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To Study Grain Interfaces and Interfacial Defects in Nanocrystalline Alloys by Positron Diffusion

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ABSTRACT: The positron annihilation in nanocrystalline system has been discussed in terms of thermal diffusion of positrons at grain surfaces and trapping into the grain interfaces and interfacial defects. The diffusion trapping model has been applied to obtain the mean lifetime of positrons $(\bar{\tau})$ as a function of grain size and S-parameter of the annihilation radiation as a function of grain size in Fe_2O_3 nanocrystalline materials. The $\bar{\tau}$ has been found to decreases with the increase in the diameter of nanocrystalline alloys suggesting that the density of grain boundaries decreases gradually when the grain grows.

Key Words: Positron Annihilation, Nanomaterials, Grain boundaries and defects.

I. INTRODUCTION

In understanding the novel properties of nanocrystalline materials, special emphasis has been laid on the study of the atomic arrangement on the ultrafine grained boundaries. Several of the physical properties of wide band gap sulfide and oxide semiconducting nanomaterial systems are inherently related to the presence of vacancy-type defects and the experimental techniques of positron annihilation spectroscopy are found very useful in their investigations [1-3]. There are a number of changes that may accompany the nanostructure formation of materials like phase transformation, lattice contraction or expansion, inversion, free volume generation etc. Positron annihilation parameters are highly sensitive to these changes as the processes involve redistribution of the electrons and hence changes in their annihilation characteristics. The morphology as well as the sizes of the nanocrystallites play crucial roles in governing the annihilation characteristics of positrons in semiconductors. The properties of nanocrystalline alloys and thin films are a subject of intense research in recent years. They have applications in a variety of areas like information storage, color imaging, ferro-fluids, microwave devices, gas sensors, solar cell and communication technology.

Dupasquier *et al.* [4] have found that the trapping mechanism at grain boundary is diffusion controlled. They have explained the positron trapping at grain boundaries employing the standard trapping model. Similarly grain boundaries are also expected to act as trapping sites for positrons since, they are regions of low atomic density. By virtue of their rapid thermalization on entering a grain the positrons exhibit remarkable advantage of diffusing out to the grain surfaces before annihilating with the electron. Tong et al. [5] performed the positron lifetime measurements in nanoscale grain size Fe-B-Si alloy. Significant changes in the structure and properties of grain boundaries and intercrystalline regions were observed when grain was reduced below 25 nm. Chakrabati et al. [6] studied the positron lifetime and Doppler broadening line shape parameter in Fe_2O_3 nanocrystalline alloy. They observed that the positron lifetime at the grain boundaries reduces with increasing grain size, implying a reduction of the total interfacial defect volume. Nambissan has studied wide band gap sulfide and oxide semiconducting nanomaterial systems using the experimental techniques of positron lifetime and coincidence Doppler broadening measurements [7].

On theoretical side, however, little work has been done to understand the positron behaviour in nanoparticle alloys and thin films. Dryzek et al [8] developed a diffusion transition model of the trapping and annihilation of the positrons in the grain. In this work, we have attempted to establish the utility of this model for the studies of nanostructured semiconductors and highlight the role of vacancy-type defects in the modification of material properties.

II. DIFFUSION TRAPPING MODEL

A Diffusion Trapping Model has been established to understand the mechanism of defects for the modification of properties in advanced functional materials [9]. In the model considered, we assume that positrons diffuse in the perfect nanocrystalline grains in which they annihilate with annihilation rate of free positrons in the sample λ_f. The nanocrystal grain surface is the perfect sink for the positrons in which they are localized and then annihilate at a rate $\lambda_g < \lambda_f$. Let the number of trapped positrons at any given instant of time be denoted by $n_g(t)$ and $C(r,t)$ is the local positron density within the grain crystal. The change in the positron concentration inside a grain with time and space is described by the three dimensional diffusion equation:

$$D_+\nabla^2 C(r,t) - \lambda_f C(r,t) = \frac{\partial C(r,t)}{\partial t} \qquad (1)$$

$$\frac{d}{dt} n_g(t) = \alpha \oint\!\!\oint_\Sigma dS\, C(r,t) - \lambda_g n_g(t) \qquad (2)$$

$$D_+ \oint\!\!\oint_\Sigma dS\, \nabla C(r,t) + \alpha \oint\!\!\oint_\Sigma dS\, C(r,t) = 0 \qquad (3)$$

Where D_+ is the diffusion coefficient. For the present calculation, to find out the general solutions of equations (1-3), Laplace transformation have been used and have been solved subjected to the boundary conditions. Where V_Ω is the volume of the grain having radius R and the time dependent of the total number of positrons is given by

$$n(t) = n_g(t) + \oint\!\!\oint\!\!\oint_\Omega dV\, C(r,t) \qquad (4)$$

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 nanocrystalline grains. Thus mean positron lifetime can be obtained as: where λ_f is the annihilation rate of free positrons and λg is the annihilation rate of trapped positrons in to grain boundaries and

$$\bar{\tau} = \frac{1}{\lambda_f} + \left(\frac{1}{\lambda_g} - \frac{1}{\lambda_f}\right)\left\{\frac{1}{1+((\lambda_f+s)/\alpha)B(\gamma)} \times \left[1-\left(1-\frac{B(\gamma)}{D(\gamma)}\right)\frac{1}{V_\Omega}\oint\!\!\oint\!\!\oint_\Omega dV\,\bar{g}(r,s)\right]\right\} \qquad (5)$$

$$B(\gamma) = \frac{\oint\!\!\oint\!\!\oint_\Omega dV\ \bar{f}(r,s)}{\oint\!\!\oint_\Sigma dS\ \bar{f}(r,s)} \qquad (6)$$

$$D(\gamma) = \frac{\oint\!\!\oint\!\!\oint_\Omega dV\ \bar{g}(r,s)}{\oint\!\!\oint_\Sigma dS\ \bar{g}(r,s)} \qquad (7)$$

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.

$$S = S_f + (S_g - S_f)\left[\frac{1}{1+((\lambda_f+s)/\alpha)B(\gamma)}\left\{1-\left(1-\frac{B(\gamma)}{D(\gamma)}\right)\frac{1}{V_\Omega}\oint\!\!\oint\!\!\oint_\Omega dV\,\bar{g}(r,s)\right]\right. \qquad (8)$$

III. RESULTS AND DISCUSSION

Employing the procedure as described above, the $\bar{\tau}$ have been calculated in Fe_2O_3 and ZnS nanocrysatals as a function of grain size. The transition rate α_{fg} is understood to be proportional to D_+, whose dependence on the temperature is given by $D_+ \propto T^{-1/2}$.

If the diffusion length L_+ competes the size of the grain the probability of the transition rate from free to grain boundary is high. Thus, α_{fg} could be described as

$$\alpha_{fg} = 100\frac{L_+}{\tau_f} \qquad \text{,where } L_+ = \sqrt{D_+\tau_f} \qquad (9)$$

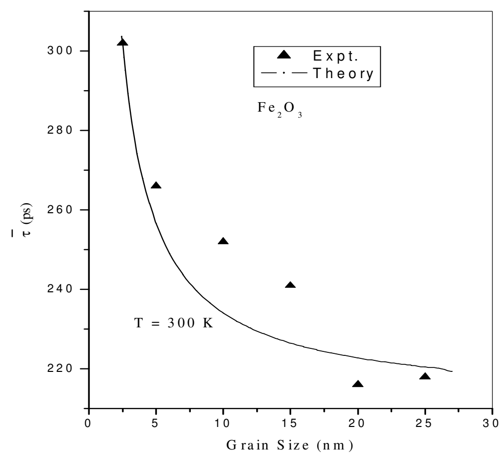

Fig. 1. Comparison of calculated mean positron lifetime ($\bar{\tau}$) as a function of grain size in Fe_2O_3 nanocrystalline alloy with the experimental observations of Chakrabarti *et al* [6].

Figs. 1 show the calculated mean positron lifetime as a function of grain size in ZnS and Fe_2O_3 nanocrystalline systems. In Fig. 2 calculated results of $\bar{\tau}$ have been compared with the experimental data of Chakrabati et al. [6] and found in good agreement with observed results. The figures show that the $\bar{\tau}$ decreases with increase grain size of Fe_2O_3. This could be understood from the fact that the density of grain boundary decreases gradually as the grain grows thus reducing the trapping centers. The $\bar{\tau}$ falls rapidly at low grain size, after this it decreases slowly. It can be shown that if the size of the nanocrystal grain is less than thermal diffusion length of positrons they will diffuse out of the grains and become trapped at the grain interface. In case of when the size of the grain becomes close to diffusion length, the lifetime becomes comparable to that in the bulk [9].

IV. CONCLUSION

The present calculation shows that diffusion of positrons in nanocrysallines coupled with trapping into grain boundaries could be used to describe the positron annihilation in nanoparticle system. The number of trapping centers has been found to decrease with increase in size of nanocrystal grains. At large grain size, comparable to the diffusion length, annihilation occurs in the bulk state. However, more theoretical and experimental work needs to establish the facts.

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