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S-Parameter and Positron Lifetime Studies of Mn Doped $Zn_{1-X}O_X$

Vandana Rathore[1]
[1]*School of Engineering and Technology, Jagran Lakecity University, Bhopal-462044, India.*

Abstract:** Zinc Oxide (ZnO) is an fascinating material and have potential applications as a transparent conductive electrodes for solar cells, light emmitting diodes as well as for gas sensors. Interaction between dopant, impurities and intrinsic defects plays an essential role to enhance the electrical and optical properties of ZnO thin films. Positron annihilation spectroscopy (PAS) is a non destructive technique to study thin films and nanocrystalline materials. The mechanism of positron annihilation in oxide thin films has been discussed in terms of diffusion of positrons inside the grain boundaries, nanovoids and thermally generated vacancies. The mean positron lifetime and S-parameter as a function of grain size in pure and Mn doped ZnO thin films has been calculated by using positron diffusion model. The samples are prepared by Spray pyrolysis method and temperature dependent measurements revels information about the presence of shallow positron traps like grain boundaries and interfacial defects. The calculations of shows that mean positron lifetime decreases as the grain grows. While the S-parameter increases with the increase in the siza of grains. This increase in $\bar{\tau}$ has been ascribed to the increase in the number of thermally generated vacancies at higher temperatures. diffusion can also be closely linked with thermal defect formation at higher temperatures. Thus, information regarding grain boundaries in thin films and nano composites can be gathered by DTM (diffusion Trapping Model).

I. INTRODUCTION

Positron annihilation lifetime spectroscopy (PALS) serves as a unique tool for the characterization of lattice defects in materials science. While the annihilation lifetime yields characteristic information about the size of open-volume defects ranging from single atomic vacancies up to nanovoids, the kinematical Doppler-broadening of annihilation radiation tells about the local electron momentum distribution at the annihilation site. Annihilation lifetimes are monotonously related to the void size with a surprisingly low dependence on the material surrounding the void [1]. The semiconducting nanocrystalline thin films have great applications in electronic industry, solar cells, solar energy storage and biomedical industries. Among the nanocrystalline semiconducting materials the preparation and characterization of doped and undoped ZnO films has assumed much importance during recent years. ZnO is an important wide band gap semiconductor having wide applications in various fields such as transducers, gas sensors, transport conduction electrodes and surface acoustic wave devices etc. [2- 4]. Zinc oxide (ZnO) is a material with great potential for a variety of practical applications due to the unique physical and chemical properties such as wide and di-rect energy band gap (~3.37 eV), large exciton binding energy (~60 meV), high electron mobility, high thermal conductivity, high radiation damage resistance and biocompatibility. The recent progress in nanoscaling of ZnO structures attracts also attention towards the use of ZnO in nanotechnological applications. There-fore, mechanical, electrical and optical properties of nanostructured ZnO crystals are widely investigated in different conditions by many research groups [5-7]. Positron annihilation spectroscopy is a well established tool for the study of electronic and defect properties of solids [8–9]. The crux of this technique is that in solid materials positrons are efficiently trapped at defects such as vacancies or voids, which makes them a very sensitive probe for studying these defects. After trapping the positron will annihilate with an electron from the immediate surrounding of the defect, thus producing two 511 keV gamma-photons. The defect-related information is obtained from properties such as the lifetime of the positrons, the Doppler broadening of the photo-peak, or the angular-correlation between the two photons. Furthermore, the development in slow positron beam methods allows the extension of traditional techniques to investigation of thin films, layered structures and surfaces [10-11].

II. FORMULATION OF THE DIFFUSION TRAPPING MODEL

The mechanism of positron annihilation in nanocrystalline materials is known to be more complex than that in metals and semiconductors because, a fraction of positrons can form a bound state with an electron. In the following, we consider the case of the slow positrons incident on a thin film having size (50 nm-200 nm). The positron gets rapidly thermalized before annihilation. After slowing down within 10 ps the penetrated positrons either directly annihilate with surrounding electrons or combine with an electron to form positronium. Fractions of positrons may diffuse back to the surface and escape into the vacuum. The positrons and positronium both are known to localize in interfacial defect and nanovoids. The theoretical model is based on diffusion trapping model (DTM). When a beam of moenergetic positron is implanted into a semiconductor surface the following processes have been considered to occur before annihilation. Firstly the positrons may diffuse back to the surface and annihilate as a free particle. Secondaly it may be trapped at a defect site. In the present work, we have considered two types of defects i.e. trapping into shallow defects and in native ion vacancy defects. The rate equations have been setup to describe all the above processes and have been solved to obtain the Doppler broadening line shape parameter or S-parameter as a function of incident positron energy in undoped and ZnO doped with different types of ions. The diffusion trapping model is able to describe the positron annihilation in ZnO thin films and it has been observed that at low energy the Sparameter corresponds to positron annihilation in the surface state and for higher energy the same corresponds to the positron annihilation in the bulk material. In case of ion implanted ZnO the S-parameter was found to be dependent on the concentration of vacancy clusters. The vacancy clusters concentration was found to be related to the atomic number of the implanted ion as well as on the fluency. The three dimensional diffusion equation has been solved and the rate equations are set up to describe the tapping of positrons at interfacial defects and nanovoids. The model has been functional to calculate the mean positron lifetime ($\bar{\tau}$) in pure and Mn-doped ZnO thin films as a function of grain size. It has been also employed to explain the S-parameter configuration in pure and doped ZnO thin films. In the present work, our endeavor is to understand the consequence of positron mean lifetime on grain size and types of defects in nanocrystalline thin films of zinc oxides. In the model considered, we assume that positrons diffuse in the interfacial defects in which they annihilate with annihilation rate of free positrons in the sample λ_f *(=1/*τ_f*)*. Let *C(r,t)* is the local positron density with in the grain. The change in the positron concentration inside defects with time and space is described by the three dimensional diffusion equation:

$$\frac{\partial C(r,t)}{\partial t} = D_{+}\nabla^2 C(r,t) - \lambda_f C(r,t) - \frac{\partial}{\partial r}\left[n_{\mathrm{nv}} C(r,t)\right] \qquad (1)$$

For the present calculation, D+ is the positron diffusion coefficient and C (r,t) is the positron density as a function of both time and position. we assume that at *t = 0* the positrons are uniformly distributed and there are no positrons trapped at interfacial defects and nanovoids. Thus, the diffusion equation is solved subjected to the boundary conditions: where V_Ω is the volume of the grain having radius *R*. Thus, we obtain the solution of equation (1). When a beam of monoenergetic positrons is implanted from vacuum into the grain, the positron survives before annihilation either as a free positron or trapped at the grain boundary or into the thermally induced vacancy.

$$C(r,t) = \sum_{n=0}^{\infty} \frac{(2n+1)}{V_\Omega}\left(\frac{r}{R}\right)^{2n} \exp-\left\{D_{+}\left(\frac{3\pi}{R}\right)^2 + \lambda_f\right\}t \qquad (2)$$

In the above equations n_{fg}, n_{fv} represent the fraction of positrons trapped at the grain boundaries and into nanovoids vacancies respectively. n_{vf} represents the fraction that detrapped from vacancy to free state. α_{fg}, α_{fv} and α_{vf} represent the transition rate from free to grain boundary, free to vacancy and from vacancy to free state respectively. λ_g and λ_v are the positron annihilation rate at the grain boundary and into the vacancy respectively. The total number of positrons reaching at the grain boundary is given by

$$N(t) = \alpha_{fg} \iint ds\, C(r,t) \qquad (3)$$

The mean positron lifetime ($\bar{\tau}$) in the nanocrystalline samples can be written as:
Thus, one gets

$$\bar{\tau} = \frac{1}{\alpha_g} + \sum_{n=0}^{\infty} \frac{\mathrm{B_n}}{\mathrm{b_n}}\left(\frac{1}{\lambda_g} - \frac{1}{\alpha_g} + \frac{\alpha_{fv}}{\alpha_g \alpha_{vf}} + \frac{\alpha_{fv}}{\alpha_g \alpha_v}\right) \qquad (4)$$

In case of thin films the Doppler broadening line shape parameter or S parameter would be a linear combination of three energy-independent terms, S_s, S_p and S_f. The Doppler broadening line shape parameter of annihilation radiation i.e. S-parameter could be obtained from the equation for the positron annihilation in fine grained particles and nanocrystalline grain clusters in the following manner.

$$S = S_f + (S_g - S_f)\left[\frac{1}{1+((\lambda_f + s)/\alpha)B(\gamma)}\left\{1-\left(1-\frac{B(\gamma)}{D(\gamma)}\right)\frac{1}{V_\Omega}\iiint_\Omega dV\bar{g}(r,s)\right\}\right] \qquad (5)$$

The equation (12) has been used to obtain the mean positron lifetime in pure and doped ZnO thin films, while equation (13) has been used to calculate the S- parameter in these films.

III. RESULTS AND DISCUSSION

Diffusion Trapping Model as described above, mean positron lifetime have been calculated in pure and Mn doped ZnO thin films a function of grain size. We have used the samples which we have prepared by spray pyrolysis technique. The samples have been prepared with the appropriate temperature conditions for pure ZnO and Mn doped ZnO thin films. The doping percentage has been kept 5% and 10%. The transition rate α_{fg} is understood to be proportional to D_+, whose dependence on the temperature is given by $D_+ \propto T^{-1/2}$.

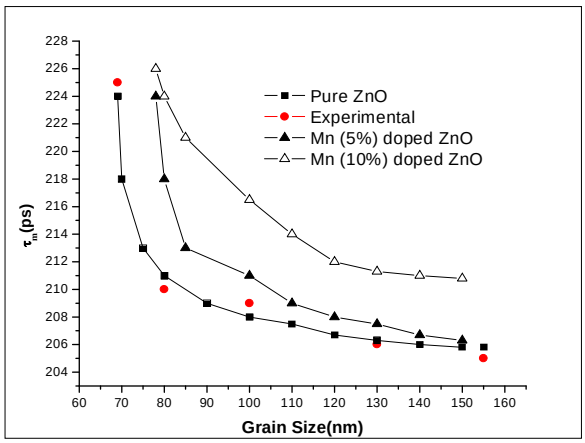

Fig.3

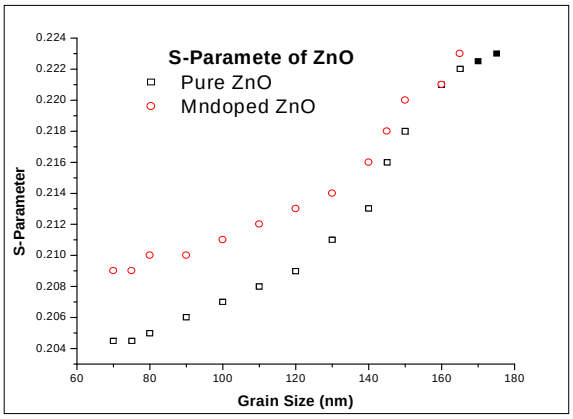

Fig.4

figure 3: comparison of calculated mean positron lifetime (τ_M) as a function of grain size in pure zno thin films and mn doped zno thin films with the experimental observations of p.m.g. nambissan [14] for zns.

figure 4: comparison of calculated S-parameter as a function of grain size in pure ZnO and Mn doped ZnO thin films.

If the diffusion length L_+ competes the size of the grain the probability of the transition rate from free to grain boundary is high. Pasquini et al [13] have shown that the trapping coefficient for the thermal vacancy shows an increasing trend as temperature rises. Further, the trapping rate is expected to be proportional to the thermal vacancy concentration.

The values of the different parameters used in the evaluation of $\bar{\tau}$ have been taken from experimental observations. Few constants have been estimated to give good results. Fig. 3 and 4 represents the results of mean positron lifetime as a function of grain size in pure and Mn doped ZnO thin films. Beside the above, we have also calculated the S-parameter as a function of grain size in pure and Mn doped ZnO thin films. The results are presented in Fig. 3 and 4. The figures show that the positron lifetime decreases with the increase in the grain size for ($T < 350\ K$). This indicates that the transition rate of positrons reaching at the grain boundary increases with increase in temperature and more positrons annihilate in side the grain. As far as the effect of grain size is concerned the lifetime has been found to be smaller corresponding to the larger grains. However, the nature of the curves remains same for the different grain sizes. The present calculation shows that the diffusion of positrons in fine-grained particles coupled with trapping into grain boundaries and thermally generated vacancies in the nanocrystallites could be used to describe the positron annihilation in nanoparticle systems. The high temperature studies of the positron lifetime in nanocrystalline grained alloys elucidate the character

of the different positron trapping sites including the trapping into thermal vacancies inside the grains. Information regarding vacancy concentration in fine-grained samples in principle could be obtained from PAS data. In case of ZnO doping the size of the nanovoid cavity changes due to the increase in doping concentration. The free volume hole concentration has been found to decrease with the increase in doping concentration. Thus positron annihilation is a powerful tool for defect studies on a nanoscopic scale. It is applicable in almost all materials which are important in material science and is more suitable for study of bulk as well as near-surface properties of thin films.

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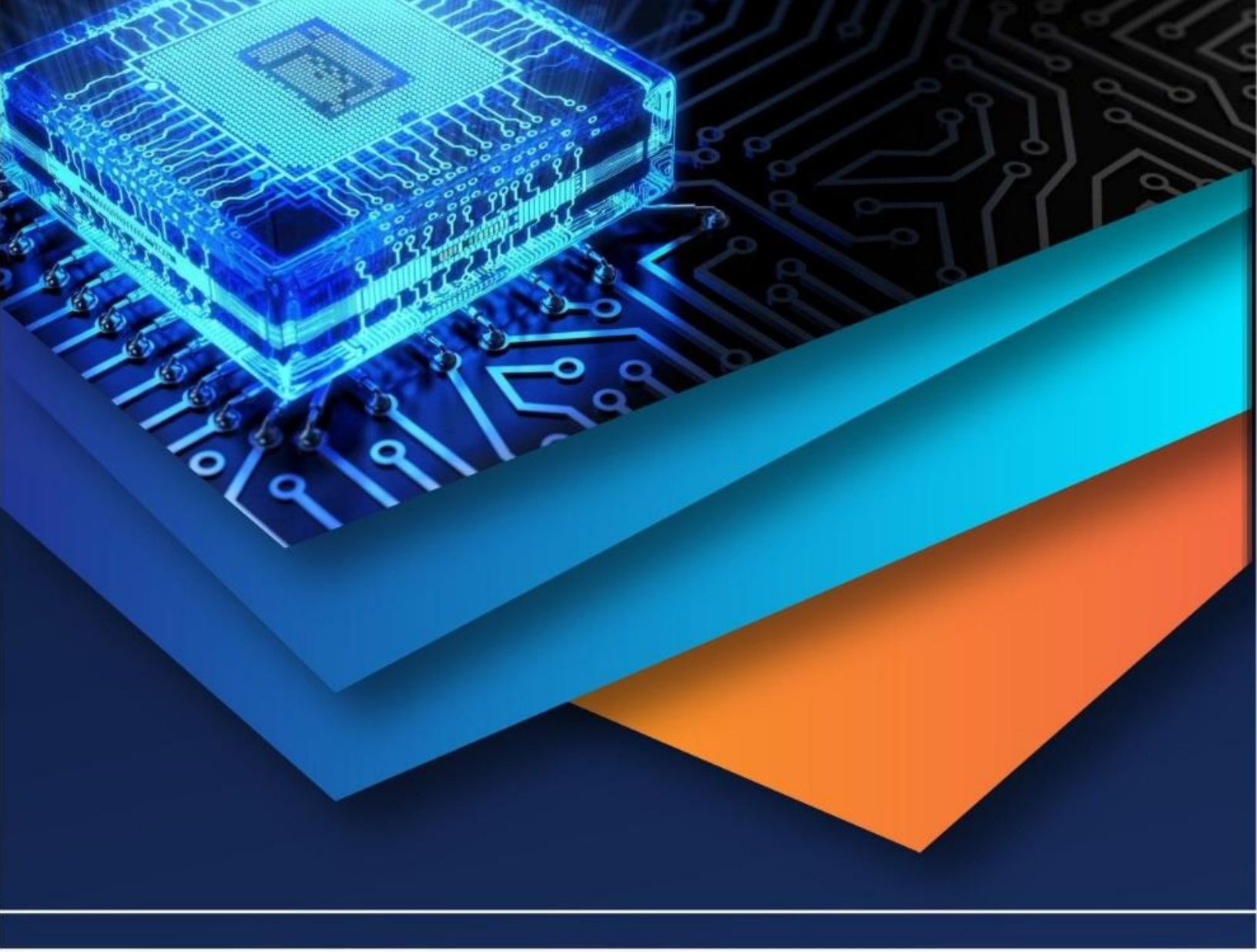

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