The Structure of Si/Ge Superlattices

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Heterostructures based on Si and Ge, deposited on (100) single crystalline Si substrate, using the Molecular Beam Epitaxy (MBE) deposition method, were analyzed by means of x-ray diffraction techniques. In this work, it were investigated different Si/Ge heterostructures, built by a superposition of two structures: (i) an internal one with a period R, formed by Si-Ge bilayers, and (ii) another with a larger periodicity D, formed by six of the former Si-Ge bilayers spaced by a Si buffer layer, whose function is to decrease the stress due to the difference in Si and Ge lattice parameters. The x-ray diffraction experimental results were computer simulated by means of kinematical and dynamical x-ray diffraction theories. The kinematical approach presented a better agreement between experimental data and simulation than the dynamical calculations. The structural parameters were obtained by at least two independent experimental data and compared with the nominal values. The superlattices with good structural properties are easily identified with this methodology, which is a non-destructive technique.

Introduction

The Molecular Beam Epitaxy (MBE) deposition method allows the growth of monolayers in atomic scale with composition control, provided a precise adjustment of the deposition parameters. Nevertheless, it is demanding to verify the real obtained structure, which requires sample's characterization after the deposition procedure. Among the non-intrusive characterization methods, x-ray diffraction has been used currently [1]. In particular, the study of superlattice's structural properties is easily accomplished by means of conventional x-ray diffraction rocking-curves, which give the relevant structural parameters: superlattice mean period, perpendicular and in- plane lattice parameters, structural strain and interface properties [1].

The epitaxial growth of heterostructures, with lattice parameter match between different semiconductor materials, were obtained in the 1970 decade [2-4], but the best use for those new materials was reached by the engineering of heterostructures with lattice parameters mismatch, i.e., the so-called strained superlattices [5-12].

Considering that the number of possibilities of combining different semiconductor materials is very large, the best strategy is to find out materials whose technology of fabrication is well developed. There is no question about the fact that silicon is the natural candidate. Among the elements that Si has crystallographic and chemical compatibility, germanium, whose lattice parameter is 4.2% larger than the Si lattice parameter, is the element that presents more similarity with silicon properties. The aim of this paper is to analyze, experimentally and theoretically, this type of structure.

Experimental

The x-ray diffraction characterization of the Si/Ge superlattices analyzed in this work were performed in two different setups: (i) a powder diffractometer at low and high angles (θ-2θ geometry) and (ii) a double crystal diffractometer (rocking- curve). Monochromatic Cu Ka radiation was used in the angular region of $2\theta \approx 1^o - 80^o$. Two samples, named JF3 and JF5, were deposited at the A.T.&T. Laboratory (N.J., USA) and studied in this work. These heterostructures have a common type of configuration, which is built by a superposition of two structures: (i) an internal one with

a period **R**, formed by Si-Ge bilayers, and (ii) another with a larger periodicity **D**, formed by six of the former Si-Ge bilayers spaced by a Si buffer layer, whose function is to decrease the stress due to the difference in Si and Ge lattice parameters. The whole system is repeated ten times. The thickness of the Si-Ge structure varies from 5 to 7 monolayers, while the Si spacer is around 360 monolayers. The nominal deposition parameters for both samples are given in Table 1.

Table 1 n_{Ge} , n_{Si} and n_{buff} are, respectively, the number of Ge, Si and buffer monolayers, R is the mean period of the internal Si/Ge superlattice, p is the number of periods of the superlattice with period R, G is the thickness of the Si buffer spacer, D = G + pR, and M number of periods with mean period D.

Sample	n_{Ge}	n_{Si}	n_{buff}	R(Å)	p	G(Å)	D(Å)	M
JF3	5.1	5.8	221	15.1	6	300.0	390.6	10
JF5	5.1	7.1	361	16.9	6	490.1	589.6	10

Results and discussion

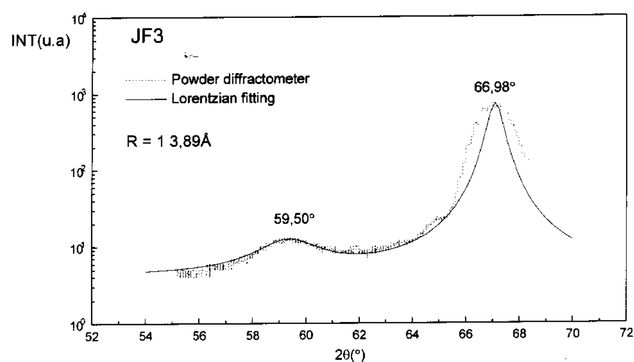
Figs. 1 presents the high angle diffractograms of samples JF3 and JF5. The data were fitted by Lorentzian functions, such that the angular position and intensity of each peak were precisely determined. Figs. 2 and 3 shows the comparison between experimental data and theoretical calculations for samples JF3 and JF5, respectively. Table 2 presents the R and D values and Table 3 shows the comparison between nominal structural parameters and those obtained from the simulation of the experimental data with the dynamical theory of x-ray diffraction.

Table 2 - R and D values obtained from the experimental x-ray diffraction data p.d.= (q-2q) diffractometer, d.c.= double crystal setup.

Sample	R(Å) high angle (p.d.)	R(Å) low angle (p.d.)	D(Å) high angle (d.c.)	D(Å) high angle (p.d.)	D(Å) low angle (p.d.)
JF3	13.89	13.10	368.6	355.3	-
JF5	16.48	16.42	570.6	570.6	571

Table 3 - Comparison: nominal (nom) structural parameters and simulation (sim).

Sample	d_{Si} (Å)	d_{Ge} (Å)	n_{Si} (ml)	n_{Ge} (ml)	n_{buff} (ml)	R_{sim} (Å)	R_{nom} (Å)	D_{sim} (Å)	D_{nom} (Å)
JF3	1.3577	1.4300	4.7	5.5	200	14.2	15.1	358.0	390.1
JF5	1.3577	1.4420	7.0	5.2	346	17.0	16.9	570.1	589.1



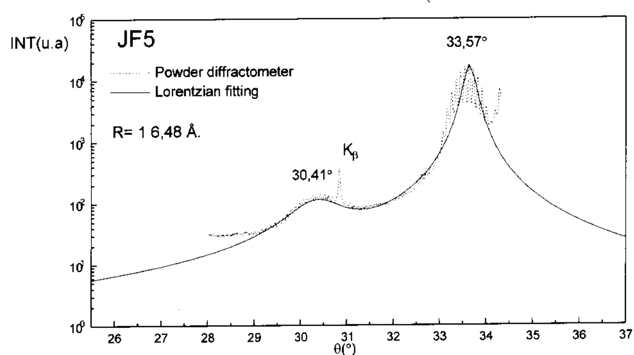


Figure 1. Powder and double-crystal diffractograms of samples JF3 and JF5.

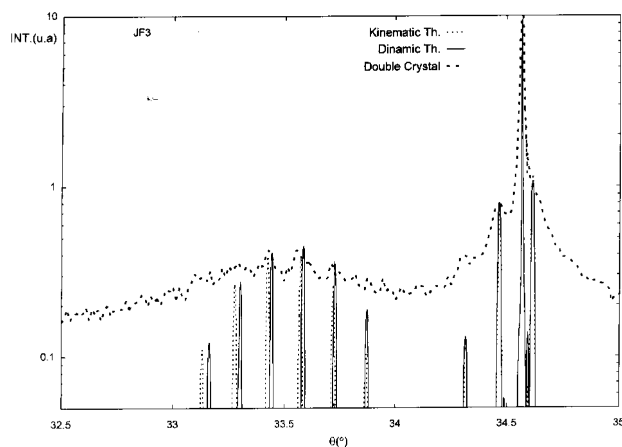


Figure 2. Experimental and theoretical results of sample JF3.

The presented results show very similar experimental R and D values, obtained from different experiments, in the case of sample JF5. This result is attributed to a better structural quality of this superlattice in comparison with sample JF3. For both analyzed heterostructures, the best fitting results were obtained using the lattice parameter of bulk Si, showing that the silicon layers are not under stress. On the other hand, the lattice spacing of the germanium layers are larger than the bulk value ($d_{400} = 1.4144$ Å), which is an indication that the Ge monolayers suffered a tetragonal distortion. The kinematical approach simulated, with a fairly good agreement, the experimental data, while the dynamical theory showed deviations in angles far from the Bragg reflection. Since the contribution of secondary reflections were disregarded in the dynamical approach, the discrepancies between experiment and theory are attributed to this approximation used in the Takagi-Taupin equations [13].

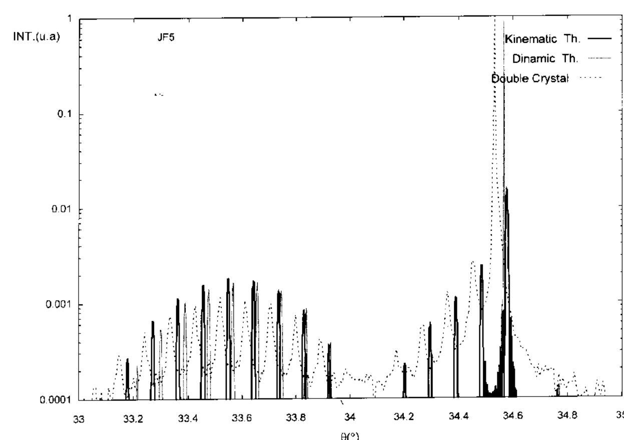


Figure 3. Experimental and theoretical results of sample JF5.

Conclusions

In this work it is shown that simple x-ray diffraction experiments can be used to characterize the structural properties of complex heterostructures, by cross-checking experimental results from different setups. The developed general simulation of the experimental data with theory is fundamental to obtain more detailed structure information. The kinematical calculations of the diffraction profiles presented better results than the dynamical approach, due to approximations used in Takagi-Taupin equations, implying that the structural properties of superlattices have to be simulated by the dynamical x-ray diffraction theory considering all secondary effects. Therefore, the use of kinematical theory are not ruled out even in the case of well deposited superlattices.

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