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Evolution of vacancies in thin film solar cells and in photochromic yttrium oxyhydride revealed by in-situ positron annihilation spectroscopy

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We apply Positron Annihilation Spectroscopy (PAS) to monitor the environmental degradation of ZnO/CIGS and perovskite thin film solar cells. Furthermore, yttrium oxy-hydride thin films are studied in view of their special photochromic properties, with the aim to elucidate the nature of vacancies in YOxHy and their evolution under in-situ UV illumination.

Our PALS study of as-deposited perovskite films using the PLEPS spectrometer reveals the presence of cation vacancies. Positron Doppler Broadening (DB-PAS) indicates that the degradation of MAPbI3 films involves the ingress of water molecules into the cation vacancies. In parallel, chemical transformations and a reduction in film thickness are observed, that proceed as a function of air exposure time.

PALS studies of ZnO:Al transparent electrode films on CIGS solar cells reveals a pronounced growth of vacancy clusters at the grain boundaries of the ZnO upon accelerated degradation at 85 oC/85% relative humidity. The growth of the vacancy clusters correlates with the observed degradation of the solar cell efficiency, pointing to a key role in the mechanism of degradation.

Finally, PALS reveals the presence of vacancies and micropores in photochromic YOxHy films. In-situ illumination DB-PAS studies show an increase in the S-parameter and a strong reduction in W, indicating that the generation of additional vacancies and/or a change in the charge state of vacancies accompanies the formation of the photochromic state.

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