EXAFS Analysis of the Local Structure of Ge_xSi_{1-x} Thin Film Alloys

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Abstract. In this work we analyzed the local structure of Ge_xSi_{1-x} ($x = 0.5$ and 0.8) ultra thin film alloys deposited on silicon substrate. The local structural parameters for the thin films were compared to the values for a bulk sample. The coordination numbers for the thin films were similar to the value of a bulk sample but the interatomic distances were different. Also, the use of a germanium solid state detector was important for EXAFS analysis of ultra thin film alloys.

Keywords: XAFS, Local Structure, Ge-Si
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INTRODUCTION

Ge_xSi_{1-x} alloys have been extensively studied for the potential applications to microelectronic and optoelectronic devices with the characteristic band gap depending on their compositions [1, 2]. The state of Ge_xSi_{1-x} alloys are mostly a miscible solid solution and the structure varies sensitively with their composition. This is very important for the device application of these materials. Especially, the local structural ordering between Ge and Si atoms can give more direct information on the characteristic of these alloys. It has been reported that the Ge-Ge and Ge-Si bond length were different and vary linearly with alloy composition from the local structural analysis of the bulk materials [3]. Frequently, the properties can be changed at the limit value of the film thickness of alloys. We are interested in the variation of the local structure of these films for the device application. In this work we analyzed the local ordering and the local structure for the ultra thin films of Ge_xSi_{1-x} alloys in this work.

EXPERIMENTS AND EXAFS ANALYSIS

Ge_xSi_{1-x} alloy films were fabricated by co-sputtering of Ge and Si targets in an RF magnetron sputtering unit. The film was deposited on Si(100) substrate with 10 nm thickness and the composition was controlled by changing RF power of each target. The compositions estimated by energy dispersion spectroscopy (EDS) and Rutherford back scattering (RBS) were $x = 0.5$ and 0.8 in Ge_xSi_{1-x}, respectively.

EXAFS experiments were carried out at the beam line 3C1 EXAFS of the Pohang Light Source (PLS). A 13-element Ge detector has been installed in the fluorescence detection mode to enhance the sensitivity of the EXAFS signal. The energy range was near the Ge K-edge (11,104 eV) and the sample was placed at room temperature during the scan.

EXAFS data were analyzed by the combined technique of conventional [4, 5] and regularization [6] methods. The local structural parameters such as bond distances and the Debye-Waller parameters were estimated from the pair distribution function (PDF) determined by the regularization method.

RESULTS AND DISCUSSION

EXAFS measurements for ultra thin and diluted samples are extremely hard because of many systematic and unexpected noises. The small step due to the dilution of sample magnifies the experimental and unexpected noises. Also the diffraction peaks coming from the silicon substrate deteriorates the EXAFS spectrum. This is the main drawback of EXAFS measurement for thin films on a substrate. The Ge detector was very useful to reduce these noise significantly. Figure 1 shows the absorption spectra for 10 *nm* Ge_xSi_{1-x} ($x = 0.5$ and 0.8) ultra thin film alloys. As shown in Fig. 1, the EXAFS data are very clean in the range to be analyzed. The difference of the step is related directly to the different concentration.

The data quality can be compared more clearly in the EXAFS spectra. The EXAFS spectra were obtained from the absorption spectra by removing the background. Figure 2 presents the k weighted EXAFS spectra for $Ge_{0.5}Si_{0.5}$ and $Ge_{0.8}Si_{0.2}$. As shown in Fig. 2, the EXAFS spectra kept the good quality even in high k except several experimental noise. We can also see the

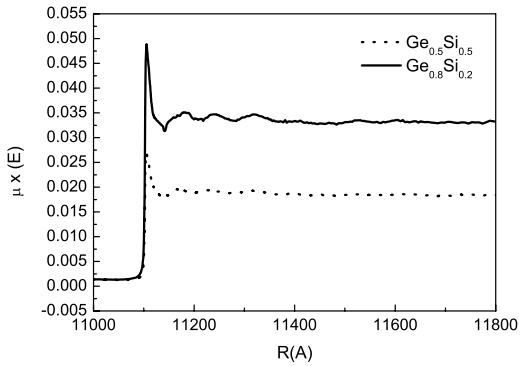

FIGURE 1. X-ray Absorption spectra of Ge_xSi_{1-x} thin films with the indicated compositions.

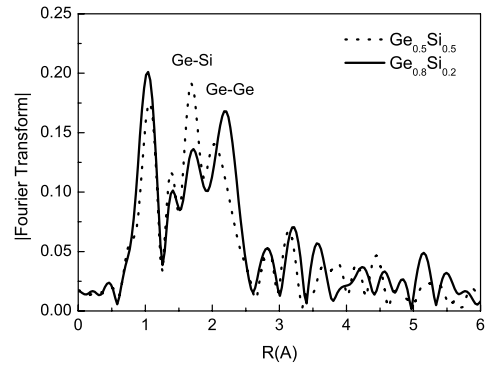

FIGURE 3. The Fourier transform of the EXAFS spectra of of Ge_xSi_{1-x} ($x = 0.5$ and 0.8) thin films.

compositional difference from the EXAFS spectra. As the Ge content increased, the phase difference increased in low k. This was expected because the reduction of Si content contributes mainly to the spectrum at low k.

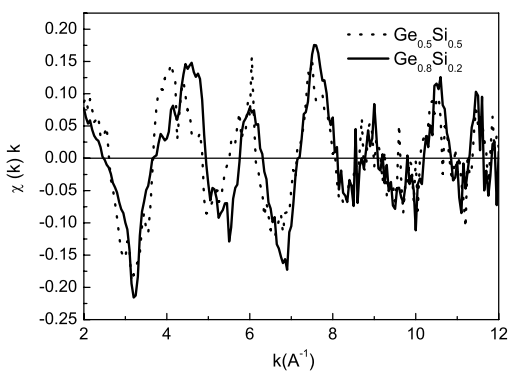

FIGURE 2. The k weighted EXAFS spectra of Ge_xSi_{1-x} thin films with the indicated compositions.

Figure 3 shows the Fourier transform of EXAFS spectra for $x = 0.5$ and 0.8, respectively. The transform range was $k = (2.2 - 12.0)\text{Å}^{-1}$ for both samples. As shown in Fig. 3, the magnitude of the Ge-Ge peak increased while the magnitude of the Ge-Si peak decreased as the concentration of germanium increased. This indicates that the number of Ge-Ge bonds increased at higher concentration of germanium, as expected. The higher shells, indicating the presence of long range order, disappeared for both compositions. The first peaks in the Fourier transform spectra caused by the instrumental noise were not considered for the analysis.

The combined Ge-Si and Ge-Ge shells were filtered by the inverse Fourier transform in the filtering range $r = (1.2 - 2.6)\text{Å}$.

Figure 4 shows the filtered EXAFS spectra with the indicated compositions. The filtered spectra show the clear difference in the local structure around Ge central atoms in $Ge_{0.5}Si_{0.5}$ and $Ge_{0.5}Si_{0.5}$ alloy films. The amplitude of the spectrum in $Ge_{0.8}Si_{0.2}$ thin film was higher that in $Ge_{0.5}Si_{0.5}$. This is due to the strong backscattering of Ge neighboring ions. The phase shifted to high k direction as the germanium concentration increased also indicates that the number of Ge-Ge bond increased.

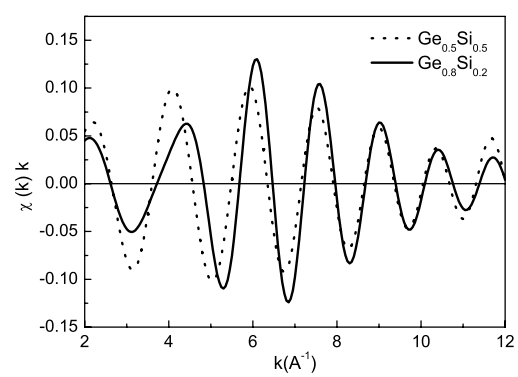

FIGURE 4. Inverse Fourier transformed spectra for Ge_xSi_{1-x} ($x = 0.5$ and 0.8) thin films.

The pair distribution functions and the local structural parameters were determined from the filtered EXAFS spectra by the regularization process with the split mode in which the kernels consist of two different kinds of atomic shells. The details have been described previously [6].

Figure 5 shows the unnormalized pair distribution functions for $Ge_{0.5}Si_{0.5}$ (dot line) and $Ge_{0.8}Si_{0.2}$ (solid line) films. As shown in Fig. 5, the width of the Ge-Ge pair is more narrow than for the Ge-Si pair. This indicates

TABLE 1. Local structural parameters for for Ge_xSi_{1-x} thin films with $x = 0.5$ and 0.8. R is the interatomic distance, and σ^2 is the Debye-Waller parameter.

Samples	N_{Ge-Ge}	R_{Ge-Ge} (Å)	$\sigma^2_{Ge-Ge}(\times 10^{-3}\text{Å}^2)$	N_{Ge-Si}	R_{Ge-Si} (Å)	$\sigma^2_{Ge-Si}(\times 10^{-3}\text{Å}^2)$
$Ge_{0.5}Si_{0.5}$	1.9 ± 0.2	2.52 ± 0.02	1.09 ± 0.05	2.1 ± 0.2	2.29 ± 0.02	2.21 ± 0.05
$Ge_{0.8}Si_{0.2}$	2.6 ± 0.2	2.47 ± 0.02	1.52 ± 0.05	1.4 ± 0.2	2.24 ± 0.02	1.35 ± 0.05

that the local ordering of germanium around germanium ion is more strong than the ordering of silicon.

The local structural parameters determined by the regularization method are shown in Table 1. The coordination numbers were 1.9 for Ge and 2.1 for Si for in $Ge_{0.5}Si_{0.5}$, respectively. These results are consistent with the values of bulk samples of $Ge_{0.43}Si_{0.57}$ in other work [3]. However, the Ge-Ge bond distance 2.52 Å is larger than that of bulk sample. The coordination numbers were 2.6 for Ge and 1.4 for Si for in $Ge_{0.8}Si_{0.2}$, respectively. The bond distances were 2.47 Å for Ge and 2.24 Å for Si. These values are not consistent with the bulk sample. The discrepancy will be related to the properties and characteristics of the ultra thin films.

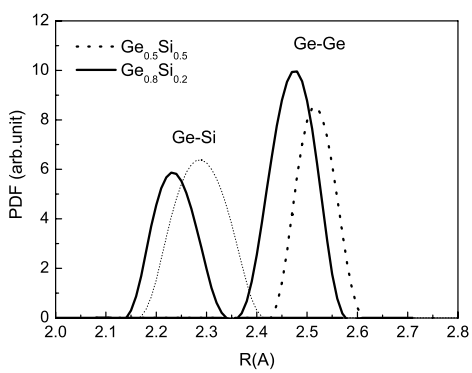

FIGURE 5. Pair distribution functions of Ge_xSi_{1-x} ($x = 0.5$ and 0.8) thin films.

CONCLUSION

In this work we analyzed the local structure of Ge_xSi_{1-x} (x=0.5 and 0.8) ultra thin film alloys deposited on the silicon substrate. The special detector was required to obtain the reasonable results for ultra thin films in the EXAFS study. Also, the combined technique of the conventional and the regularization was useful to obtain the pair distribution function and the local structural parameters such as the coordination number, bond distance and Debye-Waller parameters.

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