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Investigation of positron annihilation diffusion length in Gallium nitride

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Abstract: A number of authors reported values for positron diffusion length in Gallium nitride less than 60 nm where the expected values in semiconductors are in the range of 200 nm to 300 nm. As these values are usually obtained from fitting a theoretical diffusion model to experimental Doppler broadening results, a possibility of fitting errors exist. In this study, positron annihilation experimental results for two MBE Gallium nitride samples are used to determine diffusion length. Several models are examined and fitted to the data in order to find reasons behind such short values. The study concluded to rule out errors in theoretical fittings, confirmed the shortness and owed the shortness to trapping of positrons by line defects which have high density in this material.

Keywords: Gallium Nitride, Diffusion Length, Defects, Positron Annihilation

1. Introduction

Gallium nitride (GaN) display many valuable electronic, optical and thermal properties, which make it very important in fabricating optoelectric devices in the region of blue to ultraviolet light as well as high power devices. These properties depend mainly on the materials quality which is based on growing conditions and production methods. Intrinsic defects such as vacancies and interstitial atoms believed to form at high concentrations during crystal growth of GaN. Point defects induce localized levels into the band gap which can trap charge carriers, scatter free carriers and create a change in electrical properties. Dislocation densities as high as $10^{10} cm^{-2}$ are common in GaN films produced by metal-organic chemical vapour deposition (MOCVD), also difficulties arise in obtaining lattice matched substrates of GaN epitaxy [1-3].

When positrons are implanted into condensed matter they thermalize within about 10 ps due to inelastic collisions with electrons and ion cores then they diffuse and after a typical life time (200 ps) they annihilate with electrons, their masses are converted to two gamma rays of about 511 keV each. The important feature of positrons is their sensitivity to vacancy type defects . Essentially, vacancies are potential wells that trap slow positrons and the proportion of positrons being trapped may be revealed by an analysis of the energies of the annihilation photons. Dislocations are regarded as shallow positron traps. With a beam of controllable energies, the positrons may be implanted at various depths beneath the surface and thus be used to probe the composition and interfaces in multilayer systems [4].

GaN is a wide band gap semiconductor, it has a direct band gap of 3.4 eV, which might lead to longer epithermal positron diffusion lengths making a possibility of fabricating GaN field assisted moderator [5]. The average diffusion length " defined as the distance traveled by thermal positrons until they reach traps" reflects some of the characteristics of the material. Defect free metals (Al, Cu, Ni) are known to have values between 100 and 200 nm, values for semiconductors (Si, Ge, GaAs) are on the range 200 to 300 nm. The existence of open volume defects reduces these values by ratios of their concentration. On the other hand insulators and amorphose materials display values of 10 to 50 nm. All reported values for GaN are less than 60 nm which mean very short for semiconductors. The present study investigates all possible reasons which may be behind this shortness [6].

2. Experimental Details

The two samples used in the study were prepared using a modified molecular beam epitaxy (MBE) technique. These were grown at 700 ^{0}C under similar conditions on (111) and (001) Gallium arsenide (GaAs) substrates . The growth

rate of GaN films was $0.3\,\mu m/h$, the time was adjusted to obtain a nominal thickness of 0.5 μm . These are similar to the samples used in a previous study [7]. The samples were mounted in the variable low energy positron beam (TASITUS) at Royal Holloway University of London. This beam injects positrons with energies from 100 eV to 25 keV into a sample surface allowing depth profile of samples. Gamma rays resulting from annihilation were recorded by a high purity Germanium detector directly placed behind the sample chamber. Spectrums for 30 minutes runs were stored for 50 chosen positron energies within the range 100 eV to 25 keV. The lineshape parameters S and W were calculated for each spectrum. These parameters are sensitive to material composition and concentration of vacancy-type defects due to the fact that the motion of annihilating electron-positron pair causes Doppler shift in the annihilation radiation. The S parameter known as the law-momentum parameter is defined as the ratio of counts in a central region of the annihilation peak to the total counts in the whole peak. The high electron-momentum parameter known as W parameter is defined as the ratio of counts in specified wing regions to the total number of the counts in the peak. The valence electrons contribute to the region of S parameter because of their law momentum, where core electrons which have higher momentum values contribute to W parameter and making this parameter contain information about chemical identity of the materials atoms. The absolute values of S and W parameters themselves carry no physical meaning but their relative change convey information about the annihilation sites. In this study, these parameters are defined as the sum of counts in 17 central channels and the sum of 10 channels in each wing side divided by the sum of counts in 64 channels representing the whole annihilation peak [8].

3. Positron Diffusion in Solids

The transport of thermalized positrons in solids is described by diffusion theory. In analogy to holes in semiconductors, the movement of thermal positrons may be characterized by diffusion coefficient D_+ defined by Einstein equation:

$$D_+ = k_B T\mu/e \tag{1}$$

Where μ is the positron mobility, k_B is Boltzmann's constant ($1.38\,x\,10^{-23}\,J/K$). Generally positron diffusion is limited by phonon elastic scattering and D_+can be written as [9 -11]:

$$D_+ = \frac{2\sqrt{2\pi}\,\rho\,C_t^2\,\hbar^4}{3m_p^2\,\epsilon_d^2\,\sqrt{k_B T\,m_p}} \tag{2}$$

Where ρ is material density, C_t is longitudinal sound velocity of the material, m_p is the effective mass of positrons and ϵ_d is the deformation potential constant for positrons. The Diffusion coefficient at 300 K is in the range of 1.5 – 3.0 cm^2/sec [12]. In trap free materials, the diffusion length is related to D_+ by $L_+ = \sqrt{D_+\tau_b}$ where τ_b is the positron lifetime. The diffusion length is limited by traps in materials and when these defects (traps) have a uniform distribution then the diffusion length is reduced to an effective diffusion length L_{eff} due to trapping in defects, and they are related by :

$$L_{eff} = \left(\frac{D_+}{\lambda_b + k_D}\right)^{\frac{1}{2}} \tag{3}$$

Here λ_b is the free annihilation rate, k_D is the positron trapping rate defined as:

$$k_D = \mu_D C_D \tag{4}$$

where μ_D is the specific positron trapping rate for different types of defects and C_D is the defect concentration. The specific trapping at neutral vacancies is typically $10^{14} - 10^{15}\,sec^{-1}$ and at negative vacancies $10^{15} - 10^{16}\,sec^{-1}$. For dislocations it is typically of the order of 0,5 $cm^2 sec^{-1}$. Pure dislocation lines are regarded as shallow traps with binding energies 0.1 eV where vacancies and single jogs on the dislocation line have binding energies about 1.0 eV, these values are still smaller than values for bulk vacancies which are of the order 1,5 to 2.0 eV [13- 14]. The specific positron trapping rate μ_D and vacancy concentration C_D can be determined using the equations:

$$k_D = \mu_D C_D = \lambda_b \frac{S - S_b}{S_V - S} = \lambda_b \frac{W - W_b}{W_V - W} \tag{5}$$

Where S_b and W_b represent the parameters at the bulk (free), S_V and W_V are the values at defects (traps).

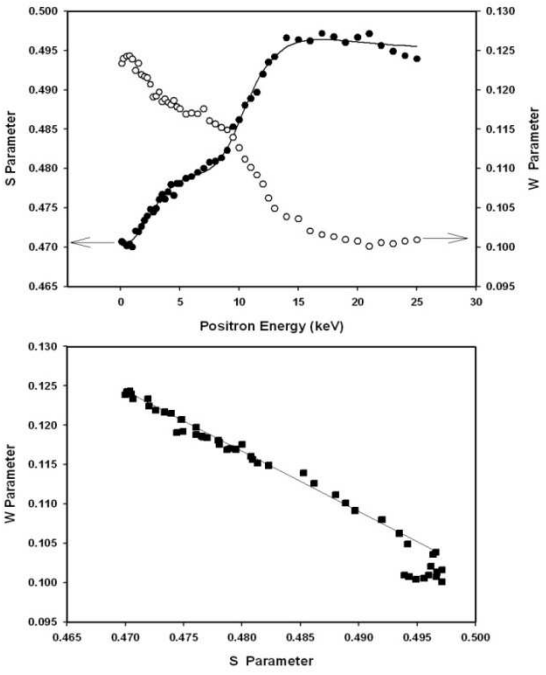

Figure.1 *The S and W parameters plotted as a function of positron impact energy for first GaN sample grown on (111) GaAs substrate. The solid line is the result of VEPFIT fitting. A plot of W versus S parameters is shown , in which a straight line indicates the existence of only single vacancy type defect.*

4. Results

Figure.1 show the calculated S and W parameters as a function of positron energy for the first sample. In the S parameter curve, the step at energies 5 to 10 keV represent the GaN film and at energies above 10 keV, signals from GaAs substrate and possible interface are seen. Similar opposite trend is also seen on W curve. The S versus W parameters are also plotted.

Results of the second sample are presented in Figure.2 . The signs of GaN film are less than 6 kev which indicates lower thickness than the first sample. The very low energy points are regarded as a contribution from epithermal positrons.

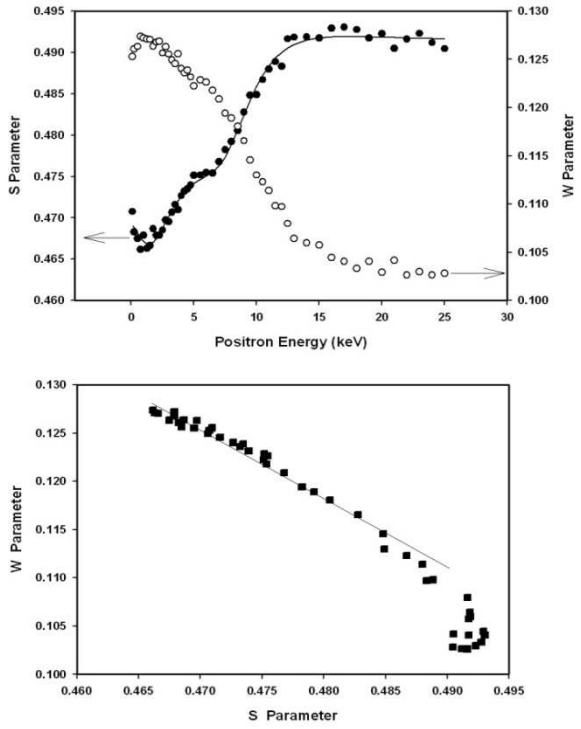

Figure.2 *The S and W parameters plotted as a function of positron impact energy for second GaN sample grown on (001) GaAs substrate. The solid line is the result of VEPFIT fitting. A plot of W versus S parameters is shown , in which a straight line in the GaN region indicates the existence of only single vacancy type defect.*

5. Discussion

The positron diffusion length is measured in solids by implanting low energy positrons at various depths and observing the fraction which diffuses back to the entrance surface. This fraction gets trapped and annihilates at this surface state. In order to obtain quantitative information, several programs are written to fit diffusion model to S and W parameters. [15]. Data sets of S parameter were fit using the code VEPFIT [16]. Fits are represented by solid lines in Figure.1 and Figure.2 . Large number of fitting trials were conducted by choosing two fitting structures, these are (surface – Layer – Substrate) and (surface – Layer – Interface – substrate). All trials to fit the data with the first structure model were unsatisfactory, it turned out that the second fitting structure model is the most suitable. The acceptable fitting result must yield self-consistent values for S and L_{eff} for each layer and carry good quisquare value. The best fits have produced values for diffusion lengths 24.2 ± 2.5 nm and 19.0 ± 1.2 nm and corresponding S values for GaN of 0.4802 ± 0.0020 and 0.4753 ± 0.0030 for the first and second samples respectively. At the interface, the obtained diffusion lengths are 0.1 nm and 0.13 nm which mean almost complete absorption of the positrons arriving at the interfaces of the two samples. We conclude that the shortness seen in the diffusion lengths is not due to errors in fitting procedures. As these samples were grown in totally similar conditions and they only differ in the substrate structure orientation , the first was grown on (111) GaAs and the second on (001) GaN, the difference in S values can only be attributed to the influence of the substrate orientation on the grown GaN layer. The lattice mismatch between GaN layer and the GaAs substrate generates a highly dislocated region in the grown layer, and distribute all over the layer after relaxation [17]. Many Authors have published short diffusion lengths in GaN, These are shown in table.1.

Table.1 *: Values of positron diffusion length in GaN as reported by different Authors.*

Author	GaN material	Diffusion length (nm)
Uodeno. A.et al.(2001) [18]	MOCVD GaN	51 ± 2
Pi. X. D. et al. (2002) [19]	MOCVD GaN	30 to 60
Weg. H. M et al. (2002) [20]		12.0 ±2
Peng .C. X et al. (2007) [21]	IF-MBE GaN	25.6 ±1.2 to 46.0±3.4
Jergensen et al.(2008) [5]	ECR-MBE GaN	19.3 ± 1.4
Uedono. A et Al. (2009) [22]	CVD- GaN	16.0 ± 1.0
Present Study	MO- MBE	24.2 ± 2.5, 19.0 ± 1

It is well known that positron annihilation spectroscopy can determine vacancy concentrations in bulk and epitaxial layers of semiconductors in the range $10^{15} - 10^{20}\, cm^{-3}$, if the concentration is beyond this range, no change in the measured S Doppler parameter nor in diffusion length is expected. The fitted values of diffusion lengths do not match with their corresponding fitted S parameters, (0.4802 , 24.2 ± 2.5 nm) and (0.4753. 19.0 ± 1 nm). Lower S value should be followed by higher L_{eff} and vice versa, this is not the case here, it is an indication that the motion of thermal positrons is influenced by a factor other than vacancies, which we suggest the dislocations. Although dislocations have lower trapping rates but their existence with very high concentrations as in GaN will scatter thermal positrons and divert their direction of motion, or these dislocations act like deep traps because vacancies tend to recide along them and convert them to negatively charged lines as reported by Pi et al. [19]. That will lead to less positron proportion

reaching the surface and result in short calculated diffusion lengths.

The existence of different vacancy-type defects that are trapping positrons in solids can be investigated through the linearity relation between S and W parameters. These relations are plotted in Figure.1 and Figure.2 and a clear linear relation is seen in the GaN region which means only single type of vacancy is present. Several studies have shown the dominant positron trapping vacancy is the Gallium vacancy (V_G) [23]. In a scanning capacitance microscopy study, there are negative charges at the dislocations and it appears that the V_G reside alongside the dislocation lines [24]. Wu, X. H. et al. [25] have measured a very high dislocation density within the first 400 nm from the substrate and the density decreases towards the surface. The influence of dislocations on diffusion length is supported by the study of Pi X. D. et al [19], in which L_{eff} increased from 30 to 60 nm after annealing the samples at 700 ^0C . As annealing at this temperature will reduce the concentration of vacancies by a large ratio but the diffusion length still remain short. Another study by Calleja et al. [26] of MBA GaN on Si substrate show large difference in the S values after annealing at different temperatures but the diffusion lengths appeared unchanged. Moutanabbir et al. [27] have observed 5.6% enhancement in S parameter after H implantation of virgin fs-GaN with 50 keV which appeared to have short diffusion length before H implantation and remained unchanged after implantation. In a study by Tuomisto [28] , GaN reference showed very short diffusion length prior to implantation with H^+ at 100 keV that resulted in $S_V/S_b = 1.055$ with no change in diffusion length. In all last mentioned studies, large variation in S parameters with negligible or no change in diffusion length, this supports the suggestion of diffusion length is influenced by additional factor other than point defects. We conclude that the shortness of the diffusion length is a result of the existence of dislocations.

6. Conclusion

The present study has confirmed the shortness of positron diffusion length in GaN, values of 24.2 ± 2.5 nm and 19.0 ± 1.2 nm are obtained. It also has ruled out the shortness is due to diffusion model fitting errors. The shortness is attributed to positrons trapped by dislocations and this is supported by the variation of S parameters in the two samples under study. The interpretation of these results in the light of related literature is satisfactory.

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