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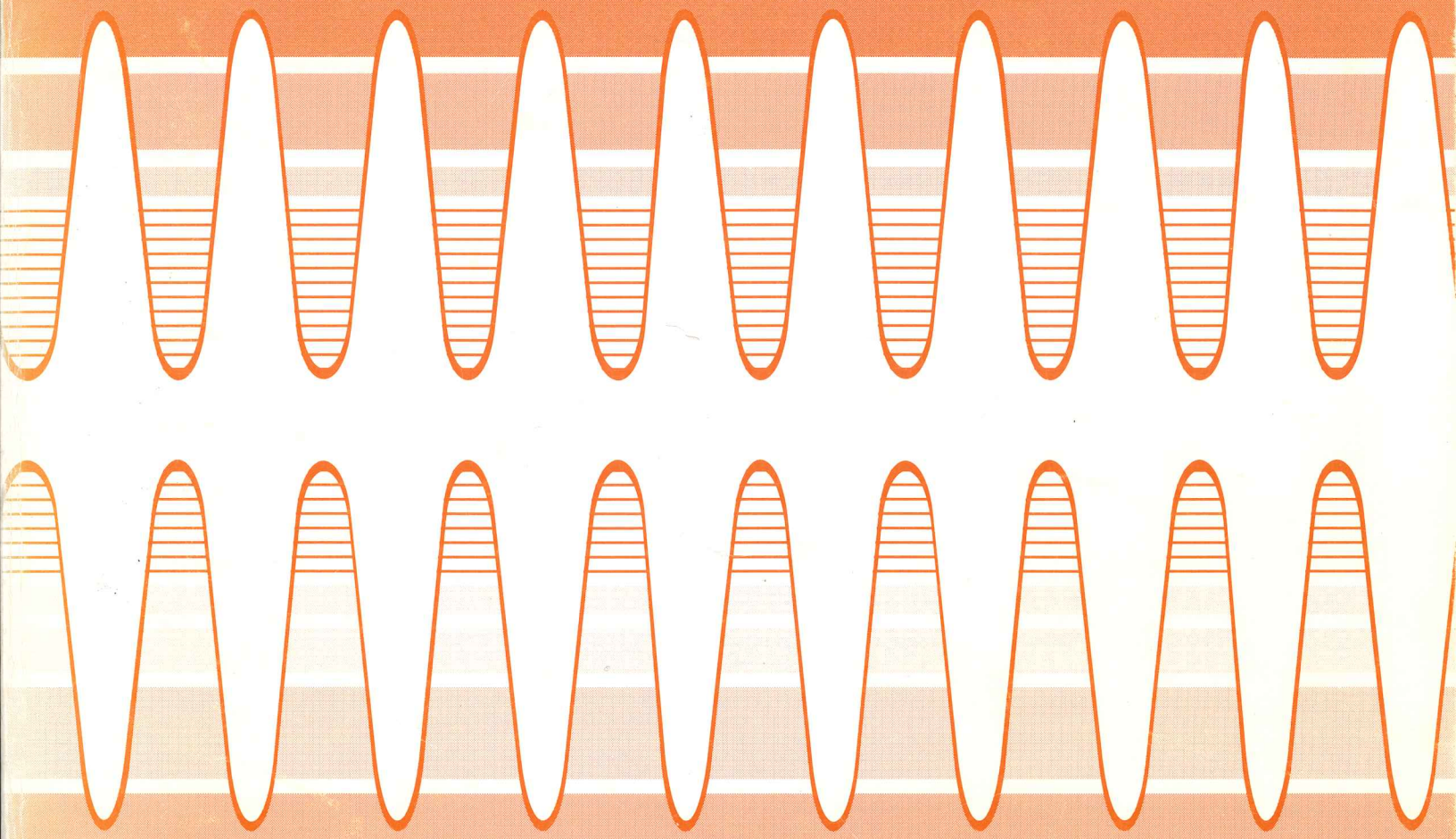

1992 ELECTRONIC MATERIALS CONFERENCE

Technical Program with Abstracts

11:20 AM, F9 †

Modulation Spectroscopy Study of Short-Period Strained Si-Ge Microstructures Grown on (001) Ge: Yichun Yin, D. Yan and Fred H. Pollak, Physics Department, Brooklyn College of CUNY, Brooklyn, NY 11210; and Mark S. Hybertsen, J.M. Vandenberg and J.C. Bean, AT&T Bell Telephone Laboratories, Murray Hill, NJ 07974.

Using various modulation methods such as electromodulation [Schottky barrier electroreflectance (SBER)] and stress-modulated reflectivity [piezoreflectance (PzR)], we have investigated a number of Si-Ge microstructures fabricated on (001) Ge. In addition to bulk Ge these samples consisted of Ge quantum wells which formed spacer layers between ordered short-period strained Si-Ge superlattice (SL) regions. No evidence for pseudo direct transitions in the Si-Ge SLs was found by either technique. We present results that the electromodulation spectra measured to date derive from a bulk-like Ge region of the samples, in contrast to the interpretation of previously published SBER data on similar samples. Furthermore, the PzR signals are due to quantum confined transitions in the Ge quantum wells. This observation of features for the Ge quantum wells has allowed us to gain information about band offsets as well as the electron-phonon interaction in the reduced dimensional system.

The possibility of achieving pseudo direct optical transitions in the Si-Ge system through artificially ordered structures has recently received considerable experimental and theoretical attention. Studies of valence-band offset and the well-known nature of the uniaxial strain in Si and Ge has established that the conduction band edge in these structures is formed from [001]-oriented Si states. Pseudomorphic, strained-layer epitaxy of a Si-Ge superlattice (SL) on a (001) Ge substrate creates a tensile, biaxial strain (in-plane) which results in a compression along the SL growth axis. Under the conditions of strain, the conduction band edge lies along the SL axis, and it will be mixed by the SL potential with zone-center states. This effect raises the possibility that the SL might be a direct-gap material. Recently it has been reported that structure in the SBER spectra at 40K of such samples was due to new optical transitions at energies theoretically predicted for SL-induced direct optical transitions at the center of the Brillouin zone. However, the interpretation of these results are complicated by the presence of Franz-Keldysh oscillations (FKO) whose origins were not clearly understood. In order to clarify this situation we performed detail SBER and PzR experiments. The latter modulation method suppresses FKO.

A detailed investigation of the SBER spectra as a function of dc bias has clearly established the origins of the signals in these samples as being due to the bulk-like Ge regions.

The observation of quantum transitions from Ge quantum wells of different well widths have allowed us to perform a number of interesting new investigations. By comparison of the observed quantum energies with a detailed theoretical calculation we have obtained important information about band offsets. In addition, the temperature dependence (10K<T<300K) of the energies and broadening parameters [G(T)] of the quantum transitions was investigated. The former variation is essentially the same as that of the direct gap of bulk Ge. The parameter G(T), which is a measure of the electron-optic phonon interaction, shows a variation with dimensionality. However, this dependence is considerably less than that for comparable GaAs/GaAlAs quantum wells. This observation will be discussed in terms of the difference between Frohlich (polar materials) and deformation potential (non-polar) electron-phonon couplings.

The samples were grown by molecular beam epitaxy at 450 °C on (001) n^+ Ge substrates ($n^+ \sim 1¥10^{17}$ cm^{-3}) followed by 1000Å of an n^+ Ge ($n^+ \sim 2¥10^{17}$ cm^{-3}) buffer on top of which was fabricated a Si-Ge microstructure capped with 1000Å of p^+ Ge ($p^+ \sim 4¥10^{18}$ cm^{-3}). For SBER measurements a semitransparent metal was evaporated onto this top layer. The Si-Ge microstructure formed the insulating region of a PIN structure. One sample category had unit cells of either three monolayers (ML) of Si and seven ML of Ge(Si_3Ge_7) or four ML of Fi and six ML of Ge(Si_4Ge_6). The samples alternated one of the above unit cells, repeated five times, with pure Ge spacer regions of various thicknesses ranging from 29ML to 143ML. The basic unit of the Si-Ge microstructure is designated $(Si_mGe_n)_5Ge_N$, where N denotes the number of MLs of the Ge spacer. The overall pattern was in turn repeated 10 or 20 times. These samples are labelled m/n/N. It is important to note that the Ge_N spacer regions form quantum wells (QW) sandwiched between Si_mGe_n SLs.

11:40 AM, F10 †

Direct Evidence by Photoluminescence of Type-I Band Alignment for Strained $Si_{1-x}Ge_x$($x \leq 0.35$) on (100) Silicon: X. Xiao and J.C. Sturm, Department of Electrical Engineering, Princeton University, Princeton, NJ 08544; L.C. Lenchyshyn and M.L.W. Thewalt, Department of Physics, Simon Fraser University, Burnaby, B.C., V5A 1S6, Canada.

The system of pseudomorphic strained $Si_{1-x}Ge_x$ on silicon substrate has been subjected to intensive studies in the past ten years. While consensus has been reached regarding the valence band alignment of the strained $Si_{1-x}Ge_x$/Si interface, alignment of the conduction band is still in dispute. While it is agreed that the conduction band offset is smaller than the valence band offset for $x<0.4$, the sign of the conduction band offset is still in dispute. Indirect evidence has been published for both type-I and type-II band alignments. In this paper, we present direct evidence obtained from band-edge photoluminescence (PL) studies of strained $Si_{1-x}Ge_x$/Si stepped quantum well structures which unambiguously indicates for the first time that the conduction band edge of strained $Si_{1-x}Ge_x$ with $x \leq 0.35$ on (100) silicon is not above that of unstrained Si, proving a type-I band alignment. Measurements of ΔE_v by internal photoemission spectroscopy are then combined with photoluminescence measurements on the same samples (measuring E_g) to experimentally determine ΔE_c vs. x.

The sign of the conduction band (CB) offset ΔE_c was determined by photoluminescence (PL) resulting from electron-hole recombination. If the CB in the $Si_{1-x}Ge_x$ is higher than that in the Si (type-II alignment), PL in the Si/$Si_{1-x}Ge_x$/Si/ structures will be due to holes in the $Si_{1-x}Ge_x$ recombining with electrons in the cladding layer (Si). If the CB in the $Si_{1-x}Ge_x$ is lower than that in the Si (type-I), both the electrons and holes will be in the $Si_{1-x}Ge_x$. These processes were distinguished by separating the strained $Si_{1-x}Ge_x$ layer from the Si with a strained $Si_{1-y}Ge_y$ layer, with $y<x$ in a stepped quantum well (STQW) structure. If the alignment is type-I, the observed PL energy in the STQW structure will be the same as the single quantum well (SQW) structure since the holes and electrons will be in the $Si_{1-x}Ge_x$ in both cases. If it is a type-II alignment, a higher PL energy will be observed in the STQW structure than that in the SQW structure, because in the STQW the PL will result from electrons in the $Si_{1-x}Ge_x$ cladding layer. Several pairs of strained SiGe samples were grown using the technique of Rapid Thermal Chemical Vapor Deposition. One of each pair was a Si/$Si_{1-x}Ge_x$/Si SQW sample, such as Si/$Si_{0.70}Ge_{0.35}$ (100Å)/Si. The second of each group was a Si/$Si_{1-y}Ge_y$/$Si_{1-x}Ge_x$/$Si_{1-y}Ge_y$ /Si($y<x$) STQW sample with the same central well Ge fraction, such as Si/$Si_{0.80}Ge_{0.20}$(100Å)/$Si_{0.70}Ge_{0.35}$(100Å)/$Si_{0.80}Ge_{0.20}$(100Å)/Si. Several pairs of samples with the central well Ge mole fraction x up to 0.35 have been studied. The layers were thick enough to complications from quantum confinement energy shift effects. Well-resolved band-edge exciton PL was observed in all samples. For each pair of samples, PL energies of the single quantum well and the stepped quantum well with an intermediate cladding layer were the same, unambiguously proving a type-I alignment.

Another set of p-$Si_{1-x}Ge_x$/p-Si samples were grown for internal photoemission measurements as well as photoluminescence measurements. Diodes were fabricated on these samples by a simple mesa etch, and their infrared photoresponse due to internal photoemission of holes from $Si_{1-x}Ge_x$ layer into the silicon were obtained at 77K using a Fourier Transformed Infrared(FT-IR) spectrometer. The long wavelength cut-off in the IR response directly gives the valence band offset (ΔE_v) of $Si_{1-x}Ge_x$/Si interface. Photoluminescence measurements were performed on the same

samples, and band gaps were obtained from the no-phonon luminescence peaks of bound excitons. Since the above experiment has determined a type-I luminescence, the conduction band offset is then given by $\Delta E_c = Eg_{Si} - Eg_{Si_{1-x}Ge_x} - \Delta E_v$. Up to x=0.35, the magnitude of this offset was found to be less than 40 meV.

In summary, the sign of the conduction band offset of the strained $Si_{1-x}Ge_x/Si(100)$ interface has been directly determined for the first time, establishing a type-I band alignment

Thursday, June 25, AM

Session G: Defects in Semiconductors: EL2

Room: Mezzanine Lounge
Session Chairman: D.J. Wolford, IBM Watson Research Center, Rt. 134, Yorktown Heights, NY 10520
Co-Chairman: M.R. Melloch, School of Electrical Engineering, Purdue University, West Lafayette, IN 47907
Co-Chairman: G.E. Stillman, 151 Microelectronics Lab., University of Illinois, Urbana, IL 61801.

8:20 AM, G1, Invited
Experiments on the Structure of the EL2 Defect in Gallium Arsenide: M.K. Nissen and M.L.W. Thewalt, Department of Physics, Simon Fraser University, Burnaby, B.C., Canada V5A 1S6.

The EL2 defect in gallium arsenide remains one of the most active topics in semiconductor physics. This defect receives much attention from experimentalists and theoreticians alike, motivated by both the technological importance of EL2 in the production of semi-insulating GaAs, and by its intriguing metastable behaviour. Despite this, controversy still flourishes over many of the fundamental properties of this defect. This talk concerns experimental work that addresses the question of the detailed structure of the defect. After reviewing some of the more important previous work and illustrating the need for new information, our recent work will be presented.

It is now widely agreed that EL2 involves an arsenic antisite. The topic of dispute is whether the arsenic antisite is either isolated or paired with another constituent atom, usually considered to be an arsenic atom in an interstitial position. The controversy has continued largely on the strength of two experiments with apparently contradictory results.

The first of these is the study under uniaxial stress of the 1.039 eV EL2 absorption line. The observed splittings were originally found to be fully consistent with an $A_1 Æ T_2$ transition in tetrahedral symmetry. No additional splittings due to orientational degeneracies could be detected and it was concluded that EL2 was the isolated antisite. This behaviour, however, has been difficult to reconcile with that observed in an optically detected electron nuclear double resonance experiment. This technique probes the hyperfine interactions from nucleii in the vicinity of the defect and hence can provide information on the structure. In addition to the results expected for an isolated antisite, there were other weaker features which were argued to indicate the presence of a nearby arsenic interstitial, reducing the symmetry of the defect to C_{3v}.

Both of these experiments have their strengths and weaknesses, but recently the uniaxial stress results were reinterpreted in a way that was consistent with the arsenic interstitial pair model. Since this experiment was its most direct evidence, the new interpretation seriously weakens the support for the isolated antisite model. Although the theoretical support for the isolated antisite has been greatly strengthened in recent years, new experimental evidence to support the model is more important now than ever.

Such a development became possible with our recent photoluminescence spectroscopy of deep levels in SI GaAs. This work included the first report of a shallow hydrogenic excited state of EL2. This is significant because the electronic transition from this state down to the EL2 ground state is much simpler to interpret than the transition responsible for the 1.039 eV absorption line, and also gives rise to sharp fine structure in the PL spectrum that is the narrowest feature yet in the optical spectroscopy of EL2. This has allowed for uniaxial stress and magnetic field perturbation studies to be done with far greater precision than has been previously possible.

As expected for an $A_1 Æ A_1$ transition in T_d symmetry, no splitting is observed under uniaxial stress and hence there is also no evidence of orientational degeneracy. The application of a magnetic field gives rise only to an isotropic splitting due to the removal of the spin degeneracy of the initial state. These results provide important new information on the structure of EL2 and give renewed strong support to the isolated arsenic antisite model.

9:00 AM, G2, Invited
***EL2*: Electronic Properties and Metastability:** Matthias Scheffler(*), Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-1000 Berlin 33, Germany.

We review the theoretical research on the *EL2* defect in GaAs. In particular we concentrate on the analysis of the electronic structure of the arsenic antisite, of various forms of the arsenic interstitial and the antisite-interstitial pair. We also discuss formation energies (abundances) and structural stabilities. The results are explained in a simple physical picture and they are put in a greater framework of defect metastability in III-V compounds.

A detailed comparison with the voluminous experimental data on *EL2* is given.

(*) Work done in collaboration with Jaroslaw Dabrowski.

9:40 AM, G3
Are EL-2 and As Precipitates in GaAs Electronically Equivalent? J.M. Woodall, A.C. Warren and P.D. Kirchner, IBM Research Division, P.O. Box 218, Yorktown Heights, NY 10598; X. Yin, X. Guo and F.H. Pollak, Physics Department, Brooklyn College, CUNY, Brooklyn, NY 11210; M.R. Melloch, School of Electrical Engineering, Purdue University, W. Lafayette, IN 47907; N. Otsuka and K. Mahalingam, School of Materials Engineering, Purdue University, W. Lafayette, IN 47907.

The MBE growth of GaAs at temperatures in the vicinity of 200C results in GaAs with an arsenic-rich stoichiometry in excess of 1%. In the as-grown condition this excess arsenic correlates with a large arsenic anti-site defect concentration. When this material is annealed at about 600 C, the excess arsenic is converted into arsenic precipitates (GaAs:As) with a concomitant decrease in the anti-site defect concentration. The question arises: Are these two forms of excess As electronically equivalent? It has been shown by a variety of electrical and optical studies on GaAs:As that the arsenic precipitates can be successfully modeled as buried Schottky barriers with a "pinned" barrier height of 0.7 eV. Less is known about the electrical behavior of the GaAs dominated by arsenic anti-site defects.

In order to address the above question we have used the electromodulation (EM) technique, i.e., photoreflectance and contactless electroreflectance, to determine the electric field distribution from the Franz-Keldysh oscillations (FKO) in thin films of both types of GaAs with excess arsenic. The MBE grown structures used in this study were as follows: an N or P buffer layer with an undoped (U) layer followed by an as-grown low temperature layer (LT) or an annealed LT (ALT) layer. Four different sequences were formed: LTUN, LTUP, ALTUN and ALTUP. The key to the experiment is the fact that if the Fermi level is pinned in the LT or ALT layers and sufficiently different from that of the doped substrate, the electric field is non-zero and constant in the "U" layer of all the structures. For this case the