Defectivity of Al:ZnO Thin Films with Different Crystalline Order Probed by Positron Annihilation Spectroscopy

R. Magrin Maffei*[a,b], M. Butterling[c], M. O. Liedke[c], S. D'Addato[a,b], A. di Bona[b], G. Bertoni[b], G. C. Gazzadi[b], S. Mariazzi[d,e], A. Wagner[c], R. S. Brusa[d,e] and S. Benedetti[b]

[a]*Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Università di Modena e Reggio Emilia, Via Giuseppe Campi 213/a, 41125 Modena, Italy*

[b]*CNR-Istituto Nanoscienze, Via Giuseppe Campi 213/a, 41125 Modena, Italy*

[c]*Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany*

[d]*Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Trento, Italy*

[e]*TIFPA/INFN Trento, Via Sommarive 14, 38123 Povo, Trento, Italy*

**Corresponding author: riccardo.magrinmaffei@unimore.it*

1 Supporting Information

ZnO Single Crystal

We performed PAS on a hydrothermally (HT) grown ZnO bulk single crystal (SurfaceNet GmbH) in order to have a reference to normalize the Doppler data. VEPALS measurements showed a single lifetime of 187 ps with almost 99% intensity in the bulk of the sample (11 keV of implantation energy), aside of the surface dynamics which we are not interested in. This lifetime is in the range of values of $183 - 189$ ps for HT-grown ZnO single crystals reported by Chen et al. [1, 2]. It is longer than typical experimental and calculated values reported for defect-free ZnO of $150 - 160$ ps [3–7] and might be related to the presence of Li_{Zn} and/or V_{Zn}:H point defects, that were reported as positron trapping defects in HT-grown ZnO in previous studies [7–11].

Fitting of the $S(E)$ and $W(E)$ curves, shown in Figure 1, yielded a diffusion length of 67.6 ± 5.2 nm, a value in line with experimental results [8–10] and far below the expected theoretical diffusion length of a defect-free ZnO bulk of 280 nm [7]. A defect density of $5.1 \cdot 10^{18}$ cm^{-3} can be then extracted. The data of the films can be still normalized to the S and W bulk parameters of our ZnO single crystal sample ($S_B^{ZnO} = 0.5042 \pm 0.0003$ and $W_B^{ZnO} = 0.0923 \pm 0.0001$), but keeping in mind that saturation trapping at such types of defects is expected to lead to a shift in the S parameter on the order of $+1\% - +2\%$ compared to defect-free ZnO [12].

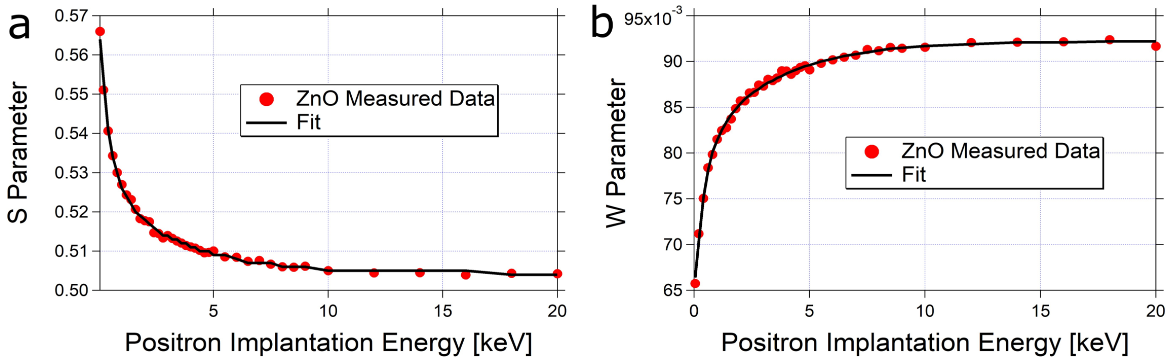

Figure 1: $S(E)$ and $W(E)$ curves for the ZnO bulk single crystal (red dots) and fits with the diffusion-annihilation model (black line). The error bars are within the dots size if not visible.

VEPALS of AZO/Quartz film grown at 75 mTorr

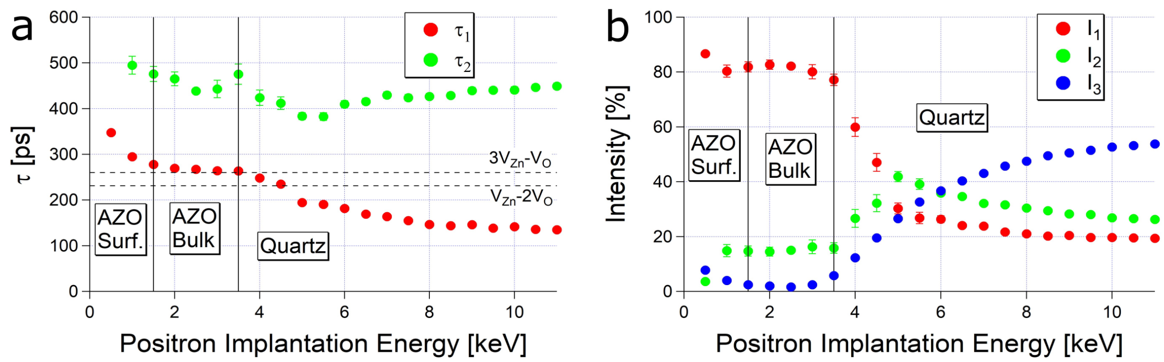

Figure 2: VEPALS depth profiles for the AZO/Quartz film grown at 75 mTorr. **(a)** Lifetimes and **(b)** intensities. Dotted lines mark the calculated lifetimes associated to the $3V_{Zn}-V_O$ and $V_{Zn}-2V_O$ vacancy clusters. Regions assigned to the layers are marked. The error bars are within the dots size if not visible.

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