Electronic Supporting Information

Transparent conducting n-type ZnO:Sc – Synthesis, optoelectronic properties and theoretical insight

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1. Scherrer's equation for estimating mean crystallite diameter from X-ray diffraction data

Where d is the average crystallite diameter, k is a constant taken to be 0.9, λ is the incident X-ray wavelength, Δ(2θ) is the full-width at half maximum of the (002) peak in radians and θ_{002} is the Bragg angle in radians, the Scherrer formula is expressed as in Equation 1.

$$d = \frac{k\,\lambda}{\Delta(2\theta)\cos\theta_{002}} \qquad \text{Equation 1}$$

2. Equation for calculation of lattice parameters for hexagonal lattice

Where d_{hkl} is the interplanar spacing and h, k, l are Miller indices, the lattice constants a and c were found by applying Equation 2 to the (002) and (101) peaks in the ZnO X-ray diffractogram.

$$\frac{1}{d_{hkl}^2} = \frac{1}{a^2}\left[\frac{4}{3}(h^2 + k^2 + hk) + l^2\left(\frac{a}{c}\right)^2\right] \qquad \text{Equation 2}$$

3. X-ray photoelectron spectroscopy

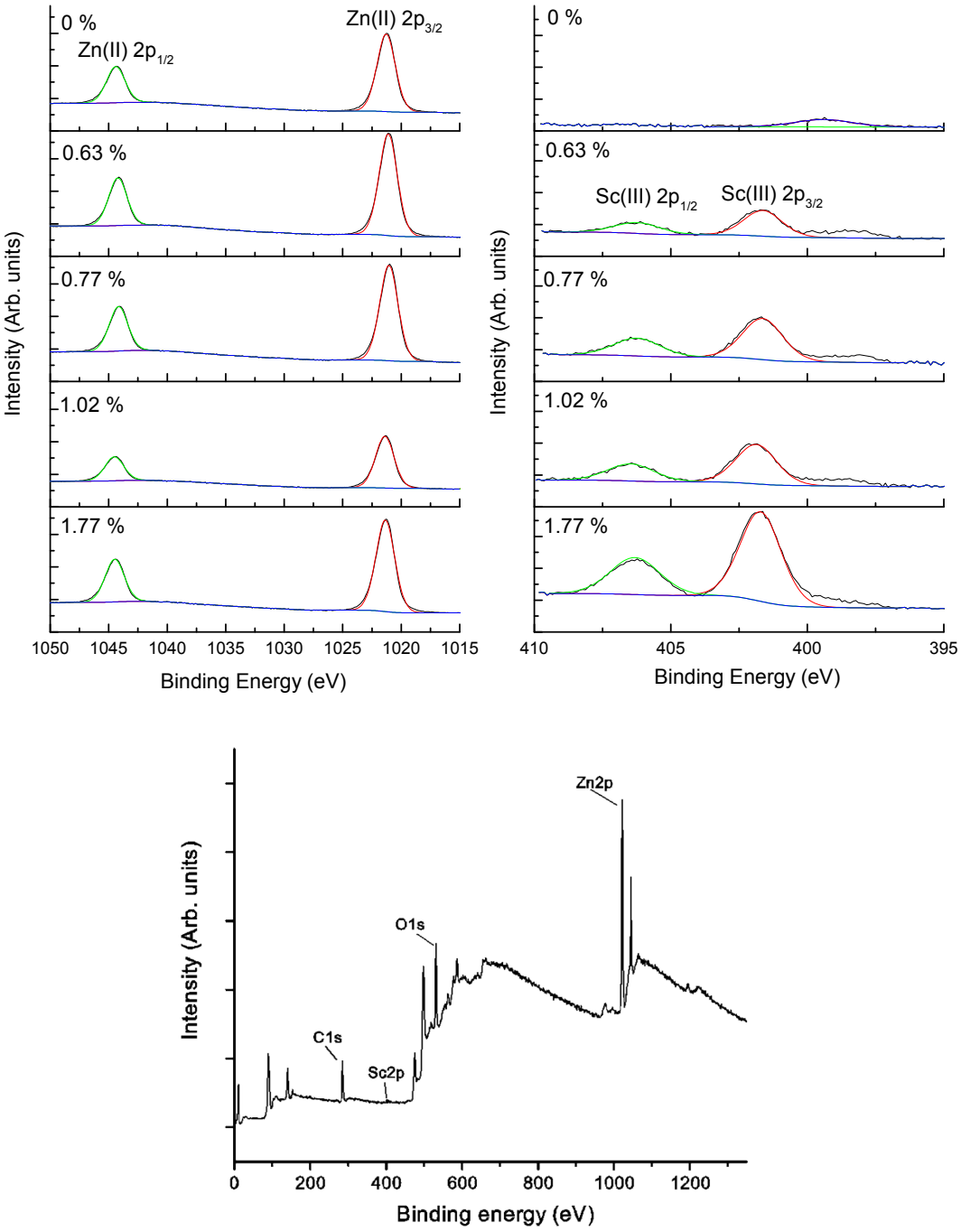

Figure 1 X-ray photoelectron spectra of Sc-doped ZnO films containing increasing amounts of bulk Sc (expressed relative to Zn in at%), at the (upper-left) Zn2p and (upper-right) Sc2p peaks, and (lower-centre) the **survey** scan.

4. Texture coefficient for hkl reflections in X-ray diffraction

The texture coefficient for each of the six diffraction peaks in the ZnO:Sc films was calculated from their intensities relative to eachother and to the standard powder pattern (ICSD 29272), as per Equation 3, in which TC(hkl) is the texture coefficient for a given reflection, I(hkl) is its intensity in the thin film sample, I_0(hkl) is that in the powder pattern and N is the number of reflections present in the powder pattern. The calculated TC(hkl) are plotted in Figure 2 against the bulk Sc concentrations in the ZnO:Sc films as obtained by EDX. Although a doping trend is not immediately obvious, there is a clear preference for c-axis orientation as indicated by the consistently strong texture coefficient for the (002) reflection.

$$TC(hkl) = \frac{I(hkl)/I_0(hkl)}{\frac{1}{N}\sum_N I(hkl)/I_0(hkl)} \qquad \text{Equation 3}$$

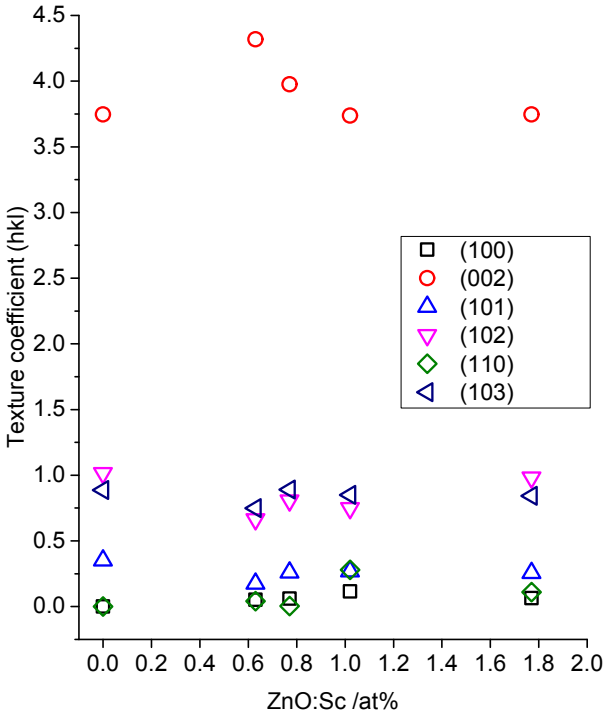

Figure 2 Texture coefficients for ZnO:Sc films containing various amounts of Sc (at%) as obtained from EDX measurements.

5. Raman scattering of films vs. bulk

Raman spectroscopy was carried out on the films using a Renishaw Invia Raman microscope fitted with a 514.5 nm green laser and a 1800 l/mm grating. Spectra were obtained at 300 s exposure time using 10 scans at 100% laser operating power. The thin films were weakly scattering, with the peak appearing at an identical position of 439 cm^{-1} in both the 1.0 at% doped ZnO:Sc film and the undoped ZnO film, while the peak occurred at 436 cm^{-1} in the ZnO powder sample. This peak is characteristic of wurtzite ZnO E_2 mode and was the strongest peak in all spectra. No obvious shifting of the E_2 mode peak was observed as a result of doping, as expected from the lack of shift in XRD due to lattice matching of Sc^{3+} ions on Zn^{2+} sites. Stronger scattering would however be required to make this judgement conclusively. Weak Raman scattering of polycrystalline ZnO films is typical for sub-micron film thicknesses.

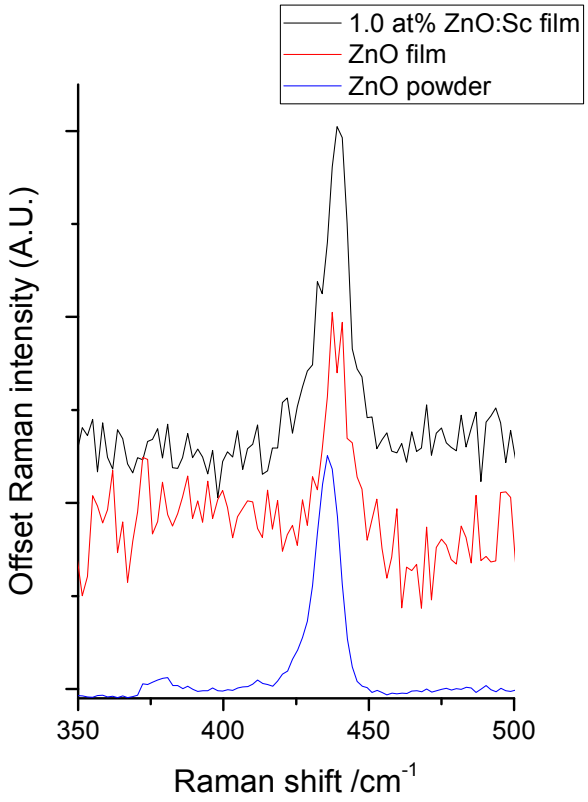

Figure 3 Raman spectra for ZnO and ZnO:Sc films as compared with the powder pattern.