Microsc. Microanal. 18 (Suppl 5), 2012

doi:10.1017/S1431927612013116

Nanostructure of the interfaces between ZnO, ZnO:Ga and ZnO:Al Films and Silicon

P. Herrero-Fernández*, J. Hernández-Moro*, F. Agulló-Rueda*, M. Gabás**, P. Díaz-Carrasco**, J.R. Ramos-Barrado** and A. R. Landa-Cánovas*

* Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Cantoblanco, 28049, Madrid, Spain
** Dpto. de Física Aplicada I, Lab. de Materiales y Superficies, Universidad de Málaga, 29071, Málaga, Spain

ZnO is a promising material for use in solar cell applications which require antireflective coatings and transparent conducting materials in front contacts. Its resistivity can be reduced by appropriate doping with different group III elements, which act as donors, without sacrificing optical transmission [1]. Besides, it constitutes a non-toxic and cheap alternative to ITO (In_2O_3:SnO_2), which is nowadays commonly used as transparent conducting oxide (TCO) in optoelectronic devices [2]. Al(III) is one of the cheapest elements on nature, and has been therefore one of the first candidates to be used as a dopant. However recent studies demonstrate that for similar amounts of dopant the use of Ga largely improves both the optical and electrical properties of the films [3]. The interface between Si (used as substrate) and the corresponding TCO is a critical part of Si-based solar cells, since the conversion efficiency may be profoundly altered by the presence of recombination centers formed at the interface. In this work we present a comparison of Si/ZnO, Si/ZnO:Ga and Si/ZnO:Al interfaces (with [dopant]/[Zn] = 2%) by using HRTEM and associated spectroscopies. Resistivity values of the films are: ρ(ZnO) = 4.4 × 10-2 Ω × cm; ρ(Ga:ZnO) = 6.3 × 10-4 Ω × cm; ρ(Al:ZnO) = 2.9 × 10-3 Ω × cm. and the films optical transmitance is larger than 80% along the visible spectrum [4].

Thin films of ZnO, ZnO:Ga and ZnO:Al were deposited by RF magnetron sputtering on Si and SiO_2 substrates for 20 minutes [4]. Cross sectional images were obtained in a JEOL 3000F. Image processing of the high-resolution images was carried out using Gatan Digital Micrograph and ImageJ software packages. Films present a crystalline wurtzite structure with the c-axis perpendicular to the substrate and some defects, mainly dislocations. They always present continuity of the (0002) planes along the whole film, as confirmed by HRTEM in Figure 1, allowing for a high conductivity along the film plane. These properties have also been confirmed by Raman spectroscopy and x-ray diffraction. In Figure 2 we present the Raman spectra of ZnO, ZnO:Ga and ZnO:Al films grown on silica, where the observed peaks correspond to a wurtzite type structure. As no TO modes are observed in the ZnO sample, this confirms that film grows along the (001) direction. Finally the fact that its full width at half maximum (FWHM) do not change significantly indicates that the crystallinity of the samples do not change appreciably with doping.

For undoped ZnO, as it can be observed in Figure 1, there is an amorphous layer of about 2 nm which presents an uniform contrast and can be identified as SiO_2. Doping introduces and additional amorphous layer at the interface whose thickness is strongly dependent on the doping cation. For ZnO:Ga the whole amorphous layer reaches ≈3 nm whilst for ZnO:Al this layer extends to ≈4 nm, as shown in Figure 1. This extra layer probably consists of amorphous doped ZnO plus the original amorphous SiO_2 layer present in pure ZnO and does not seem to affect to the resistivity values.

References

1. T. Minami, Semicond. Sci. Technol. 20: S35–S44, 2005
2. T. Minami, MRS Bull. 25: 38–44, 2000
3. M. Gabás, P. Díaz-Carrasco, F. Agulló-Rueda, P. Herrero, A. R. Landa-Cánovas and, J. R. Ramos-Barrado, Solar Energy Mater. Solar Cells 95: 2327–2334, 2011
4. M. Gabás, S. Palanco, P. Díaz-Carrasco, S. Bijani, A.R. Landa-Cánovas, P. Herrero, F. Agulló-Rueda and J.R. Ramos-Barrado, 37th Photovoltaic Specialist Conference. June 2011. Seattle USA

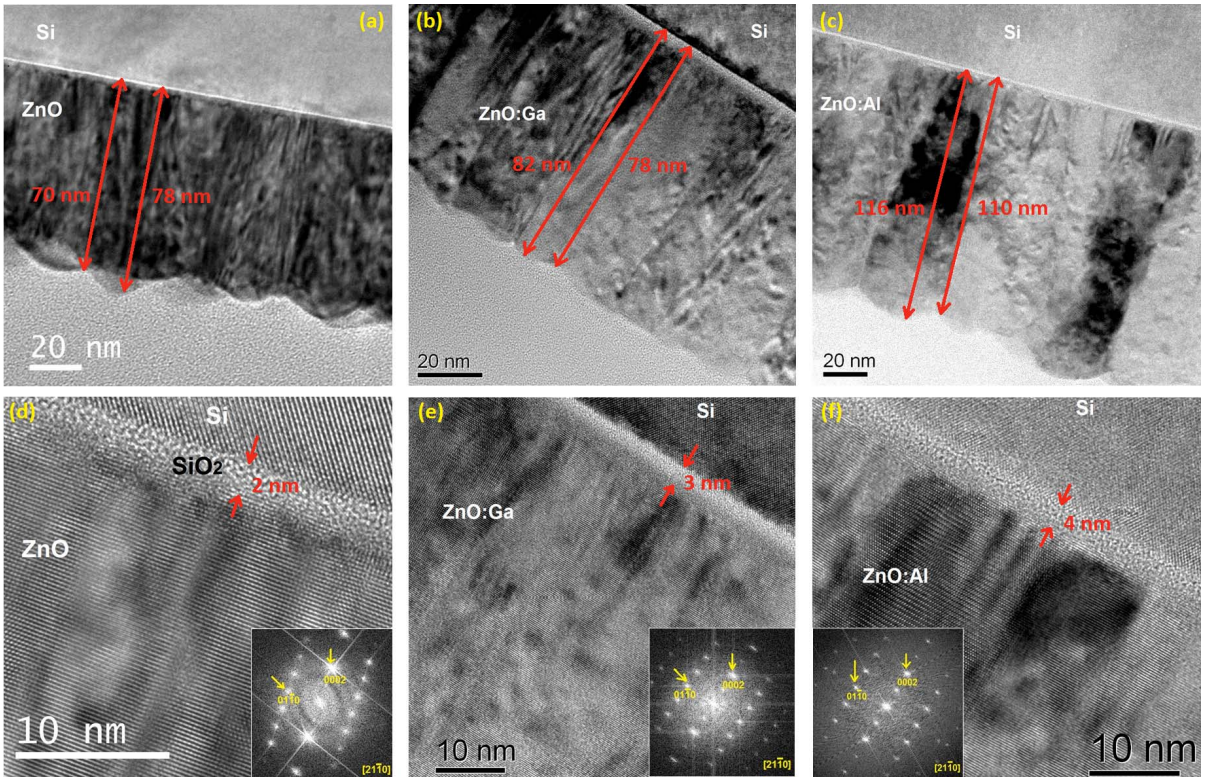

Figure 1. HRTEM images of ZnO (a, d), ZnO:Ga (b, e) and ZnO:Al (c, f) films on polished Si (100). Figs (d), (e) and (f) present a higher magnification view of the interface area.

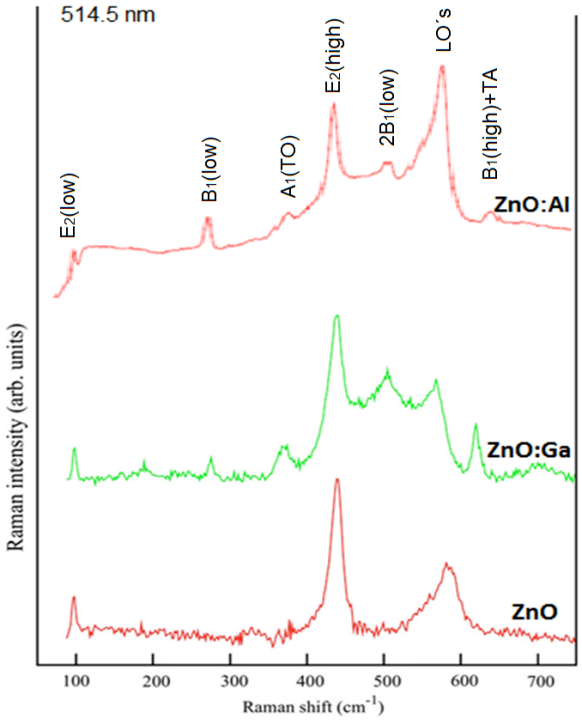

Figure 2. Raman spectra of ZnO, ZnO:Ga and ZnO:Al films grown on silica. Spectra have been vertically offset for clarity.

Acknowledgments: MAT2008-06858-C02-02 and FUNCOAT-CSD2008-00023. Technical Support from Servicio de Microscopía (ICMM-CSIC) and from Esteban Urones at I.C.T.S. Centro Nacional de Microscopía Avanzada (UCM).

https://doi.org/10.1017/S1431927612013116 Published online by Cambridge University Press