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## Microstructure of the Au/GaAs(110) interface probed using a variable-energy positron beam

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**Abstract.** A mono-energetic positron beam is used to probe the Au/GaAs(110) interface by observing the Doppler broadening of the annihilation radiation as a function of beam energy. The observed data are fitted well by a three-layer model in which the intermediate layer absorbs positrons. The annihilation radiation from this region indicates that it possesses open volume defects. This intermediate layer is attributed to both the Au–Ga alloyed structure (of  $\sim 100$  Å width) that forms close to the expected interface position as a result of atomic intermixing and an extended adjacent defect area in the Au overlayer resulting from Ga and As outmigration. The nature of the defects in these regions is discussed. While evidence is found for Au induced dissociation of the GaAs lattice, the present data are not sufficiently sensitive to give any definite conclusion regarding the presence or absence of vacancy type defects in the near-interface region of the substrate.

### 1. Introduction

The forming of a detailed knowledge of the physics and chemistry involved in the interactions between metals and semiconductors has been of great importance from the earliest days of the semiconductor industry. This general interest has prompted a vast amount of experimental and theoretical work, summaries of which may be found in a number of excellent reviews (Brillson 1982, Rhoderick and Williams 1988, Mönch 1990). However, in spite of recent advances there are some areas where knowledge remains incomplete. One such area is in understanding the mechanisms that determine Schottky barrier heights, where in general there are the conflicting mechanisms of the unified defect (UD) model (Spicer *et al* 1980, 1988) and the metal induced gap states (MIGS) model (Heine 1965, Tersoff 1984, Flores and Ortega 1992). The former model, which ascribes the observed Fermi level pinning in the semiconductor to point defects created in the near surface of the semiconductor, differs significantly from the latter, which invokes interface band structure states that originate from metallic wavefunctions that tunnel into the semiconductor. The present work owes much of its motivation to the fact that one hitherto overlooked technique, namely positron annihilation spectroscopy (PAS), may, because of its sensitivity to open volume lattice defects, have the potential to eventually differentiate between these models.

In the past ten years PAS has become a useful and non-destructive probe in detecting vacancy related defects in bulk compound semiconductors. This work, which makes use primarily of positron lifetime spectroscopy, has been reviewed generally by Dlubek and Krause (1987), and in the specific case of GaAs by Corbel *et al* (1988) and Dannefaer *et al*

(1989). The rapid development of mono-energetic positron beams over the same period has also led a number of research groups to increasingly apply PAS techniques to the study of semiconductor surface and interface structures, the most common experimental procedure being that of monitoring the Doppler broadening of the annihilation lineshape as a function of beam energy (see e.g. Schultz and Lynn 1988 and references therein). In particular the SiO<sub>2</sub>-Si system and metal-SiO<sub>2</sub>-Si systems have been extensively studied (Iwase *et al* 1985, Nielsen *et al* 1987, Uedono *et al* 1988, Baker and Coleman 1989, Smith *et al* 1990, Leung *et al* 1992) and are now sufficiently well understood to allow some microscopic models to be formed of defects that trap positrons at this interface (Au *et al* 1993). The potential of the technique has also been clearly demonstrated both in studies that show various defect structures in MBE grown Si and GaAs epilayers (see e.g. Schultz *et al* 1988, Chilton *et al* 1990) and in studies that have involved the artificial creation of defects in substrates by either ion implantation (see e.g. Keinonen *et al* 1987, Lee *et al* 1988, Takamura and Ito 1992) or surface preparation techniques (see e.g. Uedono and Tanigawa 1990, Lee *et al* 1991).

There have by comparison been only a few PAS depth profiling studies reported on metal-semiconductor systems. To our knowledge only the W/Si (Weng *et al* 1991, Tabuki *et al* 1992) and Au/Si (Corbel *et al* 1989, Mäkinen *et al* 1991) systems have received investigation with no reported studies as yet for metals deposited on III-V semiconductors. Possible reasons for this are not hard to find. Chemical structures at metal-semiconductor interfaces are mostly complex and diffuse in nature (see e.g. Brillson 1982, Rhoderick and Williams 1988) and whereas depth profiling PAS can at the moment cope with either defect concentrations that vary with depth in a single-component substrate (Mäkinen *et al* 1986), or multilayered structures where each layer is of uniform composition (Vehanen *et al* 1987), it is not clear how to deal with a chemical composition and a defect concentration that both vary continuously with depths. Expitaxial contacts, which would be ideal for preparatory studies, are not common, generally require more complex UHV preparation procedures and when formed on III-V substrates often suffer from instabilities (Sands *et al* 1990). Moreover, metal-semiconductor systems also suffer from the added complexity of having built in electric fields within the semiconductor that either force positrons away from or towards the interface (Mills and Murray 1980, Dupasquier and Quartapelle 1987, Corbel *et al* 1989). These fields, not being constant, but varying approximately linearly with position (providing that the metal itself imparts no added doping to the substrate) present an extra complexity that has as yet not been adequately dealt with.

The study presented here is one we believe gives some indication that, in spite of the above difficulties, depth profiling PAS may in the future be a useful technique in studying metal-semiconductor systems. It is carried out on the Au/GaAs(110) system, which owing to its technological importance has the advantage of having been studied by a wealth of more conventional surface analytical techniques (see e.g. Brillson 1982, Rhoderick and Williams 1988 and references therein). Even in its as deposited form this system is known to be characterized by significant Ga and As outdiffusion and subsequent intermixing with the Au overlayer (Chye *et al* 1978, Petro *et al* 1986), a fact which is linked with the high electronegativity of Au (Sinha and Poate 1978, Petro *et al* 1986). In this paper we show that the depth profiling PAS technique is not only capable of detecting the region of intermixing, but in addition is probably showing something that has escaped other spectroscopies, namely the presence of vacancy related defects, produced by Ga and As outdiffusion, in an extensive region of the overlayer.

## 2. Experimental details

The GaAs used in this experiment was obtained from the Semiconductor Processing Co. Inc., Boston, MA, USA. The wafers, which were LEC grown (110) oriented semi-insulating material with a resistivity greater than  $10^6 \Omega \text{ cm}^{-2}$ , were cut into smaller pieces of area  $1 \times 1 \text{ cm}^2$ . Each semiconductor sample was then degreased with acetone and ethanol before being etched for 1 min in first  $\text{NH}_4\text{OH}:\text{H}_2\text{O}_2:\text{H}_2\text{O}(3:1:90)$  and second  $\text{H}_2\text{SO}_4:\text{H}_2\text{O}_2:\text{H}_2\text{O}(8:1:1)$  solutions. Au was then evaporated (using a W filament heater) onto five etched samples to thicknesses of 300 Å, 600 Å, 1000 Å, 1500 Å and 3000 Å respectively. The thickness of the overlayer was measured by a quartz crystal thickness monitor placed close to the sample and at the same distance from the evaporation source. During evaporation, the pressure was kept at  $10^{-6}$  Torr. No annealing was carried out after the evaporation process.

The depth profiling PAS measurements were carried out with the variable-energy positron beam at the University of Science and Technology of China (USTC), Hefei. A detailed description of this positron beam has been given by Han *et al* (1988) but the essential features are as follows. Fast positrons from an 8 mCi  $^{22}\text{Na}$  source are implanted into a W wire mesh moderator and a small fraction ( $\sim 10^{-4}$ ) of these re-emit from the surface of the moderator with low energy,  $\simeq 2.5 \text{ eV}$ . These re-emitted slow positrons are then transported at an energy of 24 eV to the target by a curved solenoidal magnetic field. The final energy of the positrons implanted into the sample is obtained by applying the required negative potential to the sample. The positrons were implanted on the side of the sample with the metal overlayer. The beam intensity used in the present investigations was  $4 \times 10^4$  positrons  $\text{s}^{-1}$ . The annihilation gamma rays were detected by a high-purity germanium (HPGe) detector and an IBM PC/XT computer multichannel analyser system. Annihilation radiation lineshape spectra were taken with positron implanting energies ranging from 0.5 keV to 20 keV, a total of  $10^5$  counts being accumulated under the annihilation peak at each energy.

In this work the Doppler broadening of the 511 keV annihilation radiation is observed by way of the shape parameter,  $S$ , which is defined as the ratio of the area of the central region of the 511 keV peak to the total peak area (MacKenzie *et al* 1970). The width of the central region is chosen so that  $S$  is close to 0.5. It should be noted that the  $S$  parameter is not an absolute measurement and that it is used to study relative changes of the line shape of the 511 keV annihilation line for a particular experimental set-up.

## 3. Positron implantation and diffusion

As the low-energy positrons implant into the sample, they thermalize very rapidly (within 10 ps) (Schultz and Lynn 1988). The implantation profile,  $P_E(x)$ , of these thermalized positrons in a multilayer structure, in which the density varies as  $\rho(x)$ , may be described by a function of the form (Valhealahti and Nieminen 1984, Lynn *et al* 1986, Vehanen *et al* 1987, van Veen *et al* 1990)

$$P_E(x) = -(d/dx)\{\exp[-(z(x)/z_0)^m]\} \quad (1)$$

with

$$z(x) = \int_0^x \rho(\zeta)/\rho_0 d\zeta$$

where  $z_0$  is defined by  $z_0 = \bar{z}_i / \Gamma(1 + 1/m)$ ,  $\Gamma(y)$  is the gamma function,  $\bar{z}_i = AE^n/b_i$  is the mean implantation depth of each layer  $i$  in Å,  $\rho(x) = \rho_i$  is the density of layer  $i$  at depth  $x$  in  $\text{g cm}^{-3}$  and  $E$  is the positron implanting energy in keV. The constants  $m$ ,  $n$  and  $A$  are here taken as 2, 1.6 and  $400 \text{ Å g cm}^{-3} \text{ keV}^{-n}$  based on the work of Vehanen *et al* (1987), although it is noted that these parameters are in general material dependent (Asoka-Kumar and Lynn 1990, Baker *et al* 1991) and thus an exact analytical form for the implantation profile applicable to multi-layered systems has yet to be established. Systematic effects arising in the present work from the use of the material independent parameters will be commented on later.

Once thermalized, positrons undergo diffusive motion inside the sample, which may be described according to the steady state diffusion equation

$$D_+ d^2n/dx^2 - (d/dx)(v_+n) - (\kappa + \lambda_b)n = \mathcal{N}P_E(x) \quad (2)$$

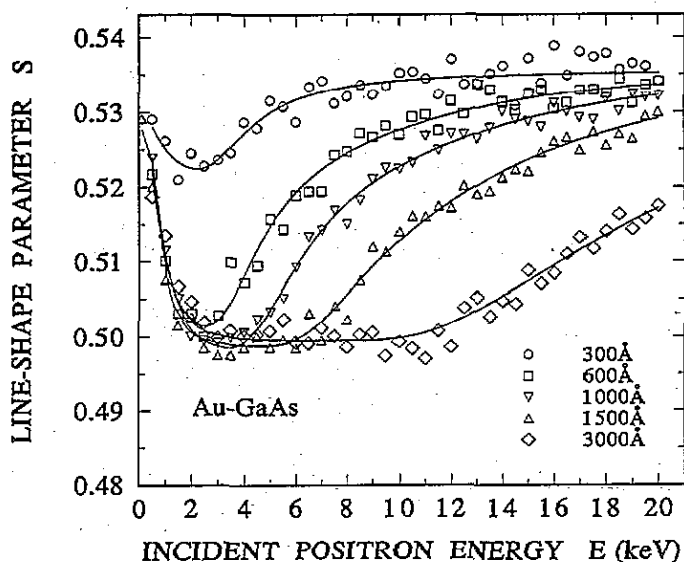
where  $n(x)$  is the time average positron density,  $\mathcal{N}$  is the positron implantation rate,  $D_+$  is the positron diffusion constant,  $v_+$  is the electric field dependent positron drift velocity,  $\lambda_b$  is the bulk annihilation rate and  $\kappa$  is the defect trapping rate. In a general system, such as a metal–semiconductor interface, where the composition is a function of depth, it is understood that  $D_+$ ,  $v_+$ ,  $\kappa$  and  $\lambda_b$  will in general all be functions of  $x$ .

The Doppler broadening parameter  $S$ , being a measure of the electron momentum distribution at the position where the positron annihilates, is the linear combination of the  $S$  parameter contributions from different annihilation states (Campbell 1977); i.e.  $S(E) = \sum_i f_i(E)S_i$  where  $f_i(E)$  is the fraction of positrons annihilating in state  $i$  characterized by the  $S$  parameter  $S_i$ . In a general multilayered structure, such as a metal–semiconductor system, the states  $i$  would correspond to positrons that annihilate from within layers (i.e. from both free and trapped states) and those that are confined to interface states. The fractions  $f_i$  can be obtained by solving the diffusion equation (2), subject to the positron implantation profile (1). For this purpose, a computer program VEPFIT has been written (van Veen *et al* 1990) to enable the fitting of experimental data. This program is very versatile, being able to take the  $S$  parameters  $S_i$ , positron diffusion lengths  $L_+ = \sqrt{D_+\tau_{\text{eff}}}$  (where  $\tau_{\text{eff}} = 1/(\kappa + \lambda_b)$ ) of each layer, drift velocities  $v_+$  in each layer and boundary positions of layers as fitting parameters. The experimental data taken in this study have all been analysed using VEPFIT.

#### 4. Results and discussion

The  $S$ – $E$  data taken for the five different samples are shown in figure 1. A general trend is seen. At low implantation energies the value of  $S$  is high (0.52–0.53) and characterizes positrons that annihilate on or close to the surface of the Au overlayer. As the energy increases more positrons annihilate in the Au and  $S$  drops, and for the thicker Au films the drop plateaus off to a value of 0.499 characteristic of the Au film. As the beam energy increases still further the  $S$  parameter begins to rise to a saturation value of 0.5355 (seen in only the thinner Au contacts) that is characteristic of the bulk GaAs.

In the Au/GaAs system, a number of possibilities exist for injected positrons. They may (i) annihilate in the bulk GaAs in a free delocalized state, (ii) be trapped into a negative or neutral vacancy type defect in the bulk GaAs with subsequent annihilation, (iii) diffuse to the Au/GaAs interface from either the Au overlayer or the GaAs bulk and annihilate from some interface state, (iv) annihilate in the Au overlayer in a free delocalized state, (v) be



**Figure 1.** The lineshape parameter  $S$  as a function of the incident positron energy for the Au/GaAs system. Data for the five different Au coverages (300 Å, 600 Å, 1000 Å, 1500 Å and 3000 Å) are shown. The solid lines are those obtained using the PAET model fits (with  $\rho_I = \rho_O$ ) as discussed in the text.

trapped into a vacancy type defect in the Au with subsequent annihilation or (vi) diffuse to the Au surface with annihilation occurring from a surface state (or possibly from emitted Ps). In order to analyse the data according to this complex picture, a simple two-layer model was first constructed. In this model, the sample is considered as a system composed of two layers, namely the Au overlayer and the bulk GaAs substrate. We refer to this model as the freely diffusing interface (FDI) model, as its basic assumption is that the interface freely transmits positrons in both directions. This is an ideal situation that clearly cannot be achieved in practice even with perfect lattice matching at the interface, since in general the bulk and the overlayer will have different positron affinities (Puska *et al* 1989) allowing a positron current in only one direction. Nevertheless, the simplicity of the FDI model makes it a convenient starting point for interpreting the present  $S(E)$  data. The  $S$  parameter for the FDI model is given by

$$S = f_S(E)S_S + f_O(E)S_O + f_B(E)S_B \quad (3)$$

where  $f_S(E)$ ,  $f_O(E)$  and  $f_B(E)$  are the implantation energy dependent fractions and  $S_S$ ,  $S_O$  and  $S_B$  are the corresponding  $S$  parameters of positrons annihilating at the surface, overlayer (Au) and bulk (GaAs) respectively. The dashed line in figure 2 shows the best fit that we could achieve to the 1000 Å data using the FDI model. For this fitting the interface is fixed at its expected depth of 1000 Å and the density of the Au overlayer is taken as the single-crystal value of  $19.3 \text{ g cm}^{-3}$ . The positron effective diffusion length in the GaAs bulk was taken as  $L_B = 2270 \pm 10 \text{ Å}$ , this being the value obtained from a control experiment involving an  $S$  parameter depth scan on a sample without any Au overlayer, and one that is reasonably consistent with the room temperature value of  $D_+ = 1.6 \pm 2 \text{ cm}^2 \text{ s}^{-1}$  as obtained by Soininen *et al* (1992) and the bulk GaAs lifetime  $\tau_B = 230 \text{ ps}$  (Dlubeck and Krause 1987). It is clear from figure 2 that the FDI model can represent only the 0–2 keV data

well, and at higher energies a large discrepancy is seen. A reasonably good fit can only be achieved if the Au/GaAs interface is brought into an unrealistic depth of  $114 \pm 3 \text{ \AA}$  from the surface (the dot-dashed line in figure 2).

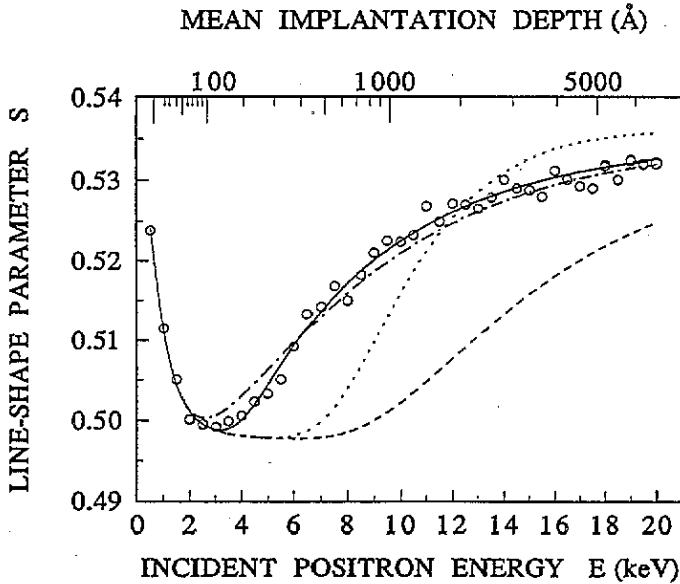


Figure 2. The lineshape parameter  $S$  as a function of the incident positron energy for the 1000 Å coverage sample. The dashed and dot-dashed lines correspond to the FDI model fit with the interface position fixed at 1000 Å and 114 Å respectively. The dotted and solid lines correspond to the PAI model with the interface fixed at 1000 Å and 345 Å respectively. The mean implantation depth scale has been calculated using (1).

We next attempted to fit the data by a model that treated the interface as a thin layer that is perfectly absorbing to positrons. This is physically more meaningful, as the expected intermixing of the Au and GaAs components would lead to a heavily defected region that would be expected to trap positrons. In this perfectly absorbing interface (PAI) model the expression for the measured  $S$  parameter is written as

$$S = f_S(E)S_S + f_O(E)S_O + f_I(E)S_I + f_B(E)S_B. \quad (4)$$

The nomenclature here is the same as in (3) with the exception of the additional term, in which  $f_I(E)$  is the fraction of positrons annihilating from the interface and  $S_I$  is the  $S$  parameter characteristic of the interface. The best PAI model fit to the 1000 Å data is shown by the dotted line in figure 2. Once again the interface position was fixed at the expected depth of 1000 Å. As VEPFIT has no built in method of allowing for a positron absorbing interface such a layer was mimicked by a third layer of 10 Å thickness having a positron diffusion length of 0.01 Å. While the PAI model gives a marginally better fit than the FDI model, it is still apparent that for the data above 2 keV there is a large discrepancy between theory and experiment. As with the FDI model, it is only by bringing the interface to an unrealistic depth ( $345 \pm 5 \text{ \AA}$ ) that a reasonable fit (solid line, figure 2) can be found. Since 1000 Å of Au is actually deposited, the implication is that both FDI and PAI models lack in some important detail.

Since discrepancies similar to those for the 1000 Å sample were found for the four other samples using both FDI and PAI models, it follows that, irrespective of the Au coverage, a model based on just two layers is in some sense incomplete. The failure of the FDI and PAI models led us to construct a further model, based on the observation (see e.g. Chye *et al* 1978, Petro *et al* 1986, Joyce *et al* 1987) that considerable atomic intermixing occurs at the unannealed Au/GaAs interface. The system was thus modelled with three layers, namely the Au overlayer ( $0 \leq x \leq T_1$ ), an extended 'interface region' attributed in some sense to Au-GaAs intermixing ( $T_1 \leq x \leq T_2$ ) and the GaAs bulk ( $x \geq T_2$ ). Since the only difference between this and the PAI model is in the extended nature of the interface, this model is referred to as the PAEI (perfectly absorbing extended interface) model. The  $S$  parameter for this model is still as represented by equation (4), the only difference being that now the fractions  $f_s$ ,  $f_o$ ,  $f_i$  and  $f_b$  depend on the interface boundary positions  $T_1$  and  $T_2$ .

**Table 1.** PAEI model fits with  $\rho_1 = \rho_0$ . VEPFIT analyses are given for the three-layer PAEI model.  $S_s$ ,  $S_o$  and  $S_i$  are the fitted  $S$  parameter values for the surface, overlayer and 'interfacial region' respectively.  $L_o$  is the overlayer diffusion length (or surface segregation length), which was fitted using data in the 0–2 keV range.  $T_1$  and  $T_2$  are the boundaries (as measured from the sample surface) of the 'interfacial region'.  $S_b$  and  $L_b$  were kept fixed at 0.5355 and 2270 Å respectively.

Coverage (Å)	$S_s$	$S_o$	$S_i$	$L_o$ (Å)	$T_1$ (Å)	$T_2$ (Å)	$\chi^2$
300	0.5315 (25)	0.5214 (10)	0.5340 (9)	20.0 (4.0) <sup>a</sup>	215 (20)	316 (205)	52.7
600	0.5336 (22)	0.5002 (8)	0.5268 (7)	13.9 (2.5) <sup>a</sup>	255 (11)	617 (95)	45.7
1000	0.5349 (24)	0.4976 (7)	0.5265 (7)	17.5 (2.2) <sup>a</sup>	412 (15)	1059 (140)	20.7
1500	0.5383 (20)	0.4986 (5)	0.5257 (8)	12.3 (2.0) <sup>a</sup>	770 (22)	1629 (171)	39.2
3000	0.5303 (24)	0.4994 (4)	0.5239 (14)	17.0 (2.3) <sup>a</sup>	1933 (157)	3085 (420)	45.2

<sup>a</sup> Fixed parameter.

The PAEI model was fitted to the data in the following way. As with the PAI model the positron diffusion length  $L_i$  in the interface region, was taken to be 0.01 Å so as to represent close to perfect absorption. The bulk parameters  $S_b$  and  $L_b$  were also kept unaltered at 0.5355 and 2270 Å respectively. For each sample the overlayer diffusion length parameter,  $L_o$ , was fixed at the values found in fitting the FDI and PAI models. These values (see table 1) had been obtained by fitting only the 0–2 keV data, as strong parameter intercorrelations prevented VEPFIT from freely fitting this parameter correctly when all the data (0–20 keV) were used. All other parameters were freely fitted. In using the PAEI model some assumption must be made about the density of the interfacial region. This will clearly be a function of position throughout the region, approaching the Au value on the overlayer side and the GaAs value on the substrate side. Since VEPFIT requires a definite value of density for each specified layer, in the first approximation some average value must be taken. In the first PAEI fitting we assumed the density of the 'interfacial region' to be equal to that of the Au overlayer (i.e.  $\rho_1 = \rho_0 = 19.3 \text{ g cm}^{-3}$ ). In the second case, however, an intermediate density of  $\rho_1 = 12 \text{ g cm}^{-3}$  was used, a value obtained assuming a 1:1 atomic ratio of Ga to Au, which can to some extent be justified by the observation of an AuGa phase at the interface using x-ray spectrometry (Zeng and Chung 1982). In both cases equally good fits could be found. Fitted parameters for the cases of  $\rho_1 = \rho_0$  and  $\rho_1 = 12 \text{ g cm}^{-3}$  are given in tables 1 and 2 respectively, and the lines drawn in figure 1 are those corresponding to the case  $\rho_1 = \rho_0$ . It is noted that while we have not been able to obtain an accurate density value for the AuGa phase, the fitted parameters (except  $T_2$ ) are not sensitive to the chosen



value of  $\rho_1$  and moreover, since, as is discussed below, only a small fraction ( $\sim 100 \text{ \AA}$ ) of the 'interfacial region' is likely to be of a composition requiring an intermediate density, the case of  $\rho_1 = \rho_0$  is believed to be the better of the two approximations.

**Table 2.** PAET model fits with  $\rho_1 = 12 \text{ g cm}^{-3}$ . VEFFIT analyses are given for the three-layer PAET model.  $S_S$ ,  $S_0$  and  $S_1$  are the fitted  $S$  parameter values for the surface, overlayer and 'interfacial region' respectively.  $L_0$  is the overlayer diffusion length (or surface segregation length), which was fitted using data in the 0–2 keV range.  $T_1$  and  $T_2$  are the boundaries (as measured from the sample surface) of the 'interfacial region'.  $S_B$  and  $L_B$  were kept fixed at 0.5355 and 2270  $\text{\AA}$  respectively.

Coverage ( $\text{\AA}$ )	$S_S$	$S_0$	$S_1$	$L_0$ ( $\text{\AA}$ )	$T_1$ ( $\text{\AA}$ )	$T_2$ ( $\text{\AA}$ )	$\chi^2$
300	0.5316 (26)	0.5214 (11)	0.5340 (9)	20.0 <sup>a</sup>	212 (19)	352 (350)	52.3
600	0.5327 (30)	0.5004 (9)	0.5259 (8)	13.9 <sup>a</sup>	253 (11)	685 (106)	44.4
1000	0.5344 (26)	0.4980 (8)	0.5249 (8)	17.5 <sup>a</sup>	400 (14)	1150 (141)	20.4
1500	0.5384 (21)	0.4986 (6)	0.5244 (10)	11.3 <sup>a</sup>	779 (23)	1703 (270)	41.1
3000	0.5301 (25)	0.4997 (4)	0.5207 (19)	17.0 <sup>a</sup>	1924 (60)	3120 (450)	43.8

<sup>a</sup> Fixed parameter.

The main conclusion that can be drawn from the above analysis is that a reasonable interpretation of the data can only be made if there exists an 'interfacial region' that is extended in structure and possesses an  $S$  parameter significantly larger than that of Au. Both these two characteristics are shown in figures 3(a) and 3(b) where the fitted parameters  $T_1$  and  $T_2$  and  $S_1$ , respectively, are shown plotted against deposited thickness,  $T$ , of Au for the cases of  $\rho_1 = \rho_0$  and  $\rho_1 = 12 \text{ g cm}^{-3}$ . As may be seen, both  $T_1$  and  $T_2$  follow in rough proportion the Au coverage. A consequence of this trend is that the thickness  $T_2 - T_1$  of the 'interfacial region', also increases in approximate proportion to Au coverage, a fact that will be commented on below.  $S_1$ , on the other hand, apart from the 300  $\text{\AA}$  case where it becomes double valued (see below), remains fairly constant.

Figure 3(a) shows that a major part of the 'interfacial region' occurs within the Au overlayer. Less clear, because of the errors in the parameter  $T_2$  (for the case  $\rho_1 = \rho_0$ ), is the penetration into the expected location of the GaAs substrate. The statistical likelihood of all the  $T_2$  points lying at their observed positions (i.e. on the GaAs side relative to the ideal interface position) by accident is low ( $\simeq 0.4\%$ ). Coupled with this are two systematic errors which, when considered together, tend to support the view that the 'interface region' penetrates the GaAs, namely (i) the real situation will lie somewhere between the two cases of  $\rho_1 = \rho_0$  and  $\rho_1 = 12 \text{ g cm}^{-3}$  (i.e.  $T_2$  will be somewhere between the dashed and solid lines in figure 3(a) and (ii) the Monte Carlo simulations and experiments of Baker *et al* (1991) indicate that the mean implantation depth of positrons in the Au/GaAs system is larger than predicted by the implantation profile based on the  $A$  and  $n$  parameters, 400  $\text{\AA}$   $\text{g cm}^{-3} \text{ keV}^{-n}$  and 1.6 respectively, used in this work. These authors find alternative values of  $A$  and  $n$  for positrons implanting into Au of  $885 \pm 296 \text{ \AA g cm}^{-3} \text{ keV}^{-n}$  and  $1.42 \pm 0.08$  respectively. While here we are not dealing with single-component Au, such values would nevertheless suggest that penetration depths,  $T_2$ , might be some 60–30% larger than those shown in figure 3(a) for the 300  $\text{\AA}$  and 3000  $\text{\AA}$  coverage samples respectively. Such a view, however, is not supported by the parametrization for Au given by Asoka-Kumar and Lynn (1990), namely that  $A = 261 + 974E^{-1} - 318E^{-2} \text{ \AA g cm}^{-3} \text{ keV}^{-n}$  ( $E$  in keV) and  $n = 1.64$ , which only gives an increased penetration for low energies ( $E < 5 \text{ keV}$ ). It is thus difficult to draw any firm conclusions regarding the exact location of  $T_2$  while such uncertainty exists on the exact parametrization of the positron implantation profile

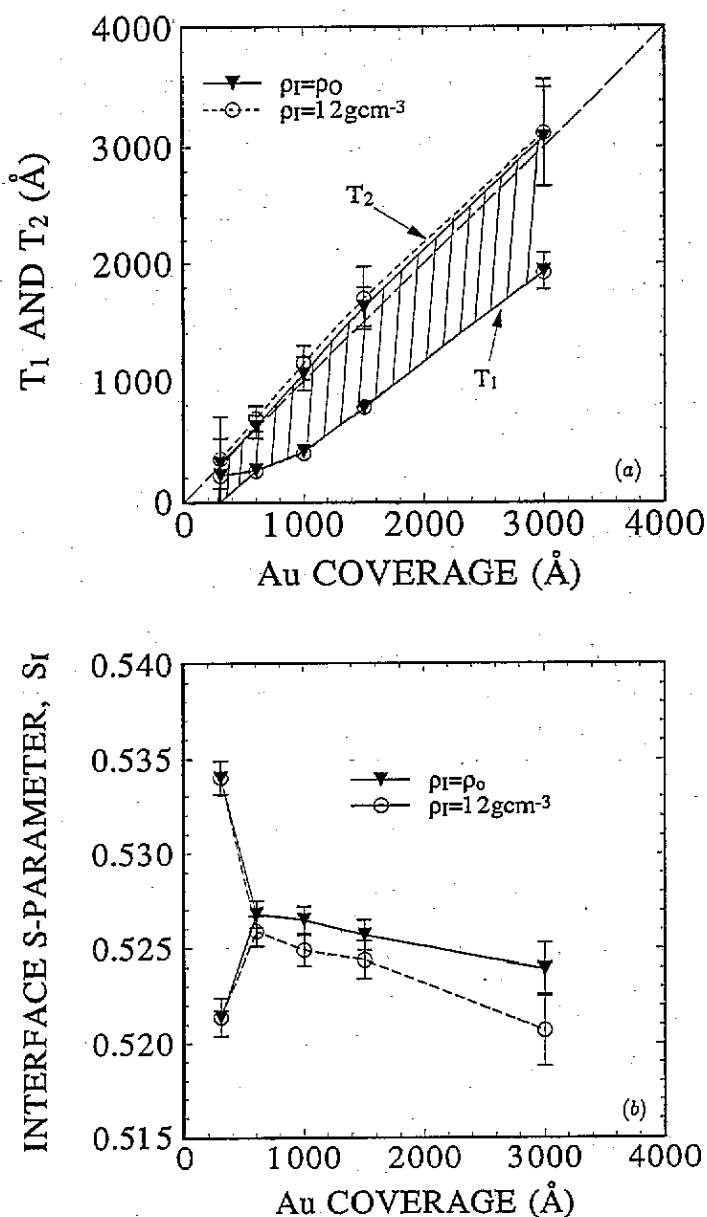


Figure 3. (a) The PAEI model fitted values of  $T_1$  and  $T_2$  as a function of Au coverage  $T$  for both cases of  $\rho_I = \rho_0$  and  $\rho_I = 12 \text{ g cm}^{-3}$ .  $T_1$  and  $T_2$  are, relative to the surface of the Au overlayer, the depths of the nearest and furthest boundaries respectively of the 'interfacial region' seen in the PAS depth scans. The shaded region indicates the extent of the 'interfacial region' (for  $\rho_I = \rho_0$ ). The long-dashed line shows the expected ideal interface location, i.e. the location of the interface if there were no intermixing of components. Note that in the case of the 300 Å sample the shaded region is drawn extending to the surface to represent the fact that the 'interfacial region' between the surface and  $T_1$  for this sample. (b) The fitted values of  $S_1$  as a function of Au coverage  $T$  for both cases of  $\rho_I = \rho_0$  and  $\rho_I = 12 \text{ g cm}^{-3}$ . In the case of the 300 Å coverage sample  $S_1$  becomes double valued, the higher value coming from the region close to the ideal interface position, and the lower value coming from the defected remainder of the Au overlayer.

for different materials and for composite systems. From the evidence presented, however, there are reasonable grounds for believing that the present 'interfacial region' penetrates the expected ideal location (i.e.  $x = T$ ) of the GaAs substrate by at least  $\sim 100 \text{ \AA}$  in all samples. Such a penetration, if real, is likely to be associated with the general dissociation of the substrate lattice caused by Ga outmigration into the metal (Sinha and Poate 1978, Kingsbron *et al* 1979).

Thus far we have referred to the intermediate layer detected in this depth profiling PAS study as the 'interfacial region', the quotes indicating that as of yet its nature and the cause behind it are uncertain. The name would appear an appropriate one since, as seen from figure 3(a), we are dealing with a region of width  $T_2 - T_1$  that is located relative to the ideal interface position,  $T$  ( $T_1 \leq T \leq T_2$ ). While this region was introduced on the basis of previous reports of Au-GaAs intermixing, some care must however be exercised in associating this layer too closely with what is normally meant by terms such as 'region of intermixing' or 'interface width'. In XPS or AES depth scans these terms usually represent the region over which the atomic fractions of substrate components drop from 90% to 10% of their bulk values. Of direct relevance to the present discussion is, for example, the fact that Chye *et al* (1978) in AES profiling the non-annealed Au/GaAs(110) system find, in accordance with the above definition, an 'interface width' of  $200 \text{ \AA}$ . Similarly, for the same system, Hiraki *et al* (1979) find a width of around  $170 \text{ \AA}$ . These values are significantly less than the interface region that our PAS data are indicating (see table 1). It is thus our conjecture that the 'interface region' we are detecting in our PAS results is a much more extensive spatial structure than what is normally meant by the term 'interface width'. The reason for observing such an extensive structure is not hard to find. It is noted that the value of  $S_1$ , while not being as high as that of GaAs, nevertheless is much higher than the average of the  $S$  parameters for Au and GaAs ( $\approx 0.517$ ). It is well known that one reason for obtaining a high  $S$  parameter is that of positron trapping into vacancy type defects (see e.g. Schultz and Lynn 1988 and references therein), and it is this that we believe is the main cause of the high  $S$  parameter characterizing the interface region. Turning this argument around, the 'interfacial region' in the context of the present discussion is that region where there is an appreciable chance of a positron trapping into an open volume defect with subsequent annihilation.

The most likely positron trapping type of vacancy type defect on the GaAs side is  $V_{\text{Ga}}$ . The reason for this is that  $V_{\text{Ga}}$  is acceptor like and usually negatively charged, and thus has an affinity for positrons. While  $V_{\text{As}}$  may also be present, it is a less likely candidate, as we are dealing with semi-insulating GaAs, and  $V_{\text{As}}$  will be in a positively charged state if the Fermi energy of the system resides close to the mid-gap position (Saarinen *et al* 1991).

On the Au side of the interface the nature of the defects trapping the positron is less certain. Xu *et al* (1987) find that Ga and As dissolve into the Au overlayer to their solubility limit, which these authors find to be  $1.3 \times 10^{-4} \text{ atoms \AA}^{-3}$  ( $1.3 \times 10^{20} \text{ cm}^{-3}$ ). This is a very high impurity level which is almost certainly going to disorder the Au matrix, causing either vacancy related centres such as  $V_{\text{Au}}$  or more complex open volume defects. Since positrons are in general sensitive to vacancy defects in solids at the 0.1–100 ppm ( $\sim 10^{16}$ – $10^{10} \text{ cm}^{-3}$ ) level (Seeger 1973) it is not surprising to find positron trapping occurring well into the Au overlayer.

The approximate proportionality, observed in figure 3(a), between coverage  $T$  and the penetration depth ( $T - T_1$ ) of the interfacial region into the Au overlayer is interesting and deserves further comment. Clearly the interface structure is not invariant under the operation of increasing the thickness of the Au overlayer as this would imply the defect causing agents (Ga or possibly As) decreasing with the same functional form relative to the

**Table 3.** PAEI model fits with added Au-GaAs alloyed layer. The VEPFIT analyses are carried out assuming a four-layer PAEI model, in which the additional fourth layer represents a region of alloying.  $S_A$  is the fitted  $S$  parameter of this region and  $T_2 = T - 50 \text{ \AA}$  and  $T_3 = T + 50 \text{ \AA}$  are its boundaries. The other parameters have the same meaning as those in tables 1 and 2.  $S_B$  and  $L_B$  were kept fixed at 0.5355 and 2270  $\text{\AA}$  respectively.

Coverage ( $\text{\AA}$ )	$S_S$	$S_O$	$S_I$	$S_A$	$L_O$ ( $\text{\AA}$ )	$T_1$ ( $\text{\AA}$ )	$\chi^2$
300	0.5336 (71)	0.5210 (28)	0.5233 (9)	0.5349 (10)	20.0 <sup>a</sup>	30 <sup>a</sup>	53.4
600	0.5334 (30)	0.4997 (11)	0.5205 (15)	0.5300 (16)	13.9 <sup>a</sup>	211 (12)	38.6
1000	0.5344 (26)	0.4980 (8)	0.5255 (16)	0.5267 (23)	17.5 <sup>a</sup>	406 (14)	20.2
1500	0.5386 (21)	0.4982 (6)	0.5277 (23)	0.5203 (40)	11.3 <sup>a</sup>	769 (21)	38.4
3000	0.5299 (25)	0.4998 (5)	0.5204 (66)	0.5340 (19)	17.0 <sup>a</sup>	2014 (71)	42.0

<sup>a</sup> Fixed parameter.

ideal interface position irrespective of coverage. If this were the case, the penetration depth ( $T - T_1$ ), being representative of where positron trapping falls below the detectable limit, would be constant. Observations such as those of Xu *et al* (1987) that Ga and As dissolve to their solubility limits in the Au also suggest a coverage dependent functional form for the fall-off in Ga and As concentrations since the amount of Ga and As dissolved must be to first order proportional to the coverage. The observed phenomenon could thus be explained if (i) the Ga and As concentrations dropped off approximately linearly throughout the overlayer but with values at any point not differing appreciably from the solid solubility limited values and (ii) such behaviour resulted in a critical concentration of vacancies (or possibly vacancy clusters or voids) being reached at some point between the interface and the surface, beyond which defect trapping becomes negligible.

The 300  $\text{\AA}$  coverage sample shows an interesting feature, namely the presence of two defected regions (see table 1 and figure 3(a)). This conclusion is drawn from the fact that both the regions ( $0 < x < T_1$ ) and ( $T_1 < x < T_2$ ) have  $S$  parameter values higher than the value associated with undefected Au (0.499). As seen from the PAEI fit of table 1 the first of these regions has an  $S$  parameter of around 0.521 and stretches from the sample surface to within  $85 \pm 20 \text{ \AA}$  of the ideal interface position after which distance an even higher  $S$  value ( $\approx 0.534$ ) is encountered, which then penetrates the substrate. Based on its value, which is close to  $S_I$ , we interpret the lower of the two  $S$  parameters as being due to vacancy related defect formation in the Au, while the higher  $S$  parameter, which occurs close to the ideal interface position is believed to be associated with that region of atomic intermixing seen by others (Chye *et al* 1978, Hiraki *et al* 1979) which we refer to here as the 'alloyed region'. We have checked to see whether there is evidence of such a higher  $S$  parameter interfacial region in the higher-coverage samples. To accomplish this within the limited statistical accuracy of our data a region of fixed boundaries spanning from  $T_2 = T - 50 \text{ \AA}$  to  $T_3 = T + 50 \text{ \AA}$  was defined. The analysis, which now incorporated four layers, can be expressed as follows:

$$S = f_S(E)S_S + f_O(E)S_O + f_I(E)S_I + f_A(E)S_A + f_B(E)S_B \quad (5)$$

where the subscripts A refers to the 'alloyed region'. The fitted values for this model are shown in table 3. It may be seen from the  $\chi^2$  values that a significantly better fit is obtained in the case of the 600  $\text{\AA}$  coverage sample and that marginal improvements are found in the higher-coverage films. Visually, except for the 600  $\text{\AA}$  sample where improvement is noticeable, the fits to the data differ little from those shown in figure 1. The fact that the two lowest-coverage fits are significantly improved by including this 'alloyed region' is we believe sufficient evidence that such a region does exist, since it is at these low coverages that the PAS depth scan has the best spatial resolution.

In recent positron lifetime experiments using similar Au coated samples, it has been possible to observe the interface positron lifetime by inducing large electric fields directed towards the interface (Shan *et al* 1993). A long-interface-lifetime component of  $\sim 400$  ps is observed. Based on the work of Hautojärvi *et al* (1977) such a lifetime would correspond to positrons trapping into microvoids of some 10 Å diameter. It is these microvoids that are probably responsible for this higher  $S$  parameter at the region close to the ideal interface position where maximum intermixing occurs. These microvoids are possibly associated with grain boundaries, or they could be due to clusters of vacancy type defects. This is a region that may be characterized by many different AuGa phases (Yoshiie *et al* 1984), and it would not be surprising to find some open volume defects at grain boundaries, especially at those bordering on the substrate lattice.

An interesting question is whether the present study can give any information on vacancy type defects in the near-interface region of the GaAs substrate, since these are of such relevance to the question of Fermi level pinning in Schottky contact formation. It has already been suggested that  $V_{\text{Ga}}^-$  could be a possible positron trap. If this defect were present in sufficient concentration as a result of the Au induced dissociation of the GaAs then an  $S$  parameter higher than  $S_B (= 0.5355)$  would be anticipated somewhere on the substrate side of the ideal interface position. Within the statistical uncertainties of the present experiment it can be said that no such region has been detected. It is clear, however, that vacancies such as  $V_{\text{Ga}}^-$  could be obscured, the most likely reason, as suggested, being that both the depth resolution and the sensitivity of the present PAS study are insufficient to bring out the necessary structural detail. Vacancy type defects could thus be present but within what we observe as the 'alloyed region' in the 300 Å and 600 Å coverage samples and would simply contribute to a slightly higher value of  $S_A$ . Such an effect would go unnoticed. In addition to this practical aspect is the observation that the solid state reaction between Au and GaAs does give rise to an irregular interface boundary as the Au dissolves the GaAs preferentially in some crystallographic directions leading to pyramidal pits (Zeng and Chung 1982, Yoshiie *et al* 1984). Thus vacancies in the substrate could exist at the same depth as some of the alloyed components and associated microvoids. Moreover, our samples were not free from a thin surface oxide when the Au was deposited, and the remnants of this oxide could well confuse the  $S$  parameter signal from the 'alloyed region', the positron binding to oxides being characterized generally by lower  $S$  parameters (see e.g. Au *et al* 1993).

To conclude the discussion of the present work some comments are made concerning the diffusion lengths of positrons in the Au overlayer. As may be seen from table 1 a value for  $L_O$  of  $16 \pm 5$  Å gives a reasonable description for all the samples. It is suggested here, however, that this value is not necessarily the diffusion length of positrons in the overlayer, as has so far been assumed, but is more likely to represent the region over which Ga (and possibly As) segregation occurs on the Au surface, which is known to have a characteristic drop-off distance in the range of 3–20 Å (Chye *et al* 1978, Hiraki *et al* 1979, Xu *et al* 1987). The VEPFIT program is not able to distinguish between an  $S$  parameter that drops off approximately exponentially in an inhomogeneous material, and positron diffusion to a surface in a homogeneous material, since these two possibilities can give rise to similar data. In support of this segregation interpretation it is first noted that the mean size of microcrystals in as deposited Au films grown under similar conditions has been reported to be around 500 Å (Yoshiie *et al* 1984). This value, being less than the typical 1000 Å diffusion length of positrons in metals, would suggest an apparent diffusion length of  $\simeq 500$  Å, the limitation of positron motion being imposed by trapping at grain boundaries. An obvious reason for observing a much smaller value for  $L_O$  would

be that the Au microcrystals were defected with positron traps, but such an explanation is inconsistent with the low overlayer  $S$  value seen in all but the 300 Å sample. Neither can such an interpretation explain why the  $L_0$  value ( $20 \pm 4$  Å) from the 300 Å coverage sample is the largest found amongst all the samples. Since this sample alone exhibits a defected 'interfacial region' all the way to the surface the  $L_0$  value would be expected to be noticeably smaller, and certainly not larger, than values obtained from the other samples. According to the 'segregation' hypothesis, however, no such problem exists. Positrons are seen as undergoing reflection on approaching grain boundaries such that, once implanted into the Au, they always annihilate from delocalized states within the microcrystals. Their diffusive motion thus goes undetected. The possibility of such confinement is to some extent supported by the positive positron work function for Au (Mills 1983). In this alternative scheme, the observed  $S$  parameter variation in the 0–2 keV range is understood to be caused by positrons implanting into both Au microcrystals and surface segregated components such as (i) Ga (As), (ii) related oxide phases  $Ga_2O_3$  ( $As_2O_3$ ), (iii) possible AuGa phases or (iv) related grain boundary microvoids. As the positron implantation energy increases, so the fraction of positrons implanting into the Au also increases and the  $S$  parameter changes from that characteristic of the surface components to that characteristic of Au. In this scheme the lightly larger  $L_0$  value of the 300 Å sample finds a natural explanation since as seen by Chye *et al* (1978) at such coverages surface segregation may still be incomplete with surface components reaching further into the overlayer.

## 5. Conclusions

Depth profiling PAS measurements have been carried out on the as deposited Au/GaAs(110) system. The results show a definite 'interfacial region' that penetrates both the Au overlayer and the GaAs substrate. The high value of the observed  $S$  parameter in the interface region of the Au overlayer leads us to conclude that the positron is being trapped by open volume defects in this region. These defects are probably vacancies, although more complex structures such as vacancy agglomerates, and possibly As aggregates at Au grain boundaries cannot be ruled out. Since the depth of penetration of the defected region into the Au increases with coverage, a picture emerges of the density of defect causing agents (Ga and As) decreasing (approximately linearly) with distance from the interface, but with the total amount of dissolved Ga and As being in proportion to the Au coverage.

The observed penetration of the 'interfacial region' into the GaAs by at least  $\sim 100$  Å, while requiring confirmation by more accurate experimental data, is probably a real effect, and attributable to the dissociation of the GaAs lattice seen by others. Coupled with this is the observation, especially noticeable in our low-coverage samples, that the interfacial region has some structure localized around the ideal interface position and of  $\sim 100$  Å width. This we have associated with the region of intermixing or alloying seen in XPS and AES depth scans. Lifetime spectroscopy data taken on the same system indicate that positrons annihilating in this region probably do so from microvoids ( $\sim 10$  Å diameter), which are likely to be associated with grain boundaries bordering on the GaAs lattice. It has not been possible to rule out, however, that some of the PAS signal from this region may also originate from positrons trapped in substrate vacancies close to the interface, or from positrons annihilating from residual oxide phases.

The present work indicates that useful data on metal–semiconductor contacts can be obtained by using PAS depth scans in spite of the general complexity of these systems. The present investigation has employed a positron beam of relatively low intensity

( $4 \times 10^4 \text{ e}^+ \text{ s}^{-1}$ ) but it is clear that the higher-statistics data available from a higher-intensity beam would undoubtedly contribute to better depth resolution and thus to a clearer understanding.

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