Extended Abstracts of the 21st Conference on Solid State Devices and Materials, Tokyo, 1989, pp. 509-512

S-E-5

Ge/Si Monolayer Superlattices on Si(100) Studied by Surface-Sensitive EXAFS

Hiroyuki OYANAGI, Tsunenori SAKAMOTO, Kunihiro SAKAMOTO,
Hirotaka YAMAGUCHI and Takafumi YAO

Electrotechnical Laboratory, Umezono, Tsukuba, Ibaraki 305, Japan

The local structure and electron states of Ge/Si monolayer superlattices epitaxially grown on Si(100) has been studied by surface-sensitive X-ray absorption fine structure in order to investigate the nature of strain-induced electron state and related optical transitions. The Ge_n/Si superlattices ($1<n<8$) prepared on a well-oriented Si(100) by MBE (molecular beam epitaxy) were studied using synchrotron radiation. We find that (1) the Ge-Ge bondlength in the superlattice relaxes and (2) there exists the substitutional disorder in the Ge layers along the [100] direction. A possible superlattice structure with a bulk-like Ge-Ge distance is ruled out. The relaxation in the momentum conservation due to the chemical disorder may enhance the amplitudes for the lowest indirect optical transition.

1. INTRODUCTION

Ge/Si strained-layer superlattices[1] exhibit unique optical properties which are absent in alloys with the corresponding composition. In particular, the origin of the lowest electroreflectance transition at 0.80 eV observed for Ge_4Si_4(100) superlattice[2] has been attracted much attention[3-6]. This transition has been interpreted as the indirect Γ_V-Δ_C excitation[3-5], while the other calculation assigned the strong 0.8 eV peak to the folded-in direct transition[6]. Previous calculations have been based on the chemically ordered superlattice structure with a strained Ge layer.

To further characterize the electron states of the Ge/Si superlattices which are dominated by strained Ge layer, the structural studies on a microscopic scale such as X-ray absorption fine structure (XAFS) is essential. This technique has been applied to the Ge/Si interface[7] and the short-range ordered structure has been confirmed for $n=1$[8]. In this paper, we report the results on the Ge_n/Si(100) superlattices ($n<8$) with an enphasis on the chemical disorder along the [100][9].

2. EXPERIMENTAL

Ge_n/Si monolayer superlattices were prepared on a well-oriented p-type Si(100) (4 ohm-cm) surface in an UHV MBE growth chamber with a base pressure of 1.3×10^{-7} Pa. After removing protective oxide layers by heating at 800°C, undoped buffer layers (2000Å) were grown at 500°C. A single-domain Si(100) 2x1 structure was obtained by annealing at 1000°C for 20 min. Si and Ge beams were obtained by a 2kW electron gun and a PBN Knudsen cell, respectively. Two-dimentional growth of Ge and Si layers were performed at 400°C monitoring the oscillation of RHEED specular beam intensity as previously reported.[7] After the Ge layer deposition, 20-22 ML's of Si were grown as a cap layer.

Surface-sensitive XAFS experiments utilized a fluorescence-detection technique and a total reflection geometry using horizontally focused synchrotron radiation from the 2.5 GeV storage ring at the Photon Factory. As a fluorescence detector, a Si(Li) solid state detector (SSD) was used to filter out the scattered photons and diffractions. Fluorescence signal and reflectivity were monitored as a function of a glancing angle at 12.3 keV so that the whole spectrum is measured within a total reflection geometry.

Invited by Symposium

3. RESULTS AND DISCUSSION

Figure 1 shows the RHEED intensity oscillations during the growth of Ge_6/Si superlattice taken from the [010] azimuth. One period of oscillation corresponds to the growth of monolayer. The RHEED oscillation during the growth of the Ge layer with T_S=400°C was observed for n<8.

Schematic of experimental set-up for surface-sensitive X-ray absorption fine structure is shown in Fig. 2. X-ray evanescent waves decay exponentially in the total reflection regime exciting only the surface region (100Å), which enhances the surface sensitivity

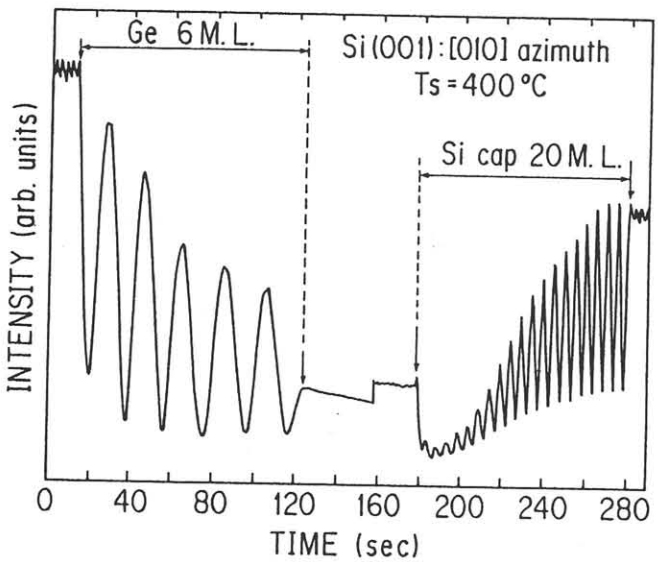

Fig. 1 RHEED intensity oscillations during the growth of Ge_n/Si superlattice (n=6).

by several orders. A typical fluorescence yield spectrum for Ge_6/Si superlattice is plotted in Fig. 3 where a high signal-to-background ratio is demonstrated.

In Fig. 4, the Ge K extended X-ray absorption fine structure (EXAFS) oscillations of Ge_n/Si superlattices are plotted as a function of photoelectron wavenumber k for (a) n=2, (b) n=4 and (c) n=8. The profile of oscillations changes from a Si-like to Ge-like pattern as the number of Ge layers increases. The backscattering amplitude of Si peaks at low k and falls off sharply with the increase of k, while that of Ge has

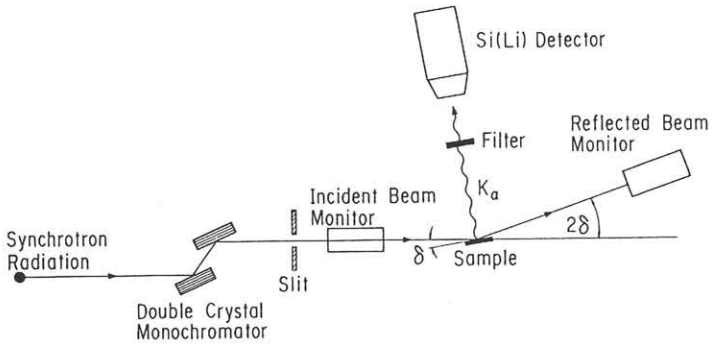

Fig. 2 Experimental set-up for surface-sensitive X-ray absorption fine structure measurement.

a maximum at k=6-7Å^{-1} and extends to k>15Å^{-1}. The change of profile thus indicates that the Ge-Ge bond increases with n.

If we neglect the chemical disorder along the [100] direction, the Si/Ge ratio is expected as 0.5 (n=2), 0.33 (n=4) and 0.14 (n=8). The EXAFS spectrum for n=2 indicates, however, that the Ge-Si bonds still dominate for n=2 in contradiction with the above estimation. Further, the EXAFS spectrum for n=2 sample is quite similar to the data for n=1[8]. These

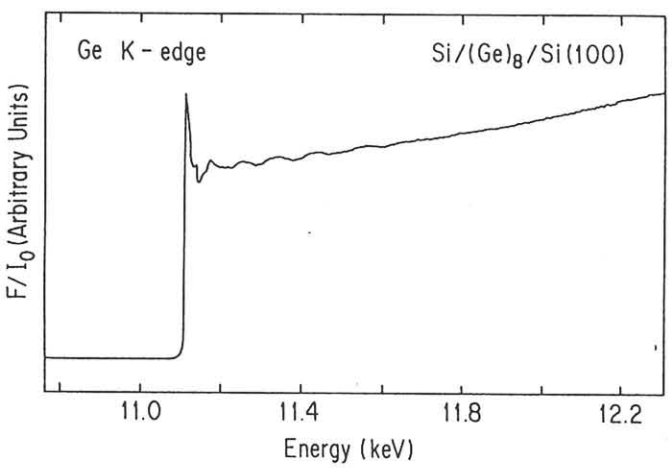

Fig. 3 Ge K fluorescence yield spectrum for Ge_8/Si monolayer superlattice plotted as a function of photon energy.

results indicate the presence of substitutional disorder along the [100] direction due to interdiffusion.

In Fig. 5, the results of Fourier transform of the Ge K-EXAFS oscillations are plotted for the Ge_n/Si superlattices with n=2, 4 and 8. The first peak position shifts to a larger R value while the peak intensity increases as n increases.

In order to match the Si layers in the plane of the interface, the Ge layers are strained to accomodate the lattice mismatch (5%) between Ge and Si, through both tetragonal deformation and bondlength relaxation. Experimentally, the Ge-Ge bondlength decreases as the Ge layers are strained, in agreement with the elastic energy minimization.[10]

On the other hand, the other calculation by Wong et al.[6] assumed a superlattice structure in which the

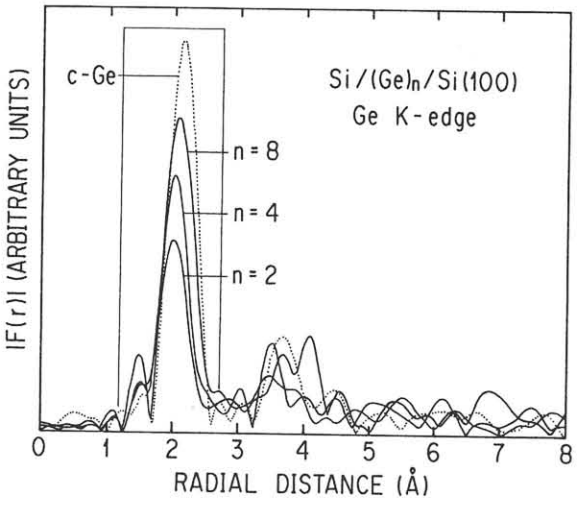

Fig. 5 Results of Fourier transform of the Ge K-EXAFS oscillations for the Ge_n/Si monolayer superlattices with n=2, 4, 8. Dotted lines indicate the results for crystalline Ge.

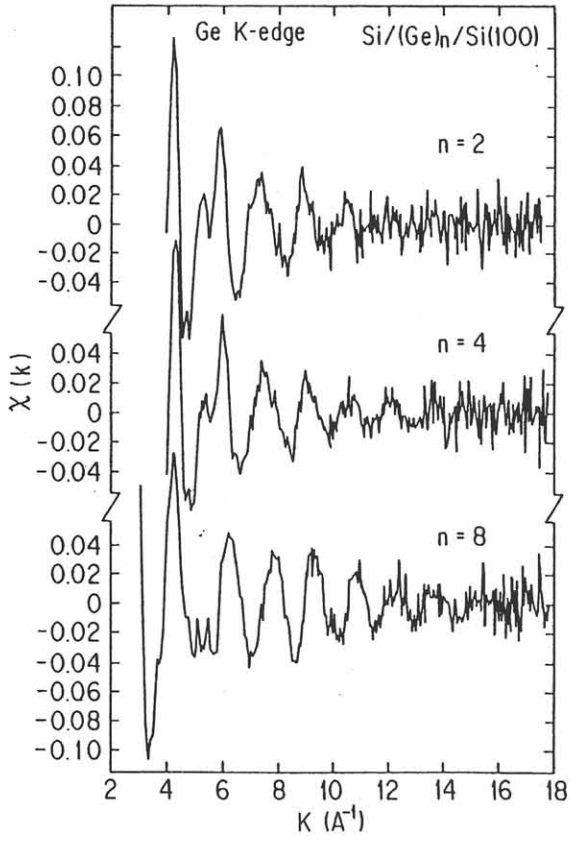

Fig. 4 Ge K-EXAFS oscillations of Ge_n/Si monolayer superlattices plotted as a function of photoelectron wavenumber k for (a) n=2, (b) n=4 and (c) n=8.

Ge-Ge bondlength of bulk Ge is conserved. However, the EXAFS results show that the Ge-Ge bondlength in the Ge_n/Si superlattices relaxes, ruling out a possible superlattice structure proposed by Wong et al.[6] However, the measured amplitudes of the lowest electroreflectance transition are much greater than the calculated intensities. The present results demonstrate that the chemical disorder exists along the perpendicular direction which relaxes the k-conservation rules along the [100] direction enhancing Γ-X mixing.

4. SUMMARY

The local structure and electron states of the Ge_n/Si (n<8) superlattices have been studied by surface-sensitive XAFS. We find that the Ge-Ge bondlength in the Ge_n/Si superlattices relaxes, i.e., the Ge-Ge distance is shortened, and there exists the substitutional disorder in the Ge layers along the [100] direction. A possible superlattice structure with a bulk-like Ge-Ge distance is thus ruled out. The relaxation in the momentum conservation due to the chemical disorder may enhance the amplitudes for the lowest indirect optical transition.

This work has been performed as a part of a project (Proposal No. 86-065, 87-065) approved by the Photon Factory Program Advisory Committee.

5. REFERENCES

1) J.Bevek,J.P.Mannaerts,L.C.Feldman, B.A.Davidson and A.Ourmazd; Appl. Phys. Lett. 49(1986)286.
2) T.P.Pearsall,J.Bevk,L.C.Feldman,J.M.Bonarand J.P.Mannaerts;Phys.Rev.Lett.58(1987)729.
3) M.S.Hybertsoen and M.Schluter,;Phys. Rev.B36,(1987)9683.
4) S.Froyen,D.M.Wood and A.Zunger;Phys. Rev. B37(1988)6893.
5) S.Satpathy,R.M.Martin and Van de Walle; Phys. Rev. B38(1988)13237.
6) K.B.Wong,M.Jaros,I.Morrison and J.P.Hagon; Phys.Rev.Lett.60(1988)2221.
7)K.Sakamoto,T.Sakamoto,S.Nagao,G.Hashiguchi, K.Kuniyoshi and Y.Bando; Jpn. J. Appl. Phys. 26(1987)666.
8)H.Oyanagi,T.Sakamoto,K.Sakamoto,T.Matsushita, T.Yao and T.Ishiguro;J.Phys.Soc.Jpn. 57(1988)2086.
9)H.Oyanagi,K.Sakamoto,T.Sakamoto,H.Yamaguchi,T.Ya o; in preparation.
10)C.G.Van de Walle and R.M.Martin;Phys.Rev. B34(1986)5621.