Recent developments in the strained layer epitaxy of germanium–silicon alloys

John C. Bean

AT&T Bell Laboratories, Murray Hill, New Jersey 07974

This paper provides a brief review of recent work on strained layer $Ge_x Si_{1-x}$ including modeling of critical thicknesses for single layers and superlattices; calculations and measurements on strain induced alteration of alloy band gap and heterostructure band alignment; and application to modulation-doped field effect transistors (MODFET) and 1.3 μm photodetector devices.

I. INTRODUCTION

It has been shown that molecular beam epitaxy (MBE) can be used to grow nominally defect-free $Ge_x Si_{1-x}$ layers commensurate with Si substrates.[1–3] Layer thicknesses can exceed calculated equilibrium limits by one and two orders of magnitude in single layers and superlattices, respectively. Although metastable, these layers have nevertheless been successfully incorporated in a number of conventionally processed devices. This paper will briefly review recent developments in the field.[4]

II. LAYER STABILITY

There have been two significant developments in our understanding of $Ge_x Si_{1-x}$/Si metastability. First, as shown in Fig. 1, we have derived a formalism that accurately models the observed single layer critical thickness values.[5,6] In contrast to earlier equilibrium approaches,[7] this kinetic model assumes that the nucleation of isolated, stress-relieving dislocations provide an effective reaction barrier to equilibrium. In lieu of a full atomistic model with thermally activated relaxation rates, this somewhat crude approach is based on the equivalence of the layer strain energy and the dislocation nucleation energy. The result involves one adjustable, but physically realistic parameter, to provide an excellent fit to data over the full composition range.

Hull *et al.* have also developed a simple predictive rule on $Ge_x Si_{1-x}$/Si superlattice stability.[8,9] This rule is based on TEM observations that superlattices do not relax to a completely strain-free state by formation of dislocations at each heteroepitaxial interface. Instead, the superlattice forms a single dislocation array at the substrate boundary. This produces a compressive/tensile strain field alternating with $Ge_x Si_{1-x}$ and Si layers to give a zero average superlattice strain. Because the driving force and relaxing dislocations are identical to the single layer case, a mathematical analogy yields the result that a superlattice will be stable if (1) individual $Ge_x Si_{1-x}$ layers are thinner than the single layer critical thickness and (2) the total superlattice thickness is less than the critical thickness for a single layer of the volume averaged superlattice composition. This rule has been tested for a variety of compositions and $Ge_x Si_{1-x}$ to Si thickness ratios and has proven moderately accurate. Slight deviations are attributed to the simplifying assumption of equal alloy and Si elastic constants.

III. BAND STRUCTURE

Our modeling of crystal growth has been paced by advances in the understanding of $Ge_x Si_{1-x}$ physics. Most importantly, strain has been shown to have huge effects on band structure. As depicted in Fig. 2 from the calculations of People[10] and the experimental data of Lang *et al.*[11,12] we now know that the strained layer band gap falls precipitously with the addition of Ge. Indeed, for Ge fractions of greater than 55%, the strained alloy band gap is smaller than that of pure bulk Ge. This may have immense practical importance.
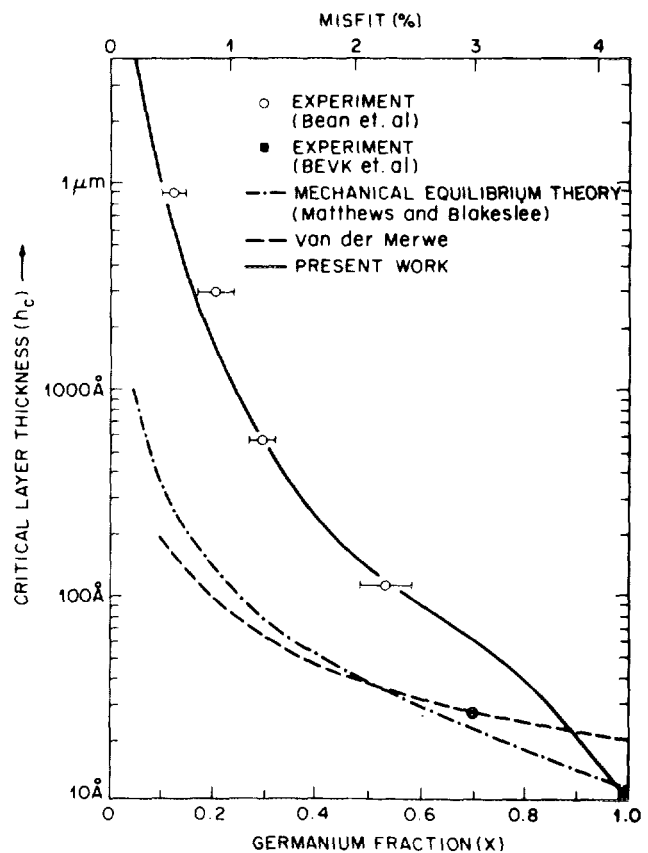

FIG. 1. Comparison of $Ge_x Si_{1-x}$ critical thickness data with equilibrium calculations of van der Merwe and Matthews (Ref. 7) and kinetic model of People and Bean (Refs. 5 and 6). O and ■ are the critical thickness data from Bean *et al.* (Refs. 2 and 4) and Bevk *et al.* (Ref. 30), respectively. ● is the thickness of the commensurate layer in the superlattice structure (Ref. 27).
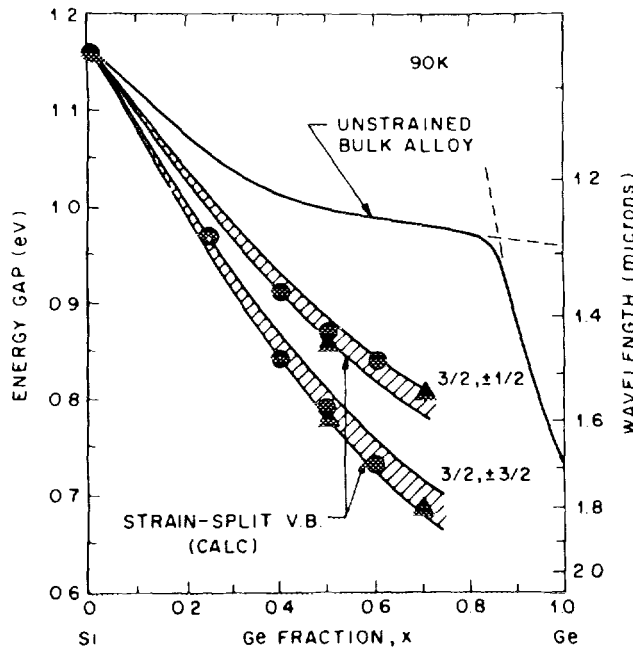
FIG. 2. Minimum band gap of strained Ge_xSi_{1-x} commensurate with the Si substrate. Calculations of People (Ref. 10) and photocurrent data of Lang et al. (Refs. 11 and 12).

A device dependent on band discontinuities will require far less concentrated alloys than originally anticipated. If the alloy dimensions are fixed, the degree of metastability will be drastically decreased. Alternately, with the more dilute alloys, thicknesses may be grossly increased to enhance device performance. Devices, such as 1.3 μm optical detectors, previously thought impossible, can now be realized in alloys of only 60%–80% Ge.

Calculations have also resolved an apparent contradiction in modulation doping results and thus highlighted another degree of freedom in the system. While the first modulation doping experiments demonstrated a strong transfer of holes from the alloy to Si, electron transfer was weak and prone to premature freeze out. This indicated an ~90%/10% split of the Ge_xSi_{1-x}/Si band discontinuity between the valence and conduction band edges, respectively, with the alloy band gap within the Si band gap ("type I" alignment).[13-15] Later n-type results[16,17] indicated electron transfer from alloy to Si, suggesting an alloy conduction band edge above that of Si ("type II" alignment). Abstreiter[17] suggested that the fundamental difference between experiments could be the presence or absence of strain in Si cladding layers. Our calculations, based on deformation potentials and pseudopotential theory, confirm this conjecture.[18] Examples of possible alignments are given in Fig. 3.

The richness of the Ge_xSi_{1-x} system may well be further extended by the existence of a strain induced, atomically ordered state. Originally indicated by TEM[19,20] and x-ray[21] data, a recent analysis of Shubnikov de Haas power loss mechanisms now invokes a piezoelectric loss mechanism that could only occur in a nonrandom polar alloy.[22] If confirmed, this ordering would open the door to a range of nonlinear optic and electro-optic phenomena previously excluded in column IV semiconductors.
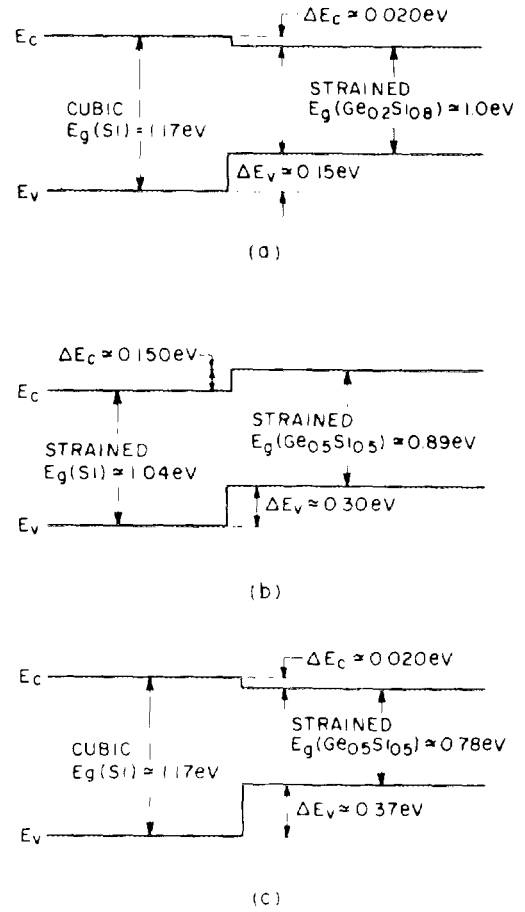
FIG. 3. Calculated band alignments (Ref. 18) for various distributions of strain between Ge_xSi_{1-x} and Si layers. (a) $Ge_{0.2}Si_{0.8}$ commensurate with unstrained Si; (b) Ge_xSi_{1-x} compressed and Si dilated to match $Ge_{0.25}Si_{0.75}$ substrate; (c) $Ge_{0.5}Si_{0.5}$ commensurate with unstrained Si.

IV. APPLICATIONS

The above results have been incorporated in a number of device structures demonstrating not only the potential of the system but the surprising robustness of these materials under conventional device processing. Modulation doped transistors have been fabricated with both p[23,24] and n[25] channels as depicted in Fig. 4. With a conventional planar Si processing sequence including lithography, etching, metallization, ion implantation, activation anneals, and thermal oxidation, the first p-MODFET had a transconductance approaching that of a p-MOSFET. Using a less conventional nonplanar fabri-
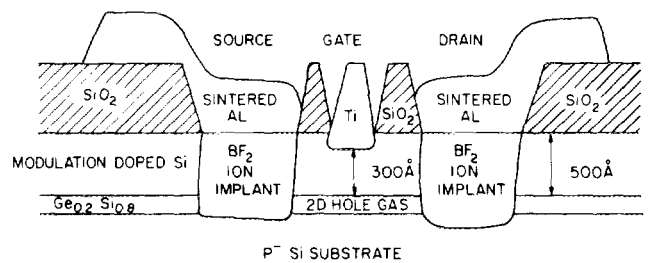

FIG. 4. Schematic cross section of p-MODFET fabricated with conventional Si processing procedures (Refs. 23 and 24).
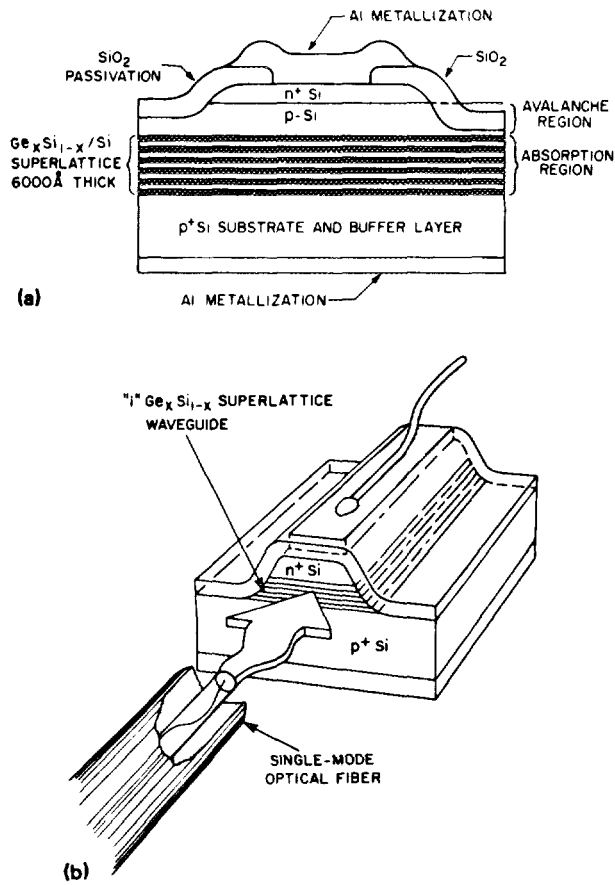
FIG. 5. Cross section (a) and perspective view (b) of Ge_xSi_{1-x}/Si light-guiding avalanche photodetector (Ref. 28).

cation process, the n-MODFET transconductances actually exceed MOSFET standards.

The radical reduction of band gap has also been exploited in a series of Ge_xSi_{1-x}/Si photodetectors for fiber optic applications.[26–29] As shown in Fig. 5, a strained layer superlattice can serve as a light-guiding absorbing layer within a silicon device structure. The light-guiding geometry not only accommodates the restrictions of absorption length and strained layer critical thickness, it also minimizes the vertical device dimension to provide for high-speed operation. Indeed, avalanche versions of this device have demonstrated a 3 dB bandwidth of over 8 GHz with a high frequency gain of 6. Over a 45 km optical fiber link, 1.3 μm laser radiation has been detected at 800 Mbyte/s with error rates of less than one part in 10^9.

In summary, the experimentally determined limits of Ge_xSi_{1-x}/Si strained layer epitaxy have now been modeled for both single layers and superlattices. Although strain can be accommodated readily in crystal growth, it has been found to have dramatic effects on band structure including gross reduction in band gap and a variable alignment in band edges. Properties have been exploited in a variety of devices.

The material has withstood conventional Si processing and demonstrated optical detector performance not far below that of the best discrete III–V devices. This is accomplished in a materials technology which can be directly merged with existing IC technology. Finally, basic studies indicate the existence of an atomically ordered state that could yield additional properties normally forbidden in column IV materials.

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