Extended Abstracts of the 1993 International Conference on Solid State Devices and Materials, Makuhari, 1993, pp. 962-963

High Resolution X-ray Triple Axis Diffractometry of Short Period Si_mGe_n Superlattices

E.Koppensteiner+, G.Bauer+, V.Holy*, and E.Kasper#
+ Johannes Kepler Universität, Altenbergerstr.69, A-4040 Linz, Austria,
Tel.:0043 732 2468 9601, Fax: 0043 732 2468 822
* Masaryk University, 61137 Brno, Czech Republic
# Daimler Benz AG Research Center, D-7900 Ulm, Germany

We present a novel x-ray diffraction method suitable for a precise analysis of strain, strain gradients and for an estimation of mosaicity in complex multilayer structures, which is used to analayze MBE grown short period Si_mGe_n superlattices (SL´s, m and n number of monolayers). Recently substantial progress has been achieved in the growth of strained Si/Ge heterostructures: through the use of thick graded SiGe alloy buffers the number of threading dislocations was shown to be reduced by several orders of magnitude in comparison to heterostructures grown on about 200 Å buffers with constant Ge content. The strain symmetrized Si/SiGe structures and Si_mGe_n SL´s grown on the graded alloy buffers have also superior electronic porperties as evidenced e.g. by the observation of efficient photoluminescence as well as electroluminescence, even at room temperature [1]. We have recently shown [2] that by the use of triple axis x-ray diffractometry, which allows the determination of the diffusely scattered intensity distribution around reciprocal lattice points, the strain status of the buffer and of the SL layers can be directly obtained with higher precision than previously possible with double crystal diffraction methods.

In the refined buffer concept on top of the graded alloy buffer B1 a further SiGe alloy buffer B2 is deposited, which should have a constant Ge content corresponding exactly to the mean Ge content of the stack of SL layers in order to achieve the goal of a freestanding SL. We report on structural studies on several Si_6Ge_4 and Si_9Ge_6 short period SL´s, which were used for the luminescence studies reported in [1] as well, employing the novel triple axis diffractometry. For the measurements a Bartels type four crystal monochromator was used in the primary beam, whereas in the secondary beam either a slit with an opening angle of *180 arcsec* (conventional double crystal (DCD)technique) or a two reflection Ge (220) channel cut analyzer crystal (triple axis diffractometry (TAD) optics: detector opening angle:*12 arcsec*) was employed. In order to obtain reciprocal lattice maps, $\omega/2\Theta$ scans (i.e.: in direction radial from the origin of the reciprocal lattice(000)) are performed for different ω offsets (i.e.:transverse, along a circle with center (000),[2]). In the following we demonstrate the method of reciprocal space mapping on three nominally identical Si_9Ge_6 superlattices (samples A,B, and C, the SL part of which is grown at 500°C,470°C and 450°C,100 periods, B1: step graded buffer with Ge content increased stepwise by 3% per 50 nm up to 650 nm, followed by buffer B2 nominally 40% Ge content, 550 nm thick, prior to growth of the SL one monolayer of Sb is deposited) by comparing TAD with DCD measurements (Figs.1a: periods of the SL´s A,B,and C from the DCD and TAD $\omega/2\Theta$ scans: 22.02Å, 23.57Å and 23.96Å). Already in single $\omega/2\Theta$ scans, the higher resolution offered by the TAD method allows to differentiate between the diffraction peak originating from the (004) Bragg reflection from the buffer B2 and from the main superlattice peak SL0, even for slight differences in the mean Ge content and strain status of the SL layers in comparison to the buffer B2 (Fig.1b). Furthermore, reciprocal space maps around the (004) and (224) reflections are used to determine independently the in plane lattice constants a_p of the buffer B2 and of the SL as well as the lattice constants along growth direction a_n (Fig2). Mere inspection of the relative positions of the extrema of the reflections from the Si substrate, the buffer B2 and the main SL peak SL0 in the (224) reciprocal lattice map (Fig.2,rhs) indicates that not only the mean Ge content of the SL #C is different from that of B2. B2 is nearly fully relaxed, however, since the center of SL0 does not coincide with the line ||[224] through the Si substrate reflection maximum, the whole SL stack is under slight biaxial compression (see Tab.I). The centrosymmetric shape of the intensity contours around the extrema proves that no strain gradient is present in the SL #C. No information on elastic constants is necessary for the exact determination of the strain status and *no assumptions* on the degree of relaxation or on the thicknesses of the constituent layers have to be made. Results are listed in Table I (where $\varepsilon_{p,n}$ denote in-plane strains and strains in growth direction; the precision of the lattice constant determination is ± 0.0003Å). We want to point out that for the strain analysis just the positions of the intensity extrema in the reciprocal lattice maps are needed.

In addition we use the whole distribution of the diffusely scattered intensity in the reciporcal space maps for the buffer and superlattice peaks B2 and SL0 to obtain further information on the defect structures present in these layers. This method can be applied for sample C, where the reciprocal lattice points from B2 and SL0 are fully separated. The correlation function G of the random deformation field due to structural defects is calculated directly from the isointensity contours. The approach is similar to the Patterson analysis well known from statistical optics. In a first step a mosaic block model, which contains the mosaic

block size 2R and the relative block tilting Δ as independent statistical parameters, has been used to estimate the defect structure (Fig.3 shows G and simulation for (004) SL0 in sample C: 2R=310 nm, Δ=370 arcsec).

We show, that the novel method of triple axis diffractometry gives precise information on the strain status and the degree of relaxation in complex multilayer structures, especially in the case of overlapping Bragg diffraction peaks from nearly freestanding, strain-symmetrized Si_mGe_n short period superlattices and from underlying buffers. Furthermore, the reciprocal space maps yield the shape of isointensity contours of scattered radiation, from which - to our knowledge for the first time for Si/Ge structures - information on the correlation function of the deformation field due to structural defects is obtained. The latter can be expressed in terms of two statistical parameters assuming a certain defect model.

[1] J.Engvall et al.Appl.Phys.Lett., in print; J.Olajos, SiMBE-5, invited paper.
[2] E.Koppensteiner et al. Appl.Phys.Lett. **62**, 1783 (1993).

Tab.I.: Structural parameters, strains and relative thicknesses of samples A,B and C.

sample	layer	a_p(Å)	ε_p(SL)	a_n(Å)	ε_n(SL)	m,n	xGe
A	Si	5.509	0.0144	5.371	-0.0111	9.18	0.386
	Ge	5.509	-0.0263	5.770	0.0198	5.82	
	B2	5.509	-	5.526	-	-	0.386
B	Si	5.502	0.0131	5.376	-0.0101	9.30	0.380
	Ge	5.502	-0.0275	5.775	0.0207	5.70	
	B2	5.501	-	5.519	-	-	0.370
C	Si	5.503	0.0132	5.375	-0.0103	9.15	0.385
	Ge	5.503	-0.0274	5.774	0.0205	5.85	
	B2	5.502	-	5.518	-	-	0.370

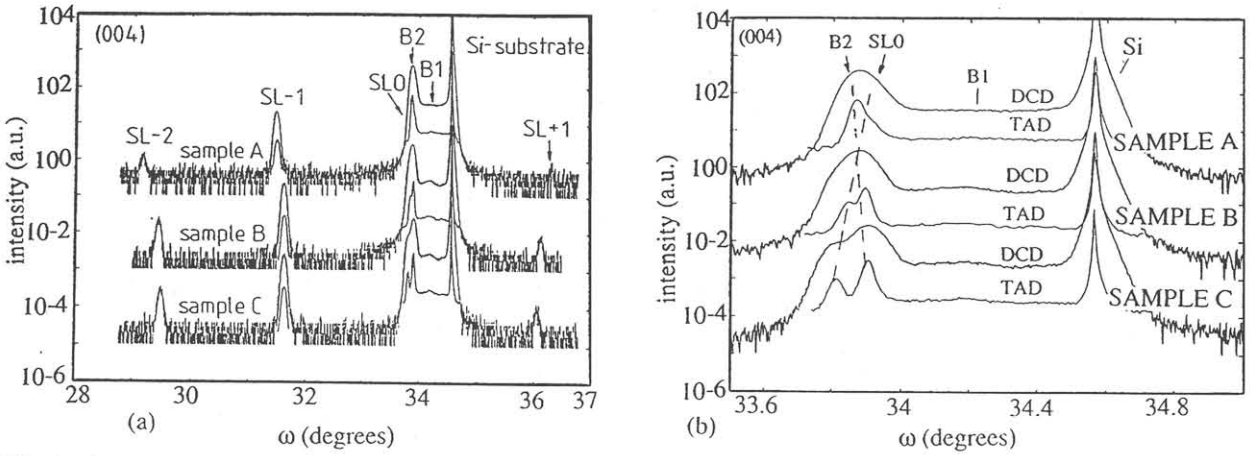

Fig.1: Double crystal and triple axis (underneath DCD) single (004) ω/2Θ scans of samples A,B and C.

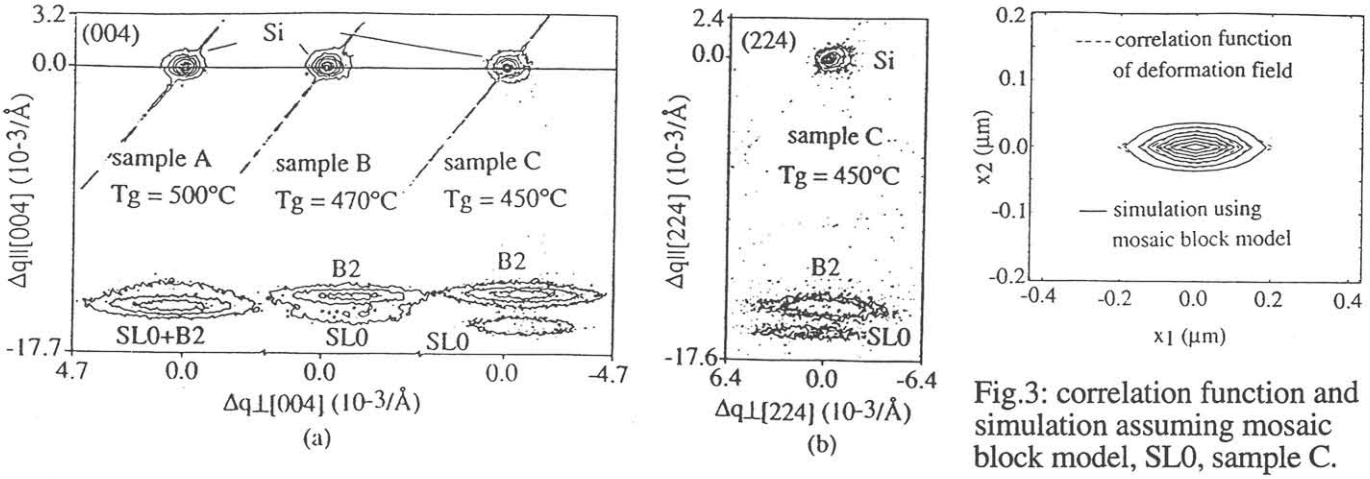

Fig.2: Reciprocal space maps around (004) (a) and (224) (b).

Fig.3: correlation function and simulation assuming mosaic block model, SL0, sample C.