Appl. Sci. Converg. Technol. 25(5): 85-87 (2016)
http://dx.doi.org/10.5757/ASCT.2016.25.5.85

Research Paper

Positron Annihilation Study of Vacancy Type Defects in Ti, Si, and BaSrFBr:Eu

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Received July 27, 2016; revised August 20, 2016; accepted August 20, 2016

Abstract Coincidence Doppler broadening and positron lifetime methods in positron annihilation spectroscopy has been used to analyze defect structures in metal, semiconductor and polycrystal, respectively. The S parameter and the lifetime (τ) value show that the defects were strongly related with vacancies. A positive relationship existed between the scanning electron microscope (SEM) images and the positron annihilation spectroscopy (PAS). According to the SEM images and PAS results, measurements of the defects with PAS indicate that it was more affected by the defect than the purity.

Keywords: Positron annihilation spectroscopy, Defects, BaSrFBr:Eu, Ti, Si

I. Introduction

Silicon single crystals are the most perfect crystal in semiconductors available nowadays. Silicon wafers are widely used in many applications, such as space, IT chips, and radiation detection. Specially, silicon crystals have attracted because of many applications including photo solar cells. Purity of a single crystal silicon is very important to use in the industries. The accumulation of defects in crystalline silicon are extensively studied phenomenon [1,2].

Titanium has the two most useful properties of the metal. They are corrosion resistance and the highest strength-to-density ratio of the metallic elements. Titanium and its alloy structure are of great interested because of their wide range of applications in sollar cells and sensors as well as the aerospace industry [3,4].

Powdered crystalline BaFBr with Eu and related X-ray storage phosphors, such as polycrystal BaSrFBr:Eu, are favored for the production of image plates for digital X-ray imaging systems. Currently BaSrFBr:Eu is being used to produce image plates for radiography [5,6]. This results in a greatly reduced X-ray dose for patients.

Positrons are of interest in many fields of science and technology, including materials science [7] and medical technology [8]. A positron may penetrate the samples and this positron rapidly loses its high kinetic energy and then diffuses through the sample until annihilation. It is localized during diffusion by positron traps at the lattice defects. Positron annihilation spectroscopy [PAS] is a well-established technique to study the electronic structure and effects in materials [9-13]. PAS is a non-destructive technique for characterizing the porosity of materials. There are two favored PAS methods for defect measurements in solids. Doppler broadening positron annihilation spectroscopy (DBPAS) measures of the annihilated electron momentum distribution. DBPAS measure the gamma ray distribution that results from annihilation events of conduction band and core-level positrons and electrons. Because gamma ray characteristics are functions of the annihilation-site electron's momentum distribution and because electron momentum distributions in the region of lattice defects are different from corresponding distributions in defect-free regions of the crystalline layer, the shape of the spectrum changes as the defect concentration changes. When a positron annihilates with an electron, two photons are emitted with a total energy of 2 m0c2-Eb, where m0c2 is the electron's rest-mass energy and Eb is the binding energy of the electron.

Using two Ge detectors in coincidence Doppler broadening (CDB) positron annihilation spectroscopy detection of annihilation photons eliminates a high degree of background signals and yields a good signal to background ratio (~106); Thus, the momentum density distribution of the positron annihilation of the electrons can be extended over abroad area of the crystalline layer. Also, the CDB technique of positron annihilation has been applied to defect analysis [14-16], and recently found to be important in identifying the impurities found in defects [17-19]. Positron annihilation lifetime spectroscopy (PALS) is a well-established technique to study electronic structures and

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vacancy-like defects in materials. The lifetime at a vacancy is larger for an open volume. The measured positron annihilation lifetimes of a sample are linked to the sizes of the defects, and the relative intensities of the defects are related to their concentrations [20].

The aims of the present study are to analyze defects in titanium, silicon, and BaSrFBr:Eu samples and to describe the positron annihilation setup. The focus of this study is to investigate the relationship between defects and scanning electron microscope (SEM) in various samples. In this work, both the CDB positron annihilation and the positron annihilation lifetime techniques measured to characterize the vacancy defects.

II. Experimental

Obtained 2 single crystal (001) Cz-grown silicon samples (5'9), each 15×15×2 mm were fabricated, for preparation SEM and PAS. The obtained titanium 15×15×1 mm samples were grown with vacuum arc remelting (VAR) method. Purity of each titanium was about 99,995%. The sample, each 20×20×0.3 mm consisted of CR MD 4.0 (AGFA) image plates. These plates, which are used in hospital, contain BaSrFBr:Eu, which emits photons in the visible range of the electromagnetic spectrum. Surface morphology of all samples was characterized by SEM.

The positron source with the active area diameter of 9.53 mm, was 22Na with activity of 25 μCi, which was covered by a thin sheet (5 μm) of the nickel foil which was then folded. A positron source was sandwiched between two identical samples so that all positrons emitted would enter the samples. Coincidence events with the following conditions were selected: 2m0c2+0.8 keV ET 2m0c2+0.8 keV. These conditions allowed us to isolate the high-momentum component from the spectrum of positron annihilation. CDB yields a good signal-to-background ratio. Positron lifetime measurements for the samples were performed. The conventional Fast-Fast Coincidence method was used at room temperature, and FWHM Gaussian resolution is 170 ps, respectively. The gamma ray was measured with a Hamamatsu 3378 PMT. Since the positron thermal permeation goes deeper than 100 μm in the sample when you want to measure in this experiment, the effect of the thickness more than 300 μm of our samples can be ignored. After the source components and background were subtracted off , the spectra were well decomposed into one or two lifetime components. The lifetime spectra were analyzed using the program PALSFIT.

III. Results and Discussion

Fig. 1. shows the representative SEM images and the typical surface morphology of (a) Ti, (b) Sn, and (c) BaSrFBr:Eu. Indeed, as revealed by SEM, a sizeable number of cracks and voids leading to relatively porous surface, together with outgrowths at the junctions of the grains in the samples are apparent. The SEM micrograph of Ti and Si in Fig. 1(a), and Fig. 1(b) show that roughness of the surface exists. Ti sample looks more fine structure than Si. On the other hand, the SEM image of BaSrFBr:Eu in Fig. 1(c) presents significant large grains. The grains of the BaSrFBr:Eu sample shown in Fig. 1(c) are irregular, with a size of about 5-10 μm. BaSrFBr:Eu is expected to exhibit a component of vacancy clusters. Thus, vacancy clusters are assumed to have been formed in a produced by the polycrystal.

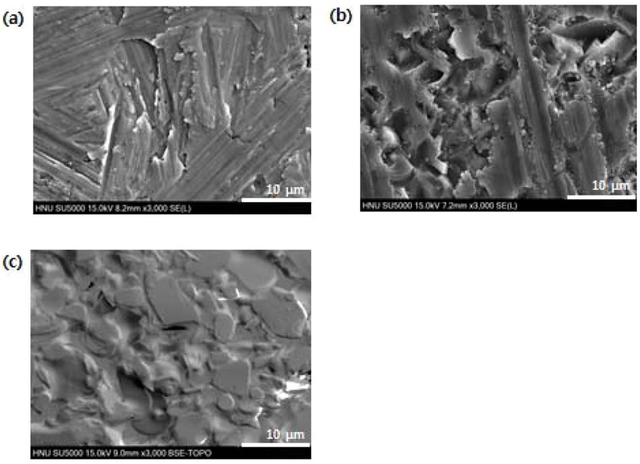

Figure 1. SEM photo micrographs showing specimens: (a) Ti, (b) Si and (c) BaSrFBr:Eu (bar=10 μm).

Table 1. S parameters, τ_1 and τ_2 lifetimes and the intensities, for Ti, Si and BaSrFBr:Eu.

Values Exposures	S. Parameter	Lifetime (ps)		(%)	
		τ_1	τ_2	I_1	I_2
Ti	$0.495 \pm 3.4 \times 10^{-4}$	138	338	94	6
Si	$0.519 \pm 3.5 \times 10^{-4}$	178	318	81	19
BaSrBr:Eu	$0.516 \pm 2.7 \times 10^{-4}$	167	415	57	40

Table 1 presents the relationship between the S parameter values of Ti, Si, and BaSrFBr:Eu. S value of Ti sample is lower than Si sample, because of the roughness, even though purity of Si is 5'9 sample. The annihilation characteristics of a positron in a medium are dependent on the local electronic properties at the site of the positron. The S parameter measurements were performed with a CDB to reduce the electronic background. Since positron annihilation spectroscopy is used to characterize atomic level defect structures in solids, the S parameter values increase in correlation with the increase in defects. The annihilation of positrons from a localized defect state is related to a significant change in the annihilation line shape. It is believed that the data of BaSrFBr:Eu indicates most of the defects generated by a component of vacancies and vacancy clusters. A defect model has been proposed by Gupta et al. [21], to explain the degradations. This model describes that the negative charges on the grain boundary are balanced by equal and opposite charges penetrating some distance into the grains. There are negatively charged ions at the grain boundary interface. This grain boundary defect model and the analogous band model are mentioned by Gupta et al. [21]. Positron will be annihilated with low energy ions. and the S parameter values are increasing. This includes both the vacancies and cluster defects are displayed at the size of the S parameter. Because image quality is important in patient diagnosis, it was measured in different ways, such as by using positron annihilation methods. To process the samples, we checked the S parameters of the sandwiched BaSrFBr:Eu layers with and without Fe sheets (with known density) in order to ensure that the positron beam had penetrated the BaSrFBr:Eu layer.

The positron lifetimes were measured at room temperature. The positron lifetimes and intensities for the Ti, Si, and BaSrFBr:Eu in Table 1, respectively. Table 1 shows the variation in lifetime and intensity of the short, bulk lifetime component ($\tau 1$, I1) and similar data for the trapped lifetime component ($\tau 2$, I2) [22,23]. For each sample, two lifetimes were resolved because two-component decomposition is possible in this case. The positron lifetime which is the inverse of the annihilation rate, is inversely proportional to the mean electron density experienced by a positron during its lifetime. The intensity indicates the fraction of annihilation taking place with a particular lifetime. The positron lifetime measurements are related to the type of defect present in the sample, a higher lifetime being an indication of larger vacancy type defects. The lifetime component $\tau 2$ has a value (300~400 ps) that is typical of positrons trapped in small open-volume defects and is comparable to the pressure of di-vacancies; on the other hand, the positron lifetime value of $\tau 1$ (140 ~180 ps) is related to mono-vacancies.

IV. Conclusions

Titanium, silicon, and BaSrFBr:Eu such as a metal, a semiconductor and a polycrystal material, were investigated by using SEM, CDBPAS, and PALS. Vacancies and clusters in Ti, Si, and BaSrFBr:Eu were studied systematically by the positron annihilation. S parameter of high purity Si is larger than Ti and BaSrFBr:Eu, because S parameter shows the direct evidence of the vacancies. The positron lifetime data for the samples are decomposed into two components (short and long lifetime). The short lifetimes (140~180 ps) for the samples are related with bulk mono vacancies, on the other hand, The long lifetimes (300~400 ps) related with the trapped lifetime component in the samples are vacancy clusters. The S parameter increments revealed that the increase in defects was caused by the roughness and multi-grains. Positron annihilation spectroscopy could be a non-destructive tool for measuring the porosity in the materials.

Acknowledgements

This work is supported by the 2016 Hannam University Research fund.

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