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Cd and In-doping in thin film SnO_2

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In this paper, we investigate the effects of doping in the local structure of SnO_2 by measuring the hyperfine interactions at impurity nuclei using the Time Differential Perturbed Gamma-Gamma Angular Correlation (TDPAC) method in addition to density functional theory simulations. The hyperfine field parameters have been probed as a function of the temperature in thin film samples. The experimental results reveal that ^{117}Cd/In and ^{111}In/Cd are incorporated and stabilized in the SnO_2 lattice replacing the cationic site. Significant differences in the electric field gradient were observed from TDPAC measurements with both the probe nuclei. Furthermore, the absence of strongly damped spectra further indicates that implanted Cd atoms (for ^{117}Cd/In probe nuclei measurements) easily occupy regular substitutional Sn sites with good stability. The simulated value for the electric field gradient obtained with the first oxygen neighbor removed is closer to the experimental value observed for ^{117}Cd, which also indicates this configuration as stable and present in the sample.

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