Abstract Title : **First principles study of the semiconductor to metal transition, dc conductivity and magnetism in (Al,Ti) codoped ZnO**

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Abstract

(Al,M) codoping of wurtzite type ZnO, where M= Co [1], Mn [2] or Ti[3], has attracted a great interest for both increasing the electrical conductivity whereas still preserving the semiconductor state and creating a stable ferromagnetic background. The maximum Al doping without entering the degenerate semiconductor regime has particularly been an issue of debate, with recent results evidencing a metallic state for 0.5 at. % Al [4]. In this contribution, we firstly present results of DFT calculations using the CPA approach on disordered systems with x=0.5-2.0 at. % Al in order to determine the concentration for the occurence of the semiconductor to metal (SM) transition. Using the DFT ground state parameters we calculate the dc conductivity and its temperature dependence in the variable range hopping model. We bring evidence that the SM transition as an electronic effect of Al doping takes place between 1.0 and 1.5 at % Al in the non defective crystal, which is well above the values experimentally observed. Present calculations considering both Al impurity and 3 at.% oxygen vacancies (OVs) show a significant increase in carriers concentration and support the role of carriers contributed by OVs present in the samples. Then, we perform GGA+U supercell calculations on fully relaxed (Al, Ti) codoped ZnO and show that: i) the atomic relaxations are negligible small for 2.8 % Al and 2.8 or 5.6 % Ti substituting for Zn, and ii) (Al,Ti) codoped ZnO exhibits a ferromagnetic ground state.

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