

Simulation of SiGe Epitaxial Growth for RF-Bipolar Transistors

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Abstract

A simple simulation model for the in-situ doped chemical vapor deposition of $\text{Si}_{1-x}\text{Ge}_x$ -epitaxial layers is presented that enables the calculation of the germanium and base doping profiles of modern rf-bipolar transistors from the process recipe, i.e. gas flows, deposition time and temperature. A first approach is based on the interpolation of experimental data characterizing the CVD-equipment. Although this gives already very good results for slowly varying GeH_4 -flows, abrupt turn-offs of the gas flow result in too steep profiles as compared to experiments. An extension of the model is presented that solves this problem via the introduction of a germanium surface layer that feeds a slowly decaying germanium concentration in the deposited silicon even after the germane flow has been turned off.

1. Introduction

Over the last few years advances in SiGe-heterojunction bipolar transistor research have shown that these device have a performance advantage of approx. 50-100% over comparable pure-silicon technologies, making this technology very attractive for wireless communication applications. The optimization of a reliable SiGe-bipolar process for a commercial high-volume production environment necessitates a careful engineering of both the doping *and* germanium profiles of the base (and possibly the emitter) region in order to optimize the device performance with respect to various trade-offs (f_T , f_{max} , R_{bi} , BV_{CE0} , etc.). Over the last few years TCAD simulation has proven to be a valuable tool for supporting this optimization process. Whereas *device* simulation of structures incorporating strained SiGe-layers is state-of-the-art in commercial TCAD systems, a consistent process simulation is not yet available. The reason for this is that typical process simulators can only deposit material layers with *predefined* thickness and doping concentration. However, since the formation of the base is the most critical process step for SiGe-HBTs, it is desirable to generate the germanium and doping profiles directly from the epitaxial recipe. For the CVD-process considered here [1], this includes the gas flows, pressure, temperatures and deposition time.

2. SiGe-epitaxy models

The probably most simple approach towards this problem is to model the deposition process via the analytical approximation of reference experimental data characterizing the CVD-equipment in very much the same way as a SPICE model simulates the response of a transistor from its measured characteristics. As an example, a comparison between the measured boron concentration vs. germane gas flow and its analytical approximation is given in Fig. 1.

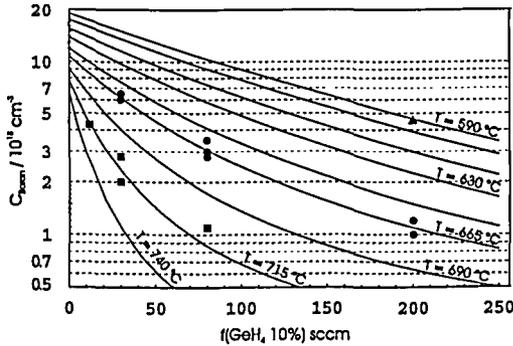


Figure 1: Comparison between measured boron concentration (symbols) and corresponding analytical approximation (lines).

Using several measurements of this kind an analytical model has been derived that allows the calculation of the germanium, boron and phosphorus concentration, as well as the deposition rate as a function of the gas flows into the reaction chamber and the processing temperature. This model is now used in the process simulator TSUPREM4 to calculate the thickness and doping information necessary to deposit—slice by slice—the various epitaxial layers. Fig. 2 shows a comparison between the results from this simple model and the corresponding experimental wafer measured by SIMS (3 keV O_2^+). The deviation from the measured signal at the right shoulder of the profiles (corresponding to the turn-on transient of the GeH_4 respectively B_2H_6 flows) is due to a SIMS knock-on effect [3]: a small part of the Ge and B atoms is not back-scattered but knocked deeper into the substrate by collisions with primary ions from the sputtering beam. Even in the case of a step-like profile this leads to an exponentially decaying tail in the measured signal. Note that a similar tail exists on the left (or turn-off side) of the Ge-profile, which can not be explained by this argument. However, the effect is an order of magnitude smaller than the peak Ge concentration and can thus be ignored.

Since the measured profile in Fig. 2 was used to calibrate the model parameters, it is more interesting to simulate a variation of this process while using the *same* model parameter set. The result of this is shown in Fig. 3 for a process recipe in which the GeH_4 -flow is turned off instantaneously. It is clear to see that the simulated Ge-profile is much steeper at the left side of the SiGe-layer. In fact, due to the very nature of the interpolation model it calculates the mole fraction of each layer according to the *momentary* GeH_4 -flow. Therefore, the simulated profile is indeed step-like and the slight rounding comes from the small but finite Ge-diffusion [2]

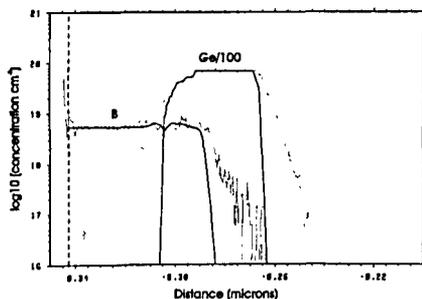


Figure 2: Comparison between measured (thick gray lines) and simulated doping and germanium profiles (thin black lines). The germanium concentration has been divided by 100 for visibility.

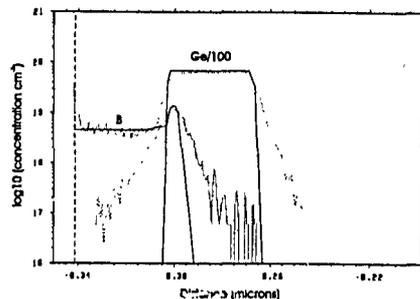


Figure 3: Same as Fig. 2, but for a recipe with instantaneous germane turn-off. The germanium concentration has been divided by 100 for visibility.

due to the epitaxial thermal budget. The possibility of a slow turn-off transient of the gas source is ruled out by the large flush-rate in the chamber (less than a second). However, from the chemistry of the deposition process [4] it is known, that the various precursor molecules (and possible gas-phase reactants thereof) are first adsorbed on the substrate surface and then broken up into fragments from which the respective atoms are eventually incorporated into the growing substrate. This leads to the conclusion that even after turn-off of the GeH_4 -flow, there is still a considerable amount of Ge atoms stored on the surface via adsorbed precursor molecules. In the course of the subsequent processing steps, these atoms either desorb from the surface or are built into the substrate, giving rise to a slowly decaying Ge concentration. For a physically rigorous treatment of this effect it would be necessary to simulate the complex chemistry and dynamics of the deposition process. This is in principal possible, and approaches in this direction have given good agreement with experiments for certain systems as e.g. $\text{GeH}_4/\text{SiH}_4$ or GeH_4/DCS [4]. However, the epitaxial process considered here [1] uses an in-situ doping of the epitaxial layer with diborane and phosphine in the gas mixture. In this case the chemical dynamics are more complicated and in fact not really known yet.

In order to solve this problem we decided to simplify the growth dynamics as much as possible. This can be done by defining a total germanium surface concentration $c_{s,\text{Ge}}$ whose time-evolution is governed by a simple rate equation, i.e. the rate of change in time of $c_{s,\text{Ge}}$ is given by a feeding rate from the gas phase germane flow and a loss rate due to incorporation of Ge-atoms into the substrate. Due to consistency with the interpolation model, this extended model has only a few parameters more which were calibrated using the Ge-profile in Fig. 3. A comparison between the experiment and the simulation with this model (c.f. Fig. 4) now shows good agreement for the left shoulder of the Ge-profile (at least in the important high-mole-fraction regime, see above). Note that as compared to Fig. 3 the width of the boron peak in the base has also increased. This is due to the fact that even after turn-off of the germane flow the enhancement of the growth rate [4] resulting from the residual Ge-atoms on the surface is still considerable.

In order to check the new simulation procedure, we have simulated several epitaxial recipes that basically vary gas flows and duration of the various deposition steps, but not the temperature profile. A typical simulation result is shown in Fig. 5. The

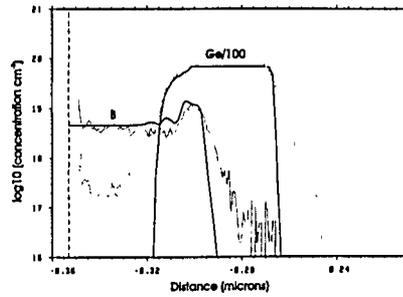
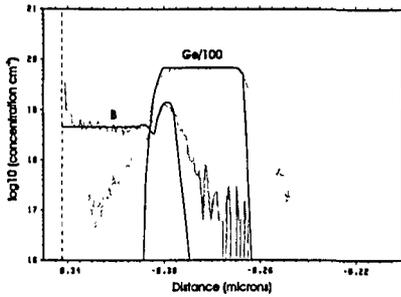


Figure 4: Same as Fig. 3, but simulated with the extended epi-model including surface adsorption effects. Figure 5: Typical simulation result for a process variation.

agreement between simulated and measured profiles is very good in the sense that in a subsequent device simulation both profiles have very similar device characteristics.

Limitations of the model: Since the model presented here is based on a simple interpolation scheme, it is clear that this approach is limited to process recipes in a parameter range close to the reference experiments. An attempt to simulate recipes with temperature profiles that were 50 °C lower and/or higher than the ones used for the reference experiments failed, because the exponentially extrapolated growth rates turned out to be too far off the experiment.

3. Conclusion

We have shown a very simple yet efficient procedure for the simulation of epitaxial growth processes, exemplified by SiGe-CVD. The model is based on the analytical approximation of experimental reference data characterizing the equipment, extended by a surface segregation model. Within the process parameter range given by the reference experiments, this model is able to calculate the germanium and doping information necessary to perform a complete process simulation of SiGe-HBT processes.

References

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