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Limits of Conductivity in ZnO Thin Films: Experiment and Theory

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Transparent conductive oxides (TCOs) have major (multi-$B) roles in applications such as flat-panel displays, solar cells, and architectural glass. The present workhorse TCO is indium-tin-oxide (ITO), but the recent huge demand for ITO has made In very expensive; moreover, it is toxic. The most commonly suggested replacement for ITO is ZnO, doped with Al, Ga, or In, and indeed the ISI lists 628 papers on Group-III-doped ZnO in 2009. However, to our knowledge, none of these papers has included calculations of donor N_D and acceptor N_A concentrations, the fundamental components of conductivity in semiconductors. We have developed a simple model for the calculation of N_D and N_A from temperature-dependent measurements of carrier concentration n, mobility μ, and film thickness d. With the inclusion of phonon scattering in the model, excellent fits of n and μ are obtained from 15 – 300 K. Experimentally, we have shown that highly conductive ZnO films can be grown by pulsed laser deposition in a pure Ar ambient, rather than the usual O_2. In a 278-μm-thick film, we have achieved a room-temperature resistivity $\rho = 1.96 \times 10^{-4}$ Ω-cm, carrier concentration n = 1.14×10^{21} cm^{-3}, and mobility $\mu = 28.0$ cm^2/V-s. From our model, we calculate $N_D = 1.60 \times 10^{21}$ and $N_A = 4.95 \times 10^{20}$ cm^{-3}; however, the model also predicts that a significant reduction of N_A would give $\mu = 42.5$ cm^2/V-s and $\rho = 7.01 \times 10^{-5}$ Ω-cm, a world record. Such a reduction in N_A may be possible by in-diffusion of Zn after growth, since there is evidence that one of the major acceptor species in these films is the Zn-vacancy/Ga_{Zn} complex. We can also decrease the resistivity by annealing in forming gas, and have recently attained $\rho = 1.46 \times 10^{-4}$ Ω-cm, n = 1.01×10^{21} cm^{-3}, and $\mu = 42.2$ cm^2/V-s, giving $N_D = 1.13 \times 10^{21}$ and $N_A = 1.09 \times 10^{20}$ cm^{-3}. In very thin films, quantum effects must be considered.