Si-Ge STRAINED LAYER SUPERLATTICES
H. Brugger, G. Abstreiter

To cite this version:

HAL Id: jpa-00226773
https://hal.archives-ouvertes.fr/jpa-00226773
Submitted on 1 Jan 1987

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
Si-Ge STRAINED LAYER SUPERLATTICES

H. BRUGGER and G. ABSTREITER

Physik-Department E16, Technische Universität München, D-8046 Garching, F.R.G.

Abstract

We report on growth and properties of Si/SiGe strained layer superlattices. Critical thicknesses and relaxation processes in single layers are studied with Raman spectroscopy, LEED, and TEM. Phonon Raman scattering is used to determine built-in strain and period length of superlattices. Transport measurements show mobility enhancement in selectively doped samples. The ordering of electronic bands due to strain yields to two-dimensional electron gases in Si.

Introduction

The proposal of periodic one-dimensional potential structures by Esaki and Tsu /1/ has initiated a vast amount of research activities on semiconductor superlattices. The artificial periodicity perturbs the band structure of the host material giving rise to narrow subbands in the conduction and valence band. Their energies are strongly affected by the thickness of individual layers resulting in a change of effective gap energy. This offers the possibility of tailoring the electronic and optical properties. Specific scientific and technological interest on strained-layer superlattices (SLS) has developed during the past few years. For thin layers the lattice mismatch of the two semiconductors involved can be accommodated by elastic deformation. The corresponding strain influences drastically the band line-up and acts as an additional parameter in band-gap engineering.

The combination of Si and Ge is very attractive due to the interesting possibility of the occurrence of a direct-gap superlattice made of indirect-gap host materials. The band-gap conversion was first discussed by Gnutzmann and Clausecker /2/ as a result of Brillouin-zone folding. The new superlattice periodicity is also reflected in the phonon properties as demonstrated by Brugger et al. /3,4/ for Si/Ge SLS.

The progress in Si-MBE made it possible to grow high-quality pseudomorphic multilayer structures Si/Si_xGe_1-x in the entire range of alloy compositions /5,6/. Si, Ge, and Si_xGe_1-x alloys have indirect band gaps, which were studied by optical absorption measurements /7/. There exists a large lattice mismatch between pure Si and Ge of about 4%. The lattice constant can be adjusted linearly with composition x between the values of the pure semiconductors. The fundamental band gap of bulk Si_xGe_1-x ranges from 0.66 to 1.12 eV and lies in the interesting range of optical fiber communication (1.3 - 1.55 μm). The possibility of monolithic integration of optoelectronic components on Si-ICs is a very stimulating prospective.

In this paper we first discuss the growth properties of lattice-mismatched Si_xGe_1-x overlayers on GaAs. Raman spectroscopy and LEED is used to determine the
critical thickness $h_c$ of single layers necessary to design appropriate commensurably grown SLS. The phonon structure is drastically influenced both by the built-in strain and the artificial period.

It is demonstrated that Raman scattering is an easy tool to determine quantitatively the stress inside the layers and the period length of SLS. These parameters are necessary in modeling band line-up and subband structure in the superlattice. The appearance of two-dimensional electron systems inside the Si-layers, as observed by Shubnikov-de Haas and cyclotron-resonance experiments /8/, can be explained consistently using the strain-effects on the band structure. The modification of the electronic band structure of ultrathin Si/Ge SLS yields to new optical transitions in the energy range below the Si band gap /9,10/.

Critical thickness and relaxation

SLS can be grown epitaxially on a substrate or on an appropriate buffer layer under adequate conditions. To achieve good electronic and optical quality, the active regions should be free of crystal defects like misfit dislocations. This is only possible if the individual layer thickness and the overall dimension of asymmetrical strained SLS remain below critical values which depend on the lattice mismatch. We briefly report on systematic studies of critical thicknesses of $\text{Si}_x\text{Ge}_{1-x}$ layers on GaAs (110) and Ge (110) surfaces. The difference in lattice constant between the overlayer and the substrate can be linearly varied in the range from nearly perfect lattice matching (Ge) to about 4% (Si). The lattice mismatch is elastically accommodated (biaxial stress) up to a critical thickness $h_c$ which depends strongly on $x$. $h_c$ is plotted versus lattice mismatch $f$ in Fig. 1, as determined by Raman scattering and LEED. The intensity of the LO-phonon in polar semiconductors, which is forbidden in first-order Raman back-scattering from (110) surfaces, turns out to be very sensitive to the creation of misfit dislocations close to the interface. The LO-intensity is proportional to the square of the electric field and consequently directly related to the band bending in GaAs close to the interface. This light scattering technique, which is called electric-field-induced Raman scattering (EFIRS), is described in more detail in Ref. /11/. EFIRS appears to be an excellent optical tool.

Fig. 1: Critical thickness of lattice mismatched $\text{Si}_x\text{Ge}_{1-x}$ overlayers on (110) GaAs

Fig. 2: High resolution TEM micrograph of a relaxed $\text{Si}_{0.5}\text{Ge}_{0.5}$ film on (110) GaAs. Misfit dislocations are indicated by arrows.
to study the band bending behaviour at the interface of semiconductor heterojunctions /12,13/ as well as to determine critical thicknesses of GaAs/Si<sub>x</sub>Ge<sub>1-x</sub> mismatched systems /14/. The experimental values of \( h_C \) are given by full dots in Fig.1. Due to the absorption of light critical thicknesses in Si<sub>x</sub>Ge<sub>1-x</sub> can only be detected if \( h_C < 200 \, \text{Å} \) or \( x < 0.4 \).

Low energy electron diffraction (LEED) has been used to get information about the change of the lateral surface lattice constant. This is observed as a shift of the LEED-spots, which can be determined easily to an accuracy of about 0.3% by analyzing the data with a vidicon camera /15/. LEED-measurements yield information about \( h_C \) from \( x < 0.2 \) up to \( x = 1 \) provided that the overlayer is of good crystalline quality. The corresponding \( h_C \)-values are given by open circles in Fig. 1.

The critical layer thickness of lattice mismatched overlayers has been calculated for example by van der Merwe on the basis of a balance between interfacial energy \((E_I \sim f)\) and areal strain energy density associated with a film of thickness \( h \) \((E_H \sim h^2)\) /16/. Such theoretical predictions are given by the solid line. The equilibrium theory results in rather low values of \( h_C \) compared to the experimental points. A reason for this underestimation is probably the neglect of an activation barrier for the generation of misfit dislocations in v.d. Merwe's theory.

Apart from the critical thickness \( h_C \) of single layers there exists another critical length \( h_{LS} \) which arises from the overall thickness of asymmetrically strained superlattices, even if the individual layers \((1,2)\) are thinner than \( h_C \). \( h_{LS} \) is found to be determined approximately by the weighted average strain in the whole structure /17/. Experimental values of \( h_{LS} \) from Si/Ge SLS are discussed in Ref. /10/.

To get information on the type of misfit dislocations we have studied strained overlayers with thicknesses above \( h_C \) by transmission electron microscopy (TEM)/18/. Fig. 2 shows the lattice-image of a GaAs (110)/Si<sub>0.5</sub>Ge<sub>0.5</sub> heterojunction. The film thickness of the alloy layer is well above the critical value \( h_C \). The Si<sub>0.5</sub>Ge<sub>0.5</sub> overlayer is of good crystal quality. Additional [111] planes, however, appear inside the film. This corresponds to a 60° mixed dislocation with slip vector parallel <110> lying in a {111} plane. The straight dislocation lines stop at the interface as marked by arrows. Due to the lattice misfit a high number of dangling bond states along the dislocation lines are generated close to the interface. The expected density increases with larger misfit \( f \) up to \( 7.4 \times 10^{13} \, \text{cm}^{-2} \) in the case of pure Si on GaAs (110).

The growth of several Si<sub>x</sub>Ge<sub>1-x</sub> films with different compositions on GaAs (110) has also been studied by phonon Raman spectroscopy. Typical spectra of thin Si<sub>0.5</sub>Ge<sub>0.5</sub> films are shown in Fig. 3. The mismatch is about 2%. The spectra were measured in situ, during growth. The corresponding thickness of the overlayer is given in Ångstroem. Si<sub>x</sub>Ge<sub>1-x</sub> alloys show a three-mode behaviour /19/. The evolution of these modes can be clearly seen in Fig. 4. The optical phonon of the GaAs-substrate is attenuated due to increasing light absorption with growing overlayer thickness. There is a characteristic shift in frequency for commensurate, i.e. elastically strained layers. The relaxation process appears as a continuous shift in phonon energies up to the values of unstrained material indicated by arrows. The strain relaxation is a gradual process completed for film thicknesses larger than 2000 Å in the case of Si<sub>0.5</sub>Ge<sub>0.5</sub>. There is, however, some evidence for a small residual strain even for large film thicknesses \( h > h_C \) /20/. Raman scattering allows a quantitative determination of built-in strain or corresponding stress. It averages the strain distribution over the layer thickness and the area of the used laser spot.

Systematic investigations of the strain-induced shift of phonon frequencies of Si<sub>x</sub>Ge<sub>1-x</sub> alloy layers are shown in Fig. 4 for \( 0 < x < 0.8 \). All three modes of the alloy films decrease monotonically with increasing \( x \). The downward shift is characteristic of tensile biaxial strain \( \epsilon = (a - a_0)/a_0 \) with \( a \) and \( a_0 \) being the in-plane lattice constant under strain and the intrinsic lattice constant of the film, respectively. The Si-Ge related mode vibration shows a nearly linear behaviour with strain. The frequency shift can be used to measure built-in strains quantitatively. A linear fit to the experimental values yields \( \Delta \omega = -8.82 \, \text{cm}^{-1} \epsilon(\%) \) for films under tensile biaxial strain grown on (110)-surfaces. The shift has opposite sign and is nearly twice as large as for Si<sub>x</sub>Ge<sub>1-x</sub> under biaxial compression grown on (100) Si surfaces as determined by Cerdeira et al. /21/.
We have also studied the phonon behaviour of ultrashort period superlattices. They were grown using MBE at a substrate temperature of 450°C and consist of 15 periods of several monolayers Si and Ge. Spectra of samples with different period length \( d = d_{\text{Si}} + d_{\text{Ge}} \) are shown in Fig. 5. The periodicity along the growth direction causes a Brillouin-zone folding and the appearance of new gaps in the phonon spectra. Doublet modes observed below 100 cm\(^{-1}\) correspond to folded LA modes. The dispersion curve of these modes can be measured \( /4/ \) and analyzed with a layered elastic continuum model \( /24/ \). The energetic positions of the back-folded modes shift to higher values with decreasing period length \( d \) as clearly seen in Fig. 5. By comparing the frequencies with calculated energies this can be used to determine accurately the period of superlattices \( /3/ \).

The peaks at higher energies (> 200 cm\(^{-1}\)) in the spectra correspond to optical phonons in the SLS. The dispersion curves of Si and Ge do not overlap in frequency. Therefore confined modes in each layer are expected (phonon quantum wells). They show up as shoulders in the Si and Ge phonon peaks as indicated by arrows. First order Raman spectra of pure Si and pure Ge exhibit a single peak at 525 cm\(^{-1}\) and at 305 cm\(^{-1}\), respectively. The strain-induced shift in energy of the Si-phonon is larger in samples 4/11 and 3/9 which were grown on a Ge(110) buffer layer compared with sample 6/11 grown on a Si\(_{0.25}\)Ge\(_{0.75}\) buffer layer. In this case also the energy of the Ge-phonon is shifted to higher energy in these layers. Caused by the finite penetration depth also the phonon structure of the buffer layer is seen (denoted by P). In addition, an interface mode (IF) is observed in between the Si and Ge modes.

The Raman spectra directly prove the possibility of growing high quality Si/Ge SLS with sharp interfaces and individual layer thicknesses of only a few monolayers. First experiments indicate new optical transitions in the energy range of about 0.7 - 0.9 eV \( /10/ \). Such energies are expected for the fundamental gap of these SLS with staggered band line-up making optical transitions indirect in real space.
Electronic transport properties have been studied in Si/Si$_{0.75}$Ge$_{0.25}$ SLS grown on Si substrates. In such samples the sign of the strain in the SiGe alloy layers is reversed. The arrangement is shown in Fig. 6. Two types of buffer layers have been used. Superlattices grown on Si are asymmetrically strained. This can be seen directly in the corresponding Raman spectrum shown in Fig. 6. The Si phonon mode of the 60Å thick layers appears at the energy as expected for unstrained bulk Si (64.5 meV). The three SiGe related modes on the other hand are shifted upwards due to biaxial compressive strain. Using a Si$_{0.75}$Ge$_{0.25}$ buffer layer leads to a smaller shift of the alloy modes. In addition, the Si mode is shifted downwards by about 1 meV for this sample. This shows the strain symmetrization in SLS grown on an Si$_{0.75}$Ge$_{0.25}$ buffer layer, whose lattice spacing lies just in between those of Si and Si$_{0.5}$Ge$_{0.5}$. The strain distribution has a strong influence on the conduction band offset, which is reflected directly in the transport properties of selectively doped samples. Successful experiments on mobility enhancements have been reported for two-dimensional electron and hole gases /8,22/.

Hall mobility, Shubnikov-de Haas oscillations, and cyclotron resonance were studied with a series of symmetrically strained Si/Si$_{0.5}$Ge$_{0.5}$ superlattices. The samples are doped selectively with Sb by secondary implantation /25/. The position of the Sb doping spike was varied with respect to the Si/SiGe layer sequence. The temperature dependence of the mobility and the measured peak value at $T = 20$ K is shown in Fig. 7. Enhanced mobilities are observed when the Sb-dopants are situated inside the SiGe layers. These samples show a monotonic increase of the mobility with decreasing temperature and saturation at low temperatures. These observations have been explained by the formation of 2D electron gases in the Si layers which are spatially separated from the charged donor impurity atoms. The two-dimensional behaviour of the carriers and the confinement in Si has been further confirmed by the angular dependence of the Shubnikov-de Haas effect and by cyclotron resonance experiments. A strain induced lowering of the Si conduction band was suggested on the basis of these experiments /23/. Careful measurements with selectively doped superlattices grown directly on Si indicate that the conduction band edges are approximately equal when Si is unstrained /26/. Built-in tensile strain in the Si layers can lower the two-fold degenerate conduction band minima (heavy

![Fig. 5: Raman spectra of Si/Ge SLS](image)

![Fig. 6: Schematic diagram of the sample structure and phonon spectra of Si/SiGe SLS](image)
mass normal to the (100) layer planes) by a few hundred meV, which favours electron confinement in the Si layers. The valence band edge is always much higher in the SiGe or Ge layers. The band offsets have been confirmed theoretically by self-consistent subband calculations /27/ and by band structure calculations /28,29/. The situation can be summarized in the following way: For unstrained Si and compressively strained SiGe the conduction band offset is very small throughout the whole range of compositions. With increasing tensile strain present in the Si layers a staggered band line-up appears with the conduction band edge much lower in Si. This is shown schematically in Fig. 8.

First applications of Si/SiGe SLS appeared already in the literature. The effect of band gap narrowing due to strain has been used for waveguide avalanche photodetectors with separate absorption and multiplications as discussed by Luryi et al. /30/.

The successful fabrication of n-channel MODFETs was recently reported by Dambkes et al. /31/, which was achieved by selective Sb-doping of a Si/SiGe/Si heterostructure as discussed above. There is also first evidence for new optical transitions in ultrashort period Si/Ge superlattices /9,10/. A clear experimental manifestation of the transition from indirect gap to direct gap semiconductor in such novel strained layer superlattices is, however, still lacking.

Acknowledgements

We thank E. Kasper, H.J. Herzog, and H. Jorke for providing part of the samples and for many stimulating discussions. We are also grateful to J. Mazur, H. Oppolzer, and H. Cerva for performing the TEM-experiments.
References:

/1/ L. Esaki and R. Tsu, IBM Res. Note, RC-2418, March 1969
/5/ E. Kasper, Surf. Sci. 172, 630 (1986), and references therein
/7/ R. Braunstein, A.R. Moore, and F. Herman, Phys. Rev. 109, 695 (1958)
/10/ K. Eberl, G. Krötz, R. Zachai, and G. Abstreiter, this conference
/16/ J.H. Van der Merwe, Journ. Appl. Phys. 34, 123 (1963)
/18/ H. Oppolzer, this volume
/29/ I. Morrison, M. Jaros, and K.B. Wong (to be published)
/30/ S. Luryi and F. Capasso, in Ref. /23/, p. 140