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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 $\mu$, and film thickness $d$. With the inclusion of phonon scattering in the model, excellent fits of $n$ and $\mu$ 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 $n = 1.14 \times 10^{21}$ 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, $n = 1.01 \times 10^{21}$ 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.