Journal of Analytical & Bioanalytical Techniques

Vador, J Anal Bioanal Tech 2023, 14:4

Review Article Open Access

X - Ray Powder Spectroscopy Serves to Study the Metal-Semiconductor Interfaces

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Abstract

Interfaces in Al/Si, Au/Si, and Au/GaAs materials have been studied using variable-energy positron annihilation spectroscopy. To discover the kind of locations that positrons were likely to sample, Doppler broadening results were analysed using computational fits of the ROYPROF programme. The positron work function of these materials was brought into consideration after it was discovered that the interfaces were working as a capturing thin layer with insignificant positrons halted in them and that their properties stemmed only from positrons diffusing to these interfaces. The interfaces are all 1 nm thick and act as an absorbing sink for all thermal positrons that diffuse in their direction, according to all fittings. This either points to the presence of open volume flaws or to a flaw in the accepted theoretical models for positron affinities. Measurements made after applying external electric fields to an Al/Si sample are used to support the conclusion. The sensitivity of interfaces in these endeavours and their significance in data analysis and the creation of fitting cods have been well shown by theoretical fittings.

Keywords: Contact; Metal-semiconductor; Defects; Positron annihilation

Introduction

The majority of electronic equipment are connected using metallic cable that creates metal-semiconductor connections, which highlights the significance of metal semiconductor interfaces. Depending on how these connections interact with the semiconductor, their characteristics can vary greatly. The development of variable low-energy positron beams made it possible to perform depth-resolved analyses of the samples' near-surface and interfacial regions. At mean energies between 0.1 and 25 keV, which correspond to mean depths from the surface to several micro metres, controllable positrons are implanted into the materials. When being injected into a material, energetic positrons quickly collide with electrons in both elastic and inelastic collisions. It takes this process around 10 p seconds. The positron is then reduced to thermal energy through phonon scattering. The positron will annihilate with an energetic electron following some diffusion at these low velocities. Hence, the motion of the lattice electrons will be mostly responsible for the Doppler broadening of the two annihilation photons. However, positrons will sample a different distribution of electron velocities if they are caught in point defects like vacancies. This can be seen in the reduced broadening of the 511 keV photon spectra captured by germanium detectors [1,2]. The measurement of Doppler broadening associated with the mean electron momentum at the annihilation sites, which is commonly denoted by the single-number parameter S, in the analysis of annihilation gamma ray energy spectra provides information on atomic-scale structure. The central region of the annihilation peak's counts divided by the peak's overall counts is the definition of the Doppler broadening S-parameter. It is simple to identify areas of the sample where positrons are annihilated by studying the spectra, but only by fitting these data with a theoretical fitting can quantitative information and conclusions be drawn [3]. There are numerous studies of various positron interfaces in the literature, and the internal electric field linked to energy band bending is thoroughly investigated [4,5] through [6]. However, the discussion on the necessity of First-Principles calculations is gaining more attention in the modelling of interfaces [7]. Because the interaction of positrons with surfaces is difficult to characterise, interfaces and heterostructures are regarded as complicated systems that necessitate trustworthy computational modelling in order to comprehend recorded positron annihilation parameters. How to handle interfaces where theoretical fits of positron experimental results are necessary to gain accurate information is the driving force behind these investigations.

Experimental information

At ambient temperature and a base pressure of 105 Torr, 100-nm-thick Al or Au layers are thermally evaporated one at a time onto p-type Si (111) and n-type GaAs substrates, preparing each sample. The Si substrates were quickly dried, put into the vacuum chamber, and pumped down after being chemically cleaned with action and toluene, followed by an HF dip. The purpose of the HF treatment is to eliminate the typical oxide coating seen on silicon wafers. At Royal Holloway University of London, the samples were fed into the Herodotus positron beam sample chamber at various times. A high-purity Ge detector system recorded annihilation gamma energy spectra for each sample over the course of a half-hour for incident positron energies E ranging from 0.1 to 25 keV. Then, gamma spectra were obtained for each of the three external applied voltages (10 V, +10 V, and +45 V) while the sample aluminium on silicon structure was within the chamber. In order to establish reference parameters for the two substrates, annihilation spectra were also collected for the backs of the Si and GaAS samples.

Results

By dividing the sum of counts in 64 channels, which represent the entirety of the annihilation peak, by the sum of counts in 17 central channels, the S parameter was computed for each spectrum for all positron energies. Figure 1 displays the computed S parameter for the

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Received: 01-Apr-2023, Manuscript No: jabt-23-95295, **Editor assigned:** 03-Apr-2023, Pre QC No: jabt-23-95295(PQ), **Reviewed:** 17-Apr-2023, QC No: jabt-23-95295, **Revised:** 21-Apr-2023, Manuscript No: jabt-23-95295(R), **Published:** 28-Apr-2023, DOI: 10.4172/2155-9872.1000513

Citation: Vador P (2023) X-Ray Powder Spectroscopy Serves to Study the Metal-Semiconductor Interfaces. J Anal Bioanal Tech 14: 513.

Al/Si (MS) structure sample as a function of positron energy. It also displays a curve for the S parameter for bulk silicon (reference silicon), which was determined by examining the reverse of the same sample. The silicon's surface and bulk can both be observed in two distinct states. The film is represented by a distinct peak at low energy on the Al/Si MS structure curve, which is followed by the interface at roughly 5 keV. The Au film can be seen as the lower section of the curve in Figure 1 when S parameters for the Au/Si sample are plotted versus positron energy along with the curve of the bulk silicon. It depicts the variation of the S parameter in the Au/GaAs sample with respect to the positron energy. Four regions are distinguished: the new surface, the Au film (the lower part of S values), the interface (at about 9 keV), and the GaAs substrate. The GaAs rear side of the sample produced the top curve, which shows two states that are evident in accordance with the strong epithermal positron signal.

Analysis and discussion of data

The solid lines in Figure 1 show these fits. The S(E) data were fitted using the ROYPROF code [1] using the film, interface, and substrate model for MS structures and the two states model for reference bulk data. Since SiO2, which is always present on silicon wafers, has been removed by HF treatment, the data obtained for reference silicon in Figure 1 clearly show two states, surface and bulk. As the surface state is represented by the S parameter's lowest value, which is still lower than the value of bulk silicon, this can be explained by possible oxygen diffusion through the surface. The best fitting produced values for silicon's S surface, S bulk, and diffusion length of 0.46825, 0.49316, and 255 nm, respectively. The film, interface, and substrate positron annihilation parameters are combined to match the S-E curve for the Al/Si MS structure. The best fitting is generated when thin interface (1 nm) thick with no diffusion is performed; despite numerous tries taking into account various interface thicknesses with all potential diffusion within. Al layer's 60 nm diffusion length suggests potential positron diffusion from the film to its surroundings. Al film, the

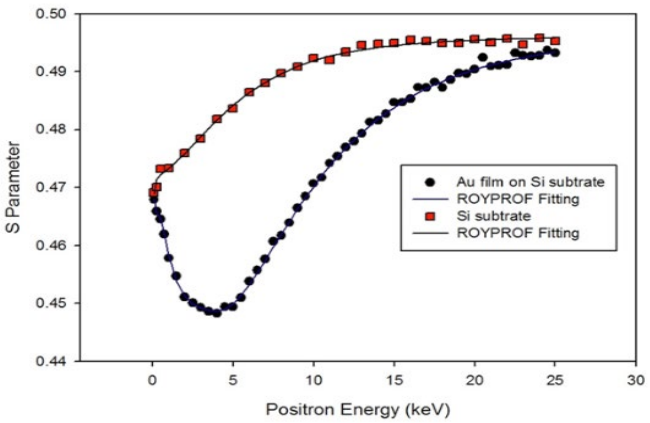

Figure 1: Modulation of the S parameter in the Au/Si sample and in the Si substrate as a function of positron energy (keV). The solid lines show where ROYPROF's data fits the data the best.

interface, and the bulk silicon all had values of 0.45785, 0.45824, and 0.49307, respectively. The interface's S value is lower than the silicon bulk's S value, which can only be explained by the presence of oxygen at the interface because trapped positrons tend to have higher S values than those from free positrons annihilating at the material bulk. For Au films coated on Si and GaAs, film thicknesses of 96 and 74 nm were produced. The discrepancy can be attributed to the nature of substrates in terms of morphology, conductance, and sticking coefficient even though the coating was carried out for the same amount of time and under comparable circumstances. Positron affinities of 6.24 eV and 7.90 eV for silicon and GaAs were reported, as well as 4.28 eV and 6.1 eV for aluminium and gold. Theoretically, and in accordance with Equation (4), thermal positrons are capable of diffusing at the interface in both directions.

Conclusion

The presence of positron absorption interfaces is shown by fitting studies of positron annihilation data of various metal-semiconductor architectures. These interfaces prevent thermal positrons that are diffusing randomly or under the influence of internal fields from crossing. Further experimental data obtained by adding external electric fields to one of the structures under consideration are consistent with this conclusion. Absorbing behaviour points to either the occurrence of open volume defects or a flaw in theoretical positron affinities models. This accomplishment aids in generating computer codes, integrating existing structures, and fitting microstructure data.

Competing Interests

The authors say they have no competing interests.

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