

Properties of SiGe Alloys and Their Applications to High-Speed Devices and Circuits

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Abstract

The electrical and material properties of strained SiGe alloys have been overviewed and the historical survey of the application of SiGe alloys to high-speed devices and circuits is given.

Introduction

The demand for high-speed devices is soaring as the applications of these devices has been shifting from military to commercial market, which includes the exploding wireless and optical network systems. In the past, III-V semiconductor-based systems were deemed to be most suitable for high-speed applications. They provide not only superior carrier transport characteristics, such as high carrier mobilities required for these applications, but also provide the feasibility of bandgap engineering by proper choice of compositions with ternary and quaternary derivatives of binary compounds such as GaAs and InP. Although the technology based on these material systems suffers from their relatively high cost of production, this has not seriously hampered their use when applied for military purposes. For the commercial applications, however, the importance of the cost for implementing such systems is playing a more important role and, therefore, Si based system becomes more favored choice for this purpose. Si has been the dominant semiconductor for a long time owing to its advantages such as compatibility with high-quality oxides, mechanical stability, high thermal conductivity, matured processing technology, and low production cost. However, the relatively poor carrier transport characteristics and the lack of the availability of heterostructures have impeded the application of Si to high-frequency and high-speed applications for a long time. Recently, however, development in the growth technology of high-quality SiGe alloys on Si substrate has made such applications feasible with Si-based systems. The incorporation of SiGe layers into Si-based systems provides the possibility to enhance the performance of Si-based electronic devices by the strain-originated carrier transport characteristics improvement and the quasi electric field from the bandgap grading.

Table 1. Selected properties of bulk Si and Ge at 300K[1].

Property	Si	Ge
Crystal Structure	Diamond	Diamond
Lattice Constant [nm]	0.543095	0.564613
Conduction Band Minima	Δ valley	L valley
Energy Bandgap [eV]	1.12	0.66
Electron Mobility [$\text{cm}^2\text{V}^{-1}\text{s}^{-1}$]	1500	3900
Hole Mobility [$\text{cm}^2\text{V}^{-1}\text{s}^{-1}$]	450	1900
Dielectric Constant	11.9	16.0
Refraction Index	3.44	3.97
Intrinsic Carrier Conc.[cm^{-3}]	1.45×10^{10}	2.4×10^{13}

Basic properties of SiGe alloys

Some of the basic properties of bulk Si and Ge at 300 K are listed in Table 1[1]. The crystal structure of both Si and Ge is the diamond structure, the lattice constant of Ge being slightly larger than that of Si. The lattice mismatch of 4.18% at room temperature, which puts an upper limit on the thickness of strained SiGe layers that can be grown on Si substrate without generating dislocations, can be compared with those of widely used III-V systems: GaAs and InAs (7.16%) and GaAs and InP (3.81%). The conduction band minimum of Si occurs at the Δ point, located at $\sim 75\%$ from Γ point to X point, while that of Ge occurs at L point, and the corresponding energy bandgap is 1.12 eV and 0.66 eV, respectively, at 300 K. One of the most attractive features of Ge is its superior carrier mobility compared with Si, which is 2.6 times larger for electrons and 4.2 times larger for holes, assuming low doping concentration and room temperature.

SiGe alloys are the material system which is made out of those two major semiconductor materials. The

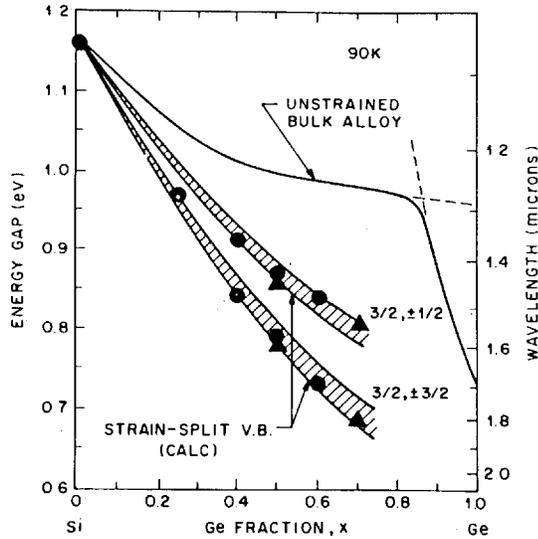


Figure 1: Energy bandgap of bulk (solid line) and compressively strained (hatched lines) $\text{Si}_{1-x}\text{Ge}_x$ alloys on Si(100) substrate at 90 K[2][3]. Symbols represent measured data.

properties of compressively strained SiGe alloys grown on Si(100) substrate, which comprise most of the SiGe alloys adopted for practical device applications, are now discussed. The bandgap of SiGe alloys has a dominant impact on the optical and electrical characteristics of the alloys. The measured and calculated bandgaps of the strained SiGe alloys are shown in Fig. 1 as a function of Ge composition x , along with that of unstrained bulk SiGe alloys[2][3]. The bandgap of unstrained $\text{Si}_{1-x}\text{Ge}_x$ alloys exhibits a slow monotonic decrease with increasing Ge composition until the composition reaches $x=0.85$, at which a steep roll-off is observed. This turning point stems from the transition of the lowest valley in the conduction band, from Si-like Δ valley to Ge-like L valley. The bandgap of strained SiGe alloys shows quite different profiles since the strain lifts the degeneracies in the conduction and valence bands, causing the relative position of the energy valleys to change. The six-fold degeneracy in the conduction band is split into four- and two-fold degeneracies, while the heavy hole band and light hole band are split in the valence band. The two bandgap curves appearing in Fig. 1 for strained alloys correspond to the heavy hole band (lower curve) and the light hole band (upper curve). The cross hatched region represents the uncertainties arising from the deformation potential employed for the calculation. The bandgap of the heavy hole band should be regarded as the actual bandgap, as this is usually defined as the energy difference between the lowest conduction band-edge and the highest valence

band-edge. The bandgap of strained SiGe alloys can be approximated by following expression at room temperature[3].

$$\Delta E_g(x) = 0.96x - 0.43x^2 + 0.17x^3 \text{ [eV]} \quad (1)$$

It is noticeable that the bandgap of the strained alloys decreases so rapidly that it becomes even smaller than that of bulk Ge when $x>0.6$. Note that the bandgap is indirect for both strained and unstrained SiGe alloys.

Once the bandgaps of SiGe alloys are determined, the next concern is how they are lined up with respect to the bandgap of Si at SiGe/Si heterojunctions, from which the band offset distribution between the conduction band and the valence band is decided. As the band offset governs the carrier transport across the heterojunctions, the band alignment is of crucial importance for electronic device applications. The calculation and measurement of the band offsets at SiGe/Si heterojunctions are quite complicated and the results differ between groups[3]-[6]. Nevertheless, they agree on the fact that most of the band offset lies on valence band, rather than conduction band, at heterojunctions between compressively strained SiGe alloys and unstrained Si. It is generally accepted that conduction band offset comprises less than 10-15% of the total band offset, depending on the Ge composition.

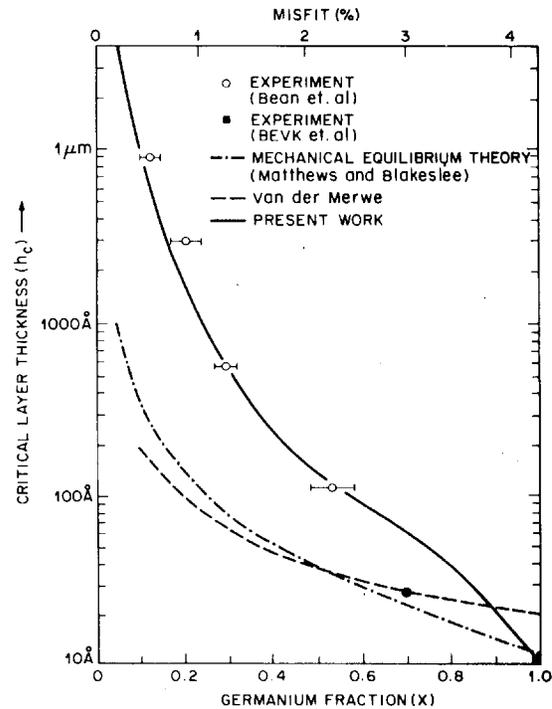


Figure 2: Critical thickness of $\text{Si}_{1-x}\text{Ge}_x$ alloys on Si(100) substrate[7]. The dashed and dot-dashed line is based on mechanical equilibrium theory while the solid line is based on meta-stable state of the layer.

According to Bean[3], the valence band offset can be approximated as a function of Ge composition x as,

$$\Delta E_v(x) = 0.84x \text{ [eV]}. \quad (2)$$

Combining Eq. 1 and Eq. 2, conduction band offset can also be expressed as a function of Ge composition:

$$\Delta E_c(x) = 0.12x - 0.43x^2 + 0.17x^3 \text{ [eV]}. \quad (3)$$

Critical thickness is another important material parameter of SiGe alloys which dictates the maximum thickness of the strained SiGe layer to be grown without relaxation, placing a limit on the device structure design. The critical thickness of SiGe alloys based on the mechanical equilibrium theory shows $1/f$ dependence, where f is the misfit between the strained epitaxial layer and the substrate. According to the calculations based on this theory, which are plotted as dashed and dot-dashed lines in Fig. 2 after two different groups[7], the critical thickness of $\text{Si}_{1-x}\text{Ge}_x$ alloy on Si(100) substrate is less than 100 \AA for $x > 0.2$, which places a severe restriction for practical device applications. However, a calculation assuming a meta-stable state of the SiGe alloys, which shows $1/f^2$ dependence and excellent agreement with experimental data, shows much larger critical thickness (plotted as solid line in Fig. 2) which exceeds 100 \AA up to $x = 0.5$. The calculation based on the meta-stable state may be used as a reference for the practical device growth and fabrication, provided the thermal budget during the epitaxial layer growth and device processing is kept low enough to maintain the meta-stable state of the strained layer.

Mobility, an important carrier transport parameter which governs the frequency response of devices, is a function of various parameters such as temperature, doping concentration, alloy composition, types of carrier (electron or hole), carrier polarity with respect to dopants (majority or minority carrier), types of strain (compressive or tensile), direction of carrier movement with respect to the strain (in-plane or out-of-plane), etc. Figure 3 illustrates a calculated result on the trend of the majority electron and hole mobilities in moderately-doped strained $\text{Si}_{1-x}\text{Ge}_x$ alloys grown on Si(100) substrate at room temperature[8]. The electron mobility initially decreases with Ge composition, then it exhibits an increase as x approaches 1. But, the mobility remains lower than that of Si ($x=0$) for almost the entire Ge composition range, indicating the existence of a strong alloy scattering. It should be noted that the out-of-plane mobility is larger than the in-plane mobility, with the bulk mobility lying in between them for the compressively strained SiGe alloys[9]-[11]. As doping concentration increases, the mobility values decrease in general and, more importantly, the Ge compo-

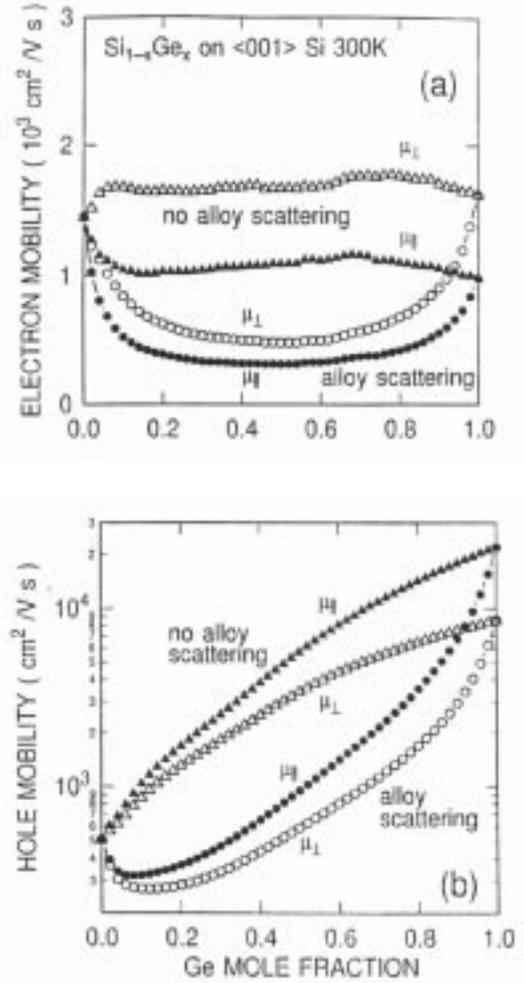


Figure 3: Carrier mobilities in strained SiGe alloys on Si(100) substrate calculated with and without alloy scattering assuming room temperature and moderate doping concentration[8]. (a) electron mobility; (b) hole mobility.

sition dependence gets weakened, leading to an almost flat mobility profile when the doping concentration exceeds 10^{19} cm^{-3} . For this heavily doped SiGe alloys, the out-of-plane mobility becomes even slightly larger than the mobility in Si[9]-[11]. The hole mobility shows similar Ge composition dependence as electron mobility, but the effect of alloy scattering is less severe for holes. It shows a small initial decrease, followed by a quick recovery (at $x \sim 0.15$) and a sharp increase, exhibiting higher mobility values than that of Si for $x > 0.3$ (Fig. 3(b)). It is interesting to note that the in-plane hole mobility is larger than the out-of-plane mobility, both of them being larger than the bulk mobility, which is different from the trend observed with the electron mobility[12]. The increase of doping concentration leads to a reduction in the hole

mobility values, but it leaves the Ge composition dependence of the mobility fairly unaltered[13]. The minority carrier mobility usually exhibits higher values than the majority counterpart, especially for higher doping concentrations, and the two mobility values cannot be assumed identical in general[11][14].

The carrier velocity becomes more important as the device dimension shrinks, since the electric field in these devices becomes large enough to saturate the carrier velocity, rendering the concept of low-field mobility less useful. According to Monte Carlo simulations by Hinckley[15], the in-plane electron velocity in compressively strained SiGe alloys is higher than that of Si, while the out-of-plane velocity is lower than that of Si. On the other hand, both in-plane and out-of-plane hole velocity in the strained SiGe alloys were calculated to be higher than that of Si, increasing with Ge composition.

A historical overview of SiGe alloys and their applications to high-speed devices and circuits

Ge was the most popular semiconductor in the early stage of semiconductor development along with Si, and efforts to make alloys out of these two dominant semiconductors have already been initiated at that time. The first synthesis of homogeneous SiGe alloys was reported by Stöhr and Klemm in 1939[16]. However, the first systematic study on the properties of SiGe alloys can be credited to Johnson and co-workers[17] who, in the 1950's, reported the Ge composition dependence of the lattice constant and bandgap of SiGe alloys for the first time. This study was followed by a number of comprehensive investigations on electronic[19] and optical[20] properties of SiGe alloys. The SiGe alloys employed in these early studies were prepared by isolated crystallization and not by epitaxial growth on Si, as is common nowadays. Thus the reported properties were limited to bulk SiGe alloys, omitting results on strained SiGe.

In the 1960's, efforts have been made by various groups to deposit SiGe alloys on Si substrates and investigate the properties of SiGe thin films. The solution technique[21][22] and the vapor deposition technique[23] were frequently adopted to deposit SiGe alloys and Ge films on Si substrates during this period. However, these studies were focused on the development of epitaxial growth techniques for SiGe alloys, neglecting the detailed analysis on the properties of the films.

More serious studies on the material properties of SiGe alloys began in the 1970's. In a series of papers, Vasilevskaya and co-workers from the Ukraine performed systematic analyses on the quality of Ge films grown by evaporation on Si substrates[24][25]. Similar studies were carried out on Ge films grown by ultra high vacuum

(UHV) evaporation by Cullis and co-workers[26] and also on SiGe alloys by Aharoni and co-workers[27]. These were followed by the first successful growth of SiGe superlattice on Si substrate by Kasper and co-workers from Germany[28], who employed UHV evaporation technique to grow $\text{Si}_{0.85}\text{Ge}_{0.15}/\text{Si}$ superlattice with periods ranging 100-800 Å on Si substrate, and made a detailed analysis of misfit dislocations in the structure. This work signaled a matured growth technique for the alloys, but the analyses were still oriented to their material characteristics, rather than electronic properties.

Monumental work on the material and electrical properties of SiGe alloys grown on Si substrates was performed by researchers in AT&T Bell laboratories in the 1980's. They made extensive analyses of the material characteristics of strained SiGe alloy films[29] and SiGe superlattices[30] grown by a molecular beam epitaxy (MBE) system, and they proceeded to investigate modulation-doped SiGe/Si structures for the first time[31], paving a way for SiGe/Si modulation-doped field effect transistors (MODFETs). This was followed by an experimental analysis on the bandstructures of strained SiGe alloys[32], and the band alignment at SiGe/Si heterojunctions[4]. The critical thickness of strained SiGe alloys on Si substrate was investigated by both experimental and theoretical techniques[7] and the optical properties of SiGe/Si superlattices were explored, leading to the development of SiGe/Si photodetectors[33]. These comprehensive studies, reported in a series of papers published in the mid- and late-1980's, have provided a solid theoretical and experimental foundation for the SiGe-based devices. The first SiGe/Si heterojunction bipolar transistor (HBT) was reported by researchers from IBM[34], and this has triggered a considerable amount of work on SiGe/Si HBTs, mainly from industries such as IBM and Daimler-Benz. IBM focused on planar-type SiGe/Si HBTs, with moderate Ge compositions ($x < 0.1$) in the base layers, grown by ultra high vacuum chemical vapor deposition (UHV-CVD) system. This technology is basically a modification of the conventional Si bipolar junction transistor technology and has led to HBTs exhibiting f_T higher than 100 GHz[35]. On the other hand, Daimler-Benz concentrated on mesa-type SiGe/Si HBTs incorporating MBE-grown base layers with higher Ge compositions ($0.3 < x < 0.4$), exhibiting f_{max} up to 160 GHz[36]. Other groups have also reported their development of SiGe/Si HBTs[37][38]. In parallel to the development of SiGe/Si HBTs, efforts have also been made to develop SiGe-based FETs in the mid 1980's[39][40], but the results were not as encouraging, since the band alignment of SiGe/Si heterojunctions is advantageous mainly for N-p-N HBTs.

In the 1990's, the technology for SiGe/Si HBTs has become matured enough to be considered for circuit

applications, and a series of successful demonstrations of circuits based on SiGe/Si HBTs have been reported. Voltage controlled oscillators (VCOs) with oscillation frequencies of 26 GHz and 40 GHz[41] and X-band mixers[42] have been realized. A narrow band amplifier for Ka-band operation[43] and a wideband amplifier operating up to Ku-band[44] have also been implemented with SiGe/Si HBTs. More recently, SiGe/Si HBT low noise amplifiers and power amplifiers for L-band wireless communication applications have been reported[45].

As commercial products based on SiGe/Si HBTs are making their way into the commercial market, it is believed that SiGe/Si HBT will be a standard npn device for future BiCMOS technologies.

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