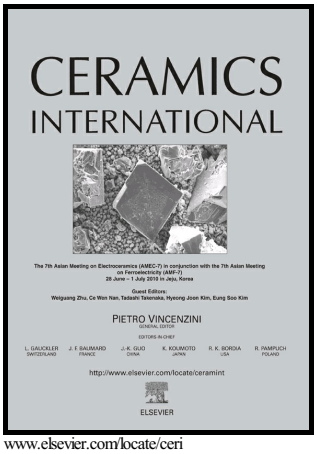

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Experimental and theoretical study on the structural, electrical and optical properties of tantalum-doped ZnO nanoparticles prepared via sol-gel acetate route

Diego Richard[a,†]*, Mariano Romero[a], Ricardo Faccio[a]

[a]*Centro NanoMat/DETEMA, Facultad de Química, Universidad de la República (UdelaR), CC 1157, Montevideo, Uruguay.*

[†] Present address: *Departamento de Física and Instituto de Física La Plata (IFLP, CONICET), Facultad de Ciencias Exactas, Universidad Nacional de La Plata, CC 67, (1900) La Plata, Argentina.*

* Corresponding author. Tel.: +54-221-4246062; Fax: +54-221-4252006.
E-mail address: richard@fisica.unlp.edu.ar

Abstract

Pure and Ta-doped ZnO were prepared by the sol-gel method in acetic medium using different annealing temperature treatments. The effects of low Ta doping on the cystallinity and electrical properties of ZnO nanoparticles were analyzed by means of X-ray diffraction and micro-Raman, UV-visible, and impedance spectroscopies.

We also performed first principles calculations in order to study the predicted changes in the structural, vibrational and electronic properties induced by the inclusion of the impurities, and to complement the experimental measurements.

We showed that above thermal treatments at 600 °C the precursor samples take the hexagonal wurtzite ZnO phase with high crystallinity. For the doped samples, we found that the synthesizing method has good Ta doping efficiency of the ZnO host structure. Also, Ta doping substantially decreases the resistivity compared to pure ZnO. These results confirm that Ta impurities can substitute Zn atoms and act as donor impurities in the host semiconductor.

Keywords: ZnO; sol-gel processes; impurities in semiconductors; tantalum; *ab initio* calculations