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Defects identification in SnO_2 semiconductor using positron annihilation techniques.

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The two-component density functional theory is employed in the modelling of defects in ion implanted SnO_2 using positrons as probes. Since defects are localized, the local density approximation (LDA) is used which is part of DFT. Although LDA gives a good approximation of positron lifetimes and electron-positron annihilation momentum density. LDA does not consider the variational nature of the charge density in constituent atoms of the sample. This has an unintended consequence of having over estimation of annihilation rates or underestimation of positron lifetimes compared to experimental values. This deficiency in LDA is corrected by using the generalized gradient approximation (GGA) which considers the variational nature of electron density. The accumulation of annihilation spectrum using coincidence setup, is utilized to allow for the determination of annihilation parameters, S and W. The spectrum consists of positron annihilations at defect sites as well as annihilations in the bulk (defect-free region). It also consists of annihilations of positrons with core electrons (high momentum electrons). The low and high momentum distribution of electrons will be used to characterize the Doppler broadening which will tell us about the quantity of radiation-induced defects in SnO_2 in terms of calculating S-parameter, which is the ratio of the annihilation centroid area to the total area of the annihilation curve. Calculated S parameters are then compared with the experimentally obtained S parameters. The nature of the defects is theoretically obtained from the annihilation rates or equivalently from the calculated positron lifetimes in SnO_2.

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