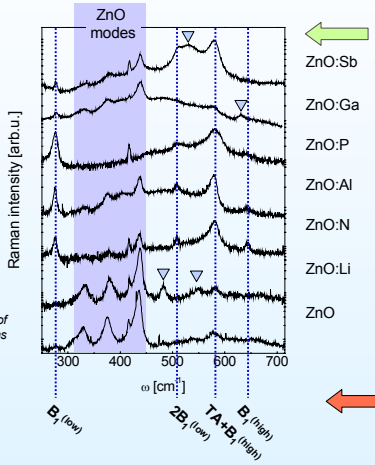


Fig.: Raman scattering spectra of several doped ZnO thin films

"N-related" additional modes (, [1]) occur in many samples, observation of dopant-specific modes ( )

Presumption [2]: Defect-induced modes ( )

[1] Kaschner et al., APL 80,1909 (2002).
[2] Bundesmann et al., APL 83, 1974 (2003).
[3] Manjón et al., JAP 97, 053516 (2005).

Calculation [3]: Defect- and impurity-activated silent modes of ZnO host lattice

IRSE

Plasmon (and phonon) properties

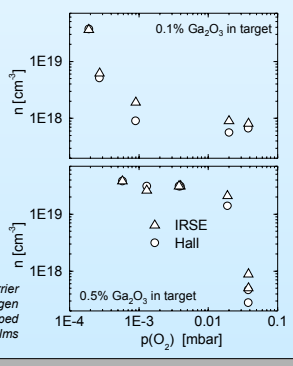


Fig.: Free charge carrier density versus partial oxygen pressure for Ga-doped ZnO thin films

Comparison of IRSE data and Hall effect results

Good agreement of n^{IRSE} and n^{Hall}

IRSE reveals anisotropy of optical mobility parameters

$$\mu_{E||c}^{opt} < \mu_{E\perp c}^{opt}$$

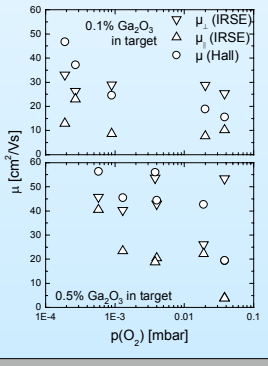


Fig.: Free charge carrier mobility versus partial oxygen pressure for Ga-doped ZnO thin films

$(Mn,Fe,Co,Ni,Cu)_xZn_{1-x}O$ thin films

Raman scattering

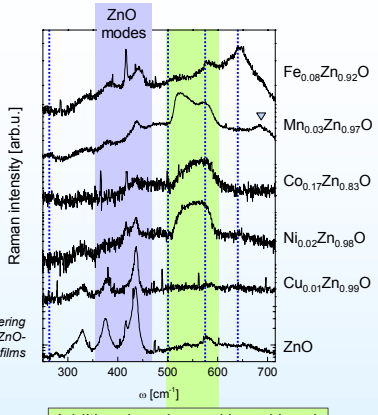
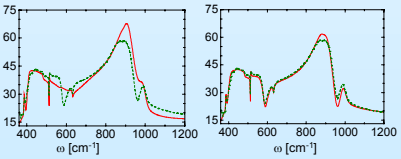


Fig.: Raman scattering spectra of several ZnO-based alloy thin films

Additional modes and broad band typical for 3d-element incorporation

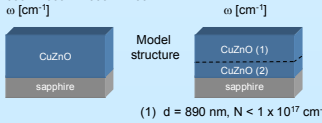
No defect-induced modes for CuZnO, ⇨ defect-decoration ?

IRSE



Figs.: IRSE spectra (Ψ only) for a $Cu_xZn_{1-x}O$ thin film.

Inhomogeneous free charge carrier distribution



(1) d = 890 nm, N < 1 x 10^{17} cm^{-3}
(2) d = 550 nm, N = 8,15 x 10^{18} cm^{-3}

One-layer-model not appropriate ⇨ Two-layer-model assumption

Printed at Rechenzentrum der Universität Leipzig