Experimental and Density Functional Theory Studies of the Structure, Optical and Electronic Properties of Wide Band Gap Oxides for Nanodevices

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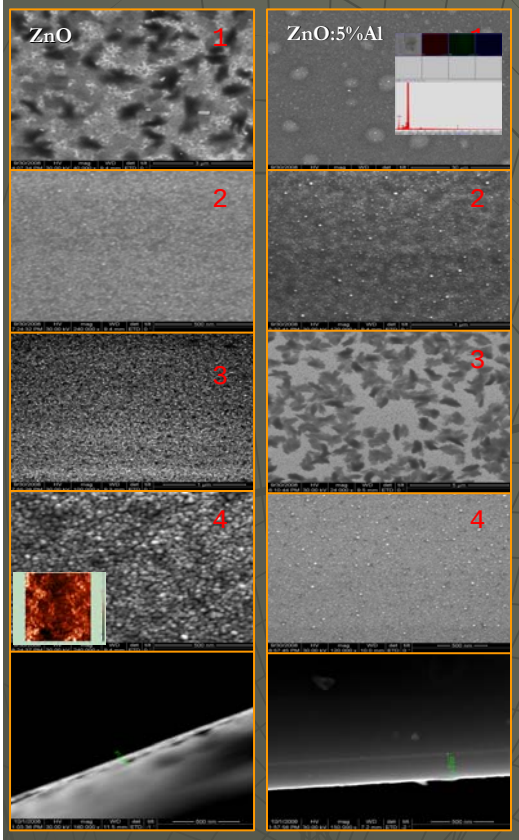
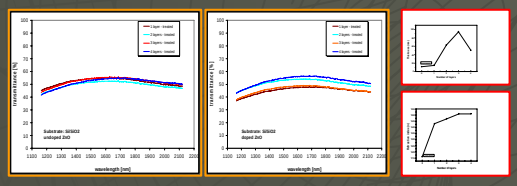
SEM, EDX, AFM, Spectroellipsometry and Spectrofotometry studies of ZnO and ZnO:5%Al obtained by sol-gel method.

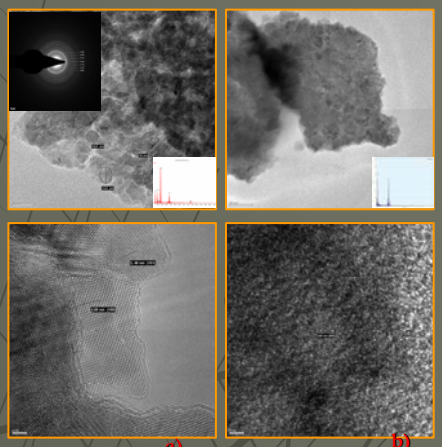


Evolution of ZnO and ZnO:5%Al thin films morphology. The films have been obtained by deposition of 4 succesive layers using sol-gel method. Each layer was treated after deposition at 500°C in ambient atmosphere for 1 hour.



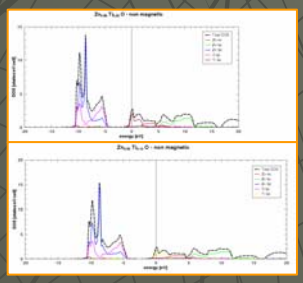
Variation of transmitance in the wavelength range 1100-2100 nm with the number of deposited layers used to obtain ZnO and ZnO: 5%Al films.

HRTEM, SAED and EDAX analyses of ZnO thin films obtained by DC and RF magnetron sputtering from Zn and ZnO targets.

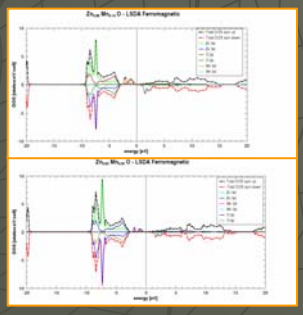


HRTEM images of ZnO films obtained by DC (a) and RF magnetron sputtering (b). The films structure is wurtzite, with nanocrystalls orientation (100) (a), and (002) (b).

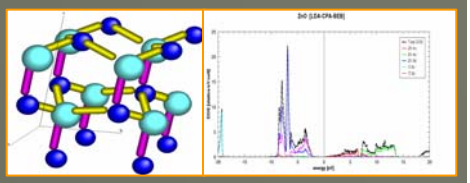
Zn:Ti



Zn: Mn

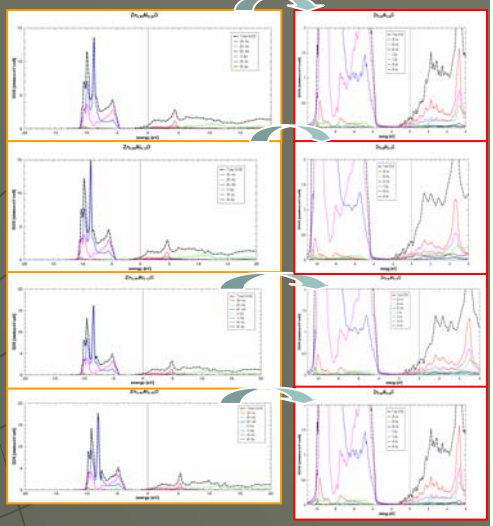


Computational study of ZnO and ZnO doped with Al, Ti and Mn.



ZnO supercell 2x2x1. ZnO crystallizes in the wurtzite structure, space group P63mc , with the lattice parameters a=3.2427 Å and c =5.1948 Å

Zn: Al



Calculation details

The ab initio self-consistent energy-band calculations were carried out in the Local Spin Density Approximation to the Density Functional Theory [1], using the Full Potential Local-Orbital (FPLO) band structure code [2]. This is an all-electron scheme based on the method of linear combination of nonorthogonal local orbitals. The site-centered potentials and densities were expanded in spherical harmonics up to lmax=12.

The exchange and correlation potential in the parametrization of Perdew and Wang 92.

Brillouin zone sampling: 16x16x16. The resulting accuracy in energy is better than 10^(-4) eV.

Basis sets: Zn, Ti and Mn: core states 1s2s2p, semicore states 3s3p, valence states 4s4p3d and polarization states 5s5p4d.

O: semicore states 1s, valence states 2s2p and polarization states 3d (to improve the completeness of the basis set).

Al: core states 1s, semicore states 2s2p, valence states 3s3p and polarization states 4s3d.

Conclusions

The comparison between total energies in spin polarized and non polarized calculations shows that the ground state is non magnetic for Al or Ti and magnetic in the case of Mn substitution for Zn ($2\% < x < 20\%$). Al substitution determines the appearance of a density of states at the Fermi level even at the lowest concentration (2%), showing the onset of metallic conduction.

The density of states at the Fermi level, N(E_F), increases as aluminum concentration increases.

References

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