

Highlights

Oxides — 2017

Morphological, Structural, and Charge Transfer Properties of F-Doped ZnO: A Spectroscopic Investigation

G.P. Papari¹, B. Silvestri², G. Vitiello^{2,3}, L. De Stefano⁴, I. Rea⁴, G. Luciani², A. Aronne², and A. Andreone¹

¹ Dip. Fisica, Università di Napoli Federico II and CNR-SPIN, UOS Napoli, Via Cinthia, I-80126, Napoli, Italy

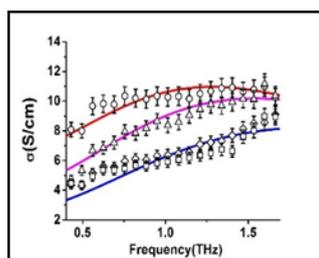
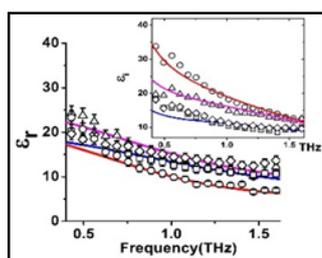
² Dip. di Ingegneria Chimica, dei Materiali e della Produzione Industriale, Università di Napoli Federico II, Piazzale Tecchio 80, I-80125 Napoli, Italy

³ CSGI, Sesto Fiorentino, Via della Lastruccia 3, Firenze, Italy

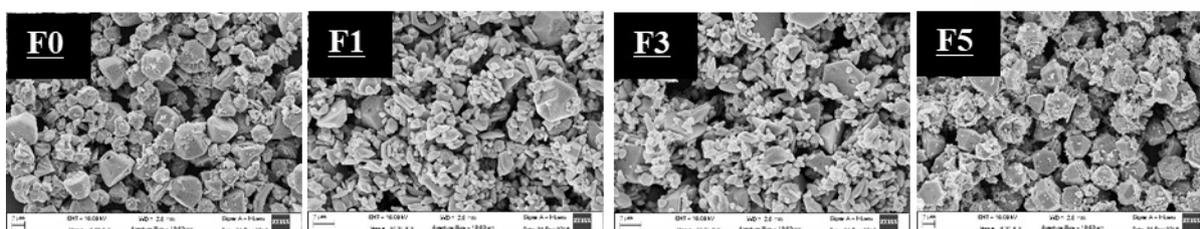
⁴ CNR-IMM, SS Napoli, Via P. Castellino 111, I-80131, Napoli, Italy

The Journal of Physical Chemistry 121, 29 (2017)

We have studied the charge transfer dynamics of ZnO powders doped with different concentration of fluorine. Time domain spectroscopy has been employed to extract the dielectric function of ZnO according to different doping levels. The appropriate application of mean field theories has confirmed the lowering of ZnO:F conductivity as the F doping is increased. Further morphological and spectroscopic techniques, like EPR, PL, XRD and SEM imaging, show that F doping promotes a granular phase and donor states in the UV band.



(a) Real part of permittivity (ϵ_1) and (b) conductivity (σ) of ZnO:F samples are reported, respectively. In the inset, the imaginary part of permittivity ϵ_2 is displayed. Circles, squares, rhombuses, and triangles correspond to F percentage of 0, 1, 3 and 5 at. % respectively. Solid curves represent the fit to the standard Drude –Smith model.



SEM images show grains with a hexagonal pyramid shape typical of mesocrystals for bare ZnO:F0. At low F at. %, ZnO grains are surrounded by smaller nanoparticles formed by the mesocrystals leaching (ZnO:F1 and ZnO:F3). The density of these nanoparticles decreases at higher fluorine concentration (ZnO:F5).

Results show that F doping does not produce any substantial change of plasma frequency but only the enhancement of scattering rate due to an increase of grain boundary density. This is in agreement with theoretical calculations asserting that the energy required to excite donor levels is on the order of 0.7 eV, and therefore, the doping mechanism is ineffective at room temperature.