Non-parabolicity and band gap renormalization in Si doped ZnO

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INTRODUCTION

EXPERIMENTAL METHODS

Films were deposited via RF magnetron sputtering using an AJA Phase II-J Orion system. The system was configured with a 'sputter-up' geometry with the substrate being suspended above two separate ceramic targets of ZnO and SiO_2 that were arranged off-centre and tilted at 5° towards the middle of the substrate. Soda-lime glass substrates (OptiWhite^{TM}, NSG) of size $100 \times 100 \times 4$ mm^3 were used throughout. They were cleaned by scrubbing with a nylon brush and a series of de-ionized water and isopropanol alcohol rinses followed by blow drying with a nitrogen gas jet. During deposition the ZnO and SiO_2 targets were sputtered from simultaneously using powers of 150 W and 50 W respectively. A growth pressure of 2mTorr Ar was used during deposition. The substrate temperature was maintained at 350 ± 5°C during growth and the substrate was kept static (i.e was not rotated). Deliberate gradients of both thickness and composition were subsequently achieved across the resultant film to generate a 'combinatorial' sample. A second film of pure SiO_2 was deposited under identical conditions (but without ZnO) to generate a reference film for calculating the % wt. profile of SiO_2 in the co-sputtered film.

A Shimadzu UV-Vis-IR 3700 spectrophotometer with mapping capability was used to measure the transmittance of the co-sputtered film over the range 250 - 2500 nm. 289 spectra were taken in total at 5 mm increments over the full sample surface. At each of these 289 points the sheet resistance was also measured using a CMT-SR2000 4-point probe mapping system. Following transmittance and sheet resistance measurements the sample was cut into one hundred 10×10 mm^2 pieces. A selection of these pieces, 10 in total, were further scribed into four 5×5 mm^2 sections and Hall measurement were performed on each of these sections. The Hall measurement was performed with custom built equipment, provided by Semimetrics Ltd., using a field strength of 0.8 T. Ellipsometry was performed on the same sections using a Woollam M2000-UI system. Ellipsometry was also used to map the thickness profile of the pure SiO_2 reference film.

RESULTS

CONCLUSIONS

The authors would like to thank ...

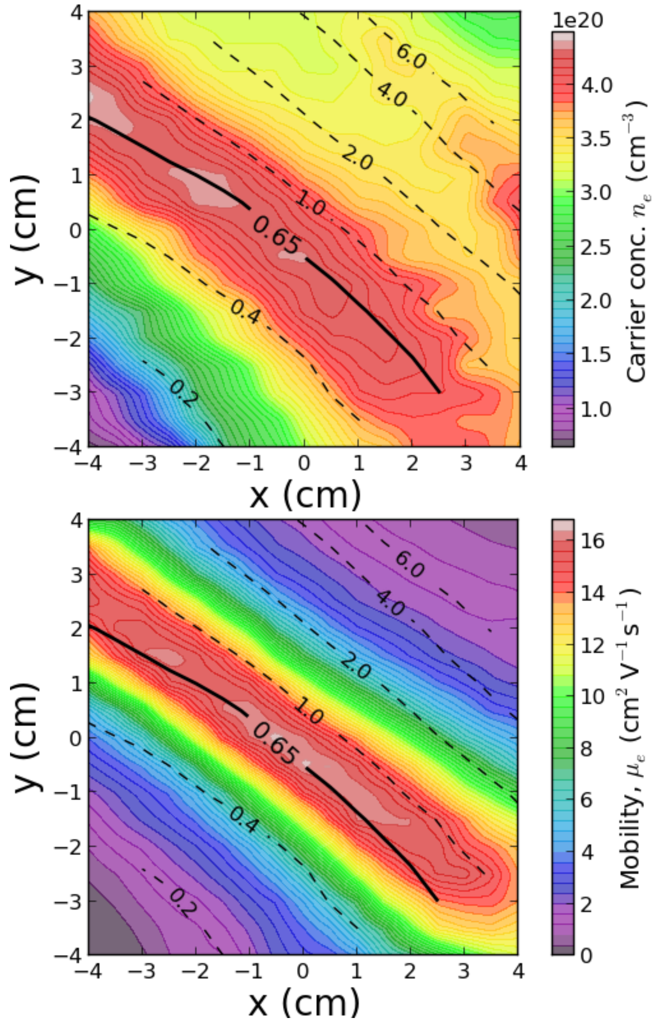


FIG. 1. Contour maps of carrier concentration and mobility over the combinatorial sample. The (–) contour lines show an overlay of the % wt. SiO_2 composition.

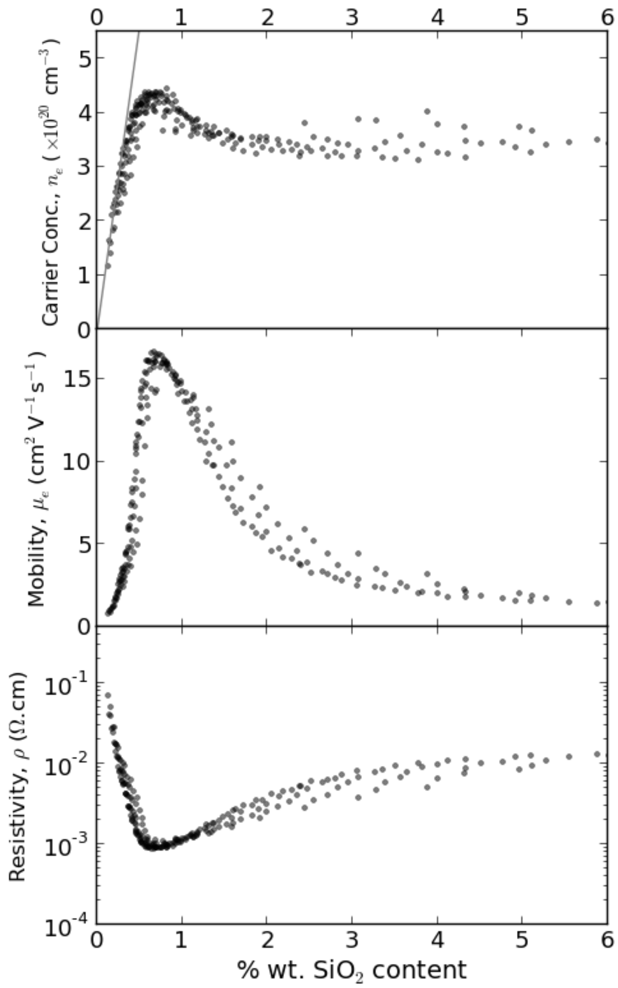


FIG. 2. Distributions of carrier concentration, mobility and resistivity with respect to % wt. SiO_2 content. The maximum values for n_e (4.4×10^{20} cm^{-3}) and μ_e (16.5 cm^{2}V^{-1}s^{-1}) coincide with a composition of 0.65% wt. SiO_2. The solid straight line in the top plot shows the maximum theoretical carrier concentration with respect to SiO_2 content should every incorporated Si atom be substituted at a Zinc site and donate 2 carriers.

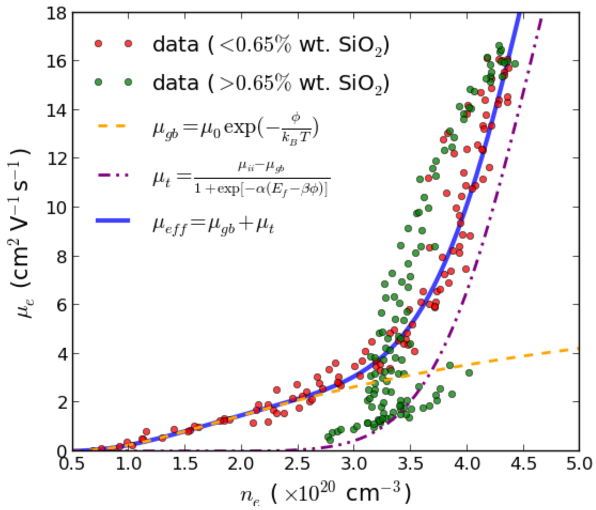
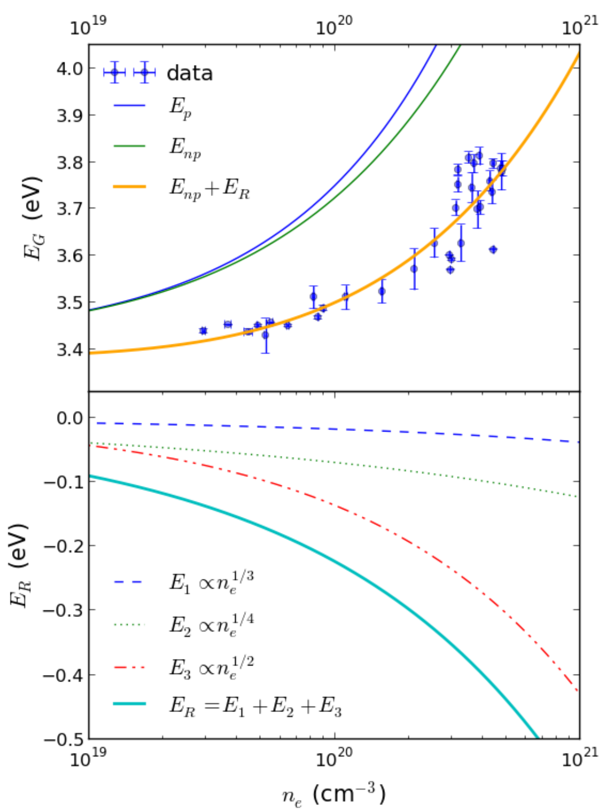

data ($<0.65\%$ wt. SiO_2)
data ($>0.65\%$ wt. SiO_2)
$\mu_{gb} = \mu_0 \exp(-\frac{\phi}{k_B T})$
$\mu_t = \frac{\mu_{ii} - \mu_{gb}}{1+\exp[-\alpha(E_f - \beta\phi)]}$
$\mu_{eff} = \mu_{gb} + \mu_t$
μ_e ($cm^2 V^{-1} s^{-1}$)
n_e ($\times 10^{20}$ cm^{-3})

FIG. 3.


data
E_p
E_{np}
$E_{np} + E_R$
E_G (eV)
$E_1 \propto n_e^{1/3}$
$E_2 \propto n_e^{1/4}$
$E_3 \propto n_e^{1/2}$
$E_R = E_1 + E_2 + E_3$
E_R (eV)
n_e (cm^{-3})