Germanium diffusion in polysilicon emitters of SiGe heterojunction bipolar transistors fabricated by germanium implantation

M. J. Mitchell and P. Ashburn[a)]
Department of Electronics and Computer Science, University of Southampton, Southampton S017 1BJ, United Kingdom

P. L. F. Hemment
School of Electronics, Computing and Maths, University of Surrey, Guildford, Surrey GU2 7XH, United Kingdom

(Received 20 May 2002; accepted 11 September 2002)

A study is made of germanium diffusion in polysilicon emitters of SiGe heterojunction bipolar transistors made by germanium implantation. Implanted Ge is found to diffuse from the single-crystal silicon substrate into deposited polysilicon emitter layers during rapid thermal anneal at 1045 °C. Measurements of germanium diffusivity in polycrystalline silicon are reported at temperatures between 800 and 900 °C and modeled by an Arrhenius relationship with a preexponential factor of $D_o = 0.026 \pm 0.023\ \mathrm{cm^2/s}$ and an activation energy of $E = 2.59 \pm 0.36$ eV. The measured diffusivity in polycrystalline silicon is $\approx 10^4$ times larger than that reported for single-crystal silicon. It is hypothesised that germanium diffusion in polysilicon occurs by diffusion along grain boundaries. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1518770]

SiGe heterojunction bipolar transistors (HBTs) are finding increasing application in high-performance integrated circuits for mobile communication systems in the 1–10 GHz range.[1] This is made possible by the very high-frequency operation that can be achieved with SiGe HBTs, for example, values of $f_{\max}$ up to 180 GHz and values of f_T up to 210 GHz[2–6] have been reported. To achieve these good performances in a SiGe HBT, the SiGe layer is produced using epitaxy, which allows very thin layers to be grown with good control over layer thickness and composition. However, germanium implantation has also been used to produce SiGe HBTs.[7,8] While this approach does not deliver such high performance as epitaxy, it does improve transistor performance using a process that is fully compatible with standard production technology, without resorting to expensive epitaxial deposition.

A feature of ion implantation is the Gaussian-like depth distributions of the implanted species and thus in a SiGe HBT produced using Ge implantation there is no silicon cap layer. In this case, the polycrystalline silicon (polysilicon) emitter is in direct contact with the synthesised SiGe layer, which means that there can be interactions between the Ge in the substrate and the polysilicon emitter. In this article, both the diffusion of Ge from a crystalline substrate into polysilicon and the diffusion of Ge in polysilicon are investigated. It is shown that significant Ge diffusion into the polysilicon emitter occurs during emitter anneal and subsequently values of Ge diffusivity in polysilicon are determined for anneal temperatures between 800 and 900 °C.

To investigate Ge diffusion from crystalline silicon into polysilicon, a $1.86 \times 10^{16}\ \mathrm{cm^{-2}}$, 200 keV Ge^+ implant was made into a (100) silicon wafer, which subsequently had a polysilicon emitter layer of thickness 0.13 μm deposited by chemical vapor deposition. Prior to polysilicon deposition, the Si was cleaned by etching to a depth of 50 nm. The wafer was annealed for 30 s at 1045 °C in dry N_2, which is typically used for the fabrication of polysilicon emitters.

To determine the diffusivity of Ge in polysilicon, a 0.35-μm layer of amorphous silicon was deposited on a (100) *p*-type Si wafer and annealed for 30 s at 1025 °C in dry N_2. This anneal has the effect of converting the layer of amorphous silicon into polysilicon. Germanium was then implanted into the polysilicon to a dose of $2 \times 10^{16}\ \mathrm{cm^{-2}}$ and at an energy of 100 keV. Finally, an oxide capping layer was deposited and the wafer sawn into 15 mm^2 test samples. The samples were then annealed in nitrogen in a furnace for 30 min at temperatures between 800 and 900 °C. The samples were loaded into the furnace at 750 °C and a ramp rate of ~5–7 °C/min used to reach the anneal temperature.

Figure 1 shows a Ge secondary ion mass spectroscopy (SIMS) profile to demonstrate the effect of a polysilicon emitter drive-in on the Ge distribution in the substrate and polysilicon layer. The sample was implanted with $1.86 \times 10^{16}\ \mathrm{cm^{-2}}$, 200 keV Ge^+ into bulk Si prior to polysilicon deposition and annealed at 1045 °C for 30 s in dry N_2. The peak Ge concentration is $1.5 \times 10^{21}\ \mathrm{cm^{-3}}$, which is equivalent to a Ge content of 3 at. %. The depth of the peak of the Ge concentration (~0.11 μm) is in good agreement with a predicted implant peak depth of 0.12 μm for a 200-keV implant. Although the polysilicon was deposited after the Ge implantation, the layer contains a significant concentration of Ge due to out diffusion during the 1045 °C anneal. This result illustrates that significant Ge diffusion into the polysilicon emitter is to be expected in transistors fabricated using Ge implantation. Diffusion of Ge in single-crystal Si has been reported by Hettich *et al.*[8] and Dorner *et al.*,[9] and at 1045 °C the diffusivity is around $4 \times 10^{-16}\ \mathrm{cm^2\,s^{-1}}$. This is

[a)]Electronic mail: PA@ECS.SOTON.AC.UK

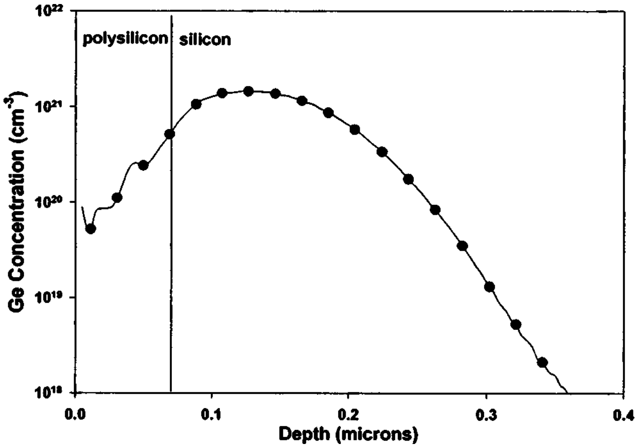

FIG. 1. Germanium SIMS profile from a sample implanted with 1.86×10^{16} cm^{-2}, 200 keV Ge$^+$ prior to deposition of a polysilicon emitter and an anneal of 30 s at 1045 °C in dry N_2. The profile shows diffusion of the germanium into the polysilicon emitter.

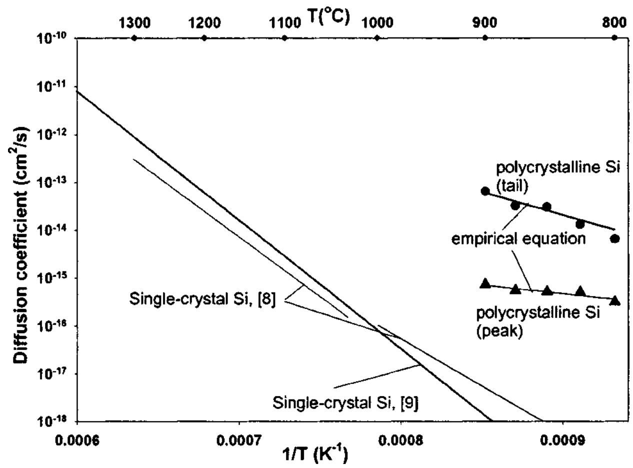

FIG. 3. Germanium diffusion coefficient in polysilicon for peak (Ge $>10^{20}$ cm^{-3}) and tail (Ge$<10^{20}$ cm^{-3}) Ge profiles as a function of reciprocal temperature, and for comparison values of germanium diffusion coefficient in single-crystal silicon (see Refs. 8, 9).

a very low value of diffusivity, and suggests that Ge diffusion in polysilicon is considerably faster than that in single-crystal Si.

Figure 2 shows Ge SIMS profiles in samples produced to quantify Ge diffusion in polycrystalline silicon. The samples were implanted with 2×10^{16} cm^{-2}, 100 keV Ge$^+$ into a 0.35-μm polysilicon layer before annealing at 800, 825, 850, 875, and 900 °C for 30 min. Each of the annealed profiles shows significant diffusion of the implanted germanium, which increases with anneal temperature. The annealed profiles have two distinct regions, one in the tail of the profile and one around the peak. The tail regions of the profiles show significant diffusion of the implanted Ge, and are similar to profiles obtained for dopant diffusion in polysilicon,[10] which occurs by a mechanism of diffusion along the grain boundaries. The peak region shows relatively little diffusion and suggests either that the Ge is trapped or segregated around the implant peak or that the Ge is diffusing only in the single-crystal grain interiors where diffusion is known to be slow.[8,9]

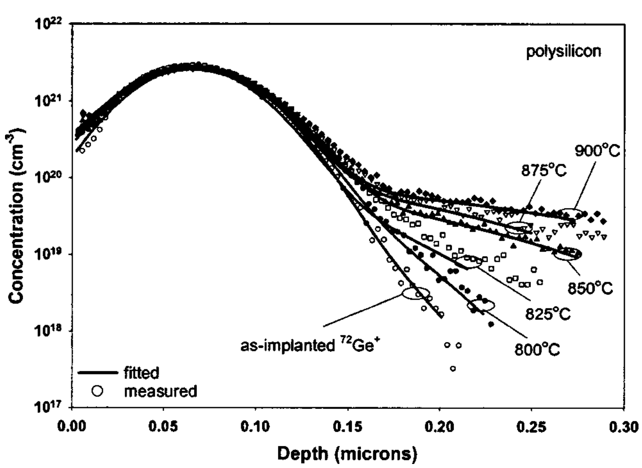

FIG. 2. Germanium SIMS profiles compared with fitted profiles for samples implanted with 100 keV 2×10^{16} cm^{-2}Ge$^+$ after polysilicon deposition and anneal for 30 min at a temperature of 800, 825, 850, 875, or 900 °C.

To extract values of diffusivity, the profiles in Fig. 2 were modeled using Eq. (1), which combines logarithmic weighted double gaussians, so that diffusion in the tail region ($<10^{20}$ cm^{-3}) can be separated from diffusion around the peak of the profile ($>10^{20}$ cm^{-3}).

$$N(x)=\frac{\Phi}{\sqrt{2\pi}(\Delta R_p^2+2D(T)t)^{1/2}} \times \exp\left\{-\frac{1}{2}\left[\frac{x-R_p}{(\Delta R_p^2+2D(T)t)^{1/2}}\right]^2\right\}. \quad (1)$$

The range and straggle were determined using the as-implanted profile with $t=0$ in Eq. (1) and a least-squares-fitting routine based on the Marquardt–Levenberg algorithm was used. In the diffused profiles, the near surface and end points of the plotted profiles (Fig. 2) were removed to reduce the noise in the data. The solid lines in Fig. 2 illustrate the fit was obtained for each of the profiles. It can be seen that a very close fit can be achieved with the experimental data.

Figure 3 summarizes the values of diffusivity obtained from fitting Eq. (1) to the profiles in Fig. 2. The values of diffusivity in the tail region can be described by an Arrhenius relationship with an activation energy (E) of 2.59 ± 0.36 eV and, a preexponential factor (D_o) of 0.026 ± 0.023 cm^2/s. For comparison, Fig. 3 also compares our measured values of diffusivity in polysilicon with measured values from the literature in single-crystal silicon.[8,9] It can be seen that the values for polysilicon are considerably higher than those for single-crystal silicon. For example, at a temperature of 900 °C, the diffusivity of Ge in polysilicon is approximately four orders of magnitude higher than that in single-crystal silicon. Similar behavior is obtained for dopant diffusion in polysilicon,[11] where arsenic and boron diffusion in polysilicon are 10^4 and 10^2 times higher in polysilicon than in single-crystal silicon, respectively, as a result of diffusion down grain boundaries. From an analogy with dopant diffusion, we hypothesise that the diffusion seen in the tail of the Ge profile is due to diffusion along the grain boundaries. Around the peak of the profile, an activation energy (E) of 0.77 ± 0.28 eV was obtained, together with a pre-exponential factor (D_o) of $1.46 \pm 0.10 \times 10^{-12}$ cm^2/s. However, the amount of diffusion around the implant peak was small and further measurements at higher temperatures are needed to be able to fully quantify the mechanisms influencing the Ge profiles around the peak.

No work has been published on Ge diffusion in polycrystalline silicon, though considerable work has been published on Ge diffusion in single-crystal silicon. For example, the isotope ^{71}Ge has been used to study silicon self diffusion[12,13] using radiotracer methods in combination with mechanical sectioning or sputter sectioning. These early studies showed significant discrepancies between results obtained by the various groups. More recently, Fahey *et al.*[14] have investigated germanium diffusion under conditions of nonequilibrium point defect concentrations in single-crystal Ge–Si grown by molecular-beam epitaxy. They concluded that germanium diffusion in single-crystal silicon occurs by both substitutional-interstitial interchange and vacancy mechanisms. Both Frank *et al.*[13] and Fahey *et al.*[14] suggest that non-Arrhenius behavior seen at about 1050 °C is caused by a change in diffusion mechanism at this temperature, although this view is not supported by Dorner *et al.*,[9] who performed a large study on ^{70}Ge using SIMS analysis.

In conclusion, the diffusion of Ge in polysilicon has been quantified to support an investigation of the anomalously high diffusion of Ge in polysilicon emitters of synthesized SiGe HBTs. Measurements of germanium diffusivity in polysilicon at volume concentrations $< 1 \times 10^{20}$ cm^{-3} have been made at temperatures between 800 and 900 °C. It is found that the diffusion can be modeled by an Arrhenius relationship with a pre-exponential factor of $D_o = 0.026 \pm 0.023$ cm^2/s and an activation energy of $E = 2.59 \pm 0.36$ eV. The measured values of diffusivity in polycrystalline silicon are approximately four orders of magnitude higher than reported values in single-crystal silicon. We hypothesis that Ge diffusion occurs along grain boundaries.

ACKNOWLEDGMENT

The EPSRC (SiGe program—Grant No. GRL50013) is acknowledged for partial funding this research.

[1] A. Schuppen, Solid-State Electron. **43**(8), 1373 (1999).
[2] K. Washio, E. Ohue, H. Shimamoto, K. Oda, R. Hayami, Y. Kiyota, M. Tanabe, M. Kondo, T. Hashimoto, and T. Harada, Tech. Dig. - Int. Electron Devices Meet. **2000**, 741.
[3] G. Freeman, D. Ahlgren, D. R. Greenberg, R. Groves, F. Huang, G. Hugo, B. Jagannathan, S. J. Jeng, J. Johnson, K. Schonenberg, K. Stein, R. Volant, and S. Subbanna, Tech. Dig. - Int. Electron Devices Meet. 1999.
[4] J. Böck, T. F. Meister, H. Knapp, D. Zöschg, H. Schäfer, K. Aufinger, M. Wurzer, S. Boguth, M. Franosch, R. Stengl, R. Schreiter, M. Rest, L. Treitinger, Tech. Dig. - Int. Electron Devices Meet. **2000**, 745.
[5] B. Martinet, H. Baudry, O. Kermarrec, Y. Campidelli, M. Laurens, M. Marty, T. Schwartzmann, A. Monroy, D. Bensahel, A. Chantre, *Proceedings of the European Solid State Device Research Conference*, (Frontier Group, France 2001), p. 97.
[6] R. Ball, Electronics Weekly, (EMBC, 2001), p. 15.
[7] S. Lombardo, A. Pinto, V. Raineri, P. Ward, G. LaRosa, G. Privitera, S. U. Campisano, IEEE Electron Device Lett. **17**, 485 (1996).
[8] G. Hettich, H. Mehrer, K. Maier, *Institute of Physics Conference Series No. 46* (Institute of Physics, University of Reading, Berkshire) p. 500.
[9] P. Dorner, W. Gust, B. Predel, U. Roll, A. Ludding, H. Odelius, Philos. Mag. A **49**(4), 557 (1984).
[10] I. R. C. Post and P. Ashburn, IEEE Electron Device Lett. **38**(11), 2442 (1991).
[11] A. G. O'Neill, C. Hill, J. King, and C. Please, J. Appl. Phys. **64**(1), 167 (1988).
[12] G. L. McVay, A. R. DuCharme, *Institute of Physics Conference Series, No. 23* (Institute of Physics, University of Reading, Berkshire, 1975), p. 91.
[13] W. Frank, U. Gosele, H. Mehrer, and A. Seeger, in *Diffusion in Crystalline Solids*, edited by G. E. Murch and A. S. Nowick (Academic, New York, 1984).
[14] P. Fahey, S. S. Iyer, G. J. Scilla, Appl. Phys. Lett. **54**(9), 843 (1989).