Simulation of Be diffusion in the base layer of InGaAs/InP Heterojunction Bipolar Transistors

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Abstract

In order to improve InGaAs/InP device fabrication processes and effectively control the performances of Heterojunction Bipolar Transistors (HBTs), one should avoid the undesired diffusion of p-type dopant during high-temperature device fabrication which often degrades the performances of compounds [1]. Consequently, the understanding and the control of p-type dopant diffusion in InGaAs epitaxial layers are necessary. All available beryllium diffusion profiles in InGaAs epitaxial layers have been simulated by using the Kick-out model $Be_i^0 \Leftrightarrow Be_s^- + I_{III}^+$.

1. Introduction

Investigations on Zn and Be diffusion mechanisms in the binary and ternary InP based compounds are still limited [2]. In GaAs, it is well accepted that the p-type dopants diffuse by the Substitutional Interstitial Diffusion mechanism (SID) [3-5]. The diffusion behaviour of beryllium in GaAs and related III-V compounds seems to be similar to that of zinc but much less well investigated and understood. We propose a Kick-out model to simulate the beryllium diffusion in InGaAs epitaxial layers. Example of atomic SIMS profiles of Be before and after annealing exhibiting significant diffusion are shown in figure 1.

2. The Kick-out mechanism

There has been a great deal of discussion in the literature concerning the fundamental type of exchange between interstitial and substitutional species in III-V materials [3-5]. For the GaAs and InGaAs cases, exchanges could take place via gallium and indium vacancies, the so called Longini and Frank-Turnbull mechanism, or via gallium and indium interstitial, the so called Kick-out mechanism. Comparing the superlattice disordering obtained from Be and Zn in-diffusion and out-diffusion experiments, Yu, Tan

and Gösele conclude that the Kick-out mechanism governs Be and Zn diffusion in GaAs and in GaAlAs [3]. In this study, we have assumed that the Be diffusion is similar in GaAs and in InGaAs, and we have considered only the Kick-out mechanism.

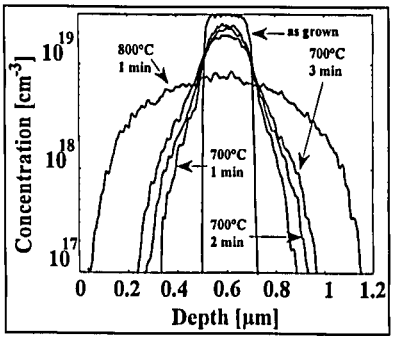

Figure 1 : SIMS Be diffusion profiles in InGaAs grown by CBE

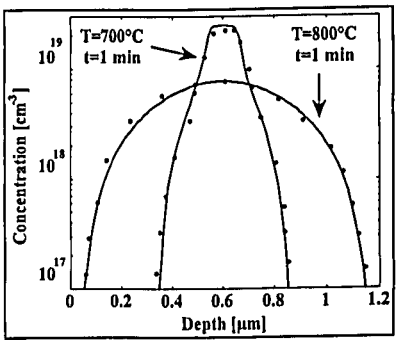

Figure 2 : Experimental Be diffusion profiles and calculated curves

The exchange between interstitial and substitutional species is given by the Kick-out mechanism :

$$A_i^{n+} \Leftrightarrow A_s^- + I_{III}^{r+} + (n - r + 1)h^+ \qquad (1)$$

where A_i^{n+} and A_s^- are interstitial and substitutional impurity atoms respectively, I_{III}^{r+} represents gallium and indium self-interstitials and h^+ is a hole; n and r are positive integers. To explain the Zn or Be diffusion profiles in GaAs compounds, several forms of Kick-out mechanisms, involving different values of n and r, have been proposed because this process requires one point defect species and one interstitial state. In the case of Be or Zn doped InGaAs and GaAs, two Be_i^{n+} and Zn_i^{n+} charges and three I_{III}^{r+} charges have been postulated Be_i^0, Be_i^+, I_{III}^0, I_{III}^+ and I_{III}^{2+}. The diffusion equations for the two mobile species are given in references 3 and 4.

3. Numerical simulation and results

An effective method of solving large parabolic systems (diffusion reaction equations) is the numerical method of lines. Using finite differences, the Partial Differential Equations (PDE) are converted into Ordinary Differential Equations (ODE). All available beryllium diffusion profiles in InGaAs epitaxial layers have been simulated by using the Kick-out model $Be_i^0 \Leftrightarrow Be_s^- + I_{III}^+$ (figure 2). Qualitative comparaisons between simulated profiles (see figures 3 and 4) with our experimental data (fig. 1) show clearly that only the mechanism $Be_i^0 \Leftrightarrow Be_s^- + I_{III}^+$ can fit correctly our experimental profiles.
The system of diffusion equations involves a number of unknown parameters that must be determined by fitting of simulated profiles with experimental data. In contrast with

silicon materials, for the III-V compounds and more particularly for $In_xGa_{1-x}As$, there is a lack in literature of a consistent set of parameters, such as the Be diffusion coefficient or equilibrium concentrations. Consequently, C_i^{eq}, D_i, $C_I^{eq}(n_i)$, D_I and K_I have been used as fitting parameters.

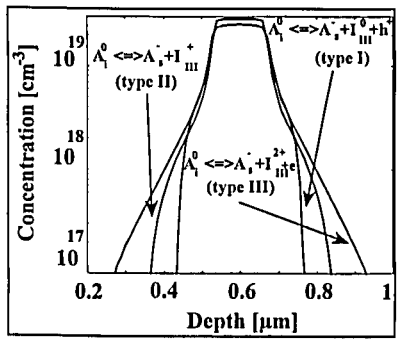

Figure 3 : Influence of species charges
Neutral beryllium interstitials

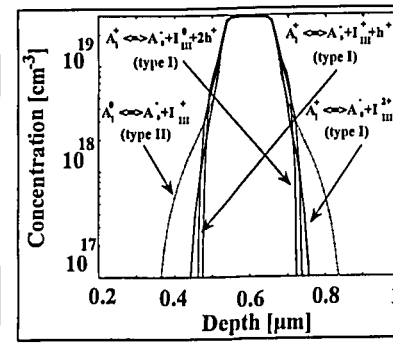

Figure 4 : Influence of species charges
Charged beryllium interstitials

In this study we have found that the p-type dopant diffusion depth is mainly determined by the diffusion coefficient $D = D_i C_i^{eq} / C_s^{eq}$. The simulated profiles seem to be approximatively insensitive to the variation of individual C_i^{eq} and D_i parameter values if their product is kept constant. This means that the same experimental profile could be fitted with several C_i^{eq} and D_i individual values. Consequently, our aim is not to propose a complete and consistent set of Be diffusion parameters but to deduce or extract some physical and absolute values in order to compare our results with published data.
With this Kick-out model, the effect of V/III ratio on diffusion profiles has been satisfactory simulated (see figure 5 and 6).

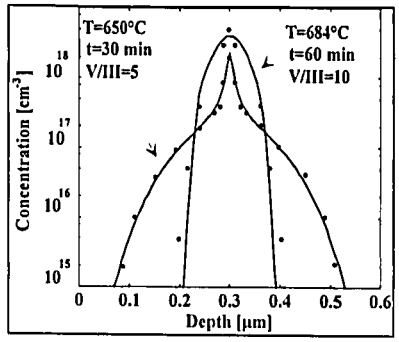

Figure 5 : Effect of V/III ratio
on diffusion profiles

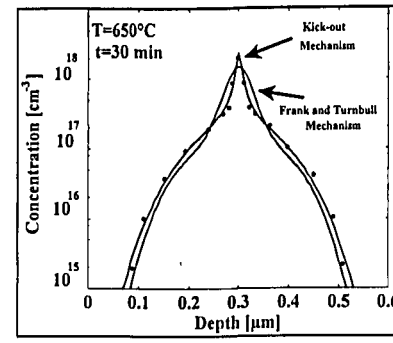

Figure 6 : Comparison between Kick-out
and Frank/Turnbull models

For the same experimental conditions (see figure 1), on figure 7, Be diffusion profiles in InGaAs grown by GSMBE are presented. We used the Kick-out model $Be_i^0 \Leftrightarrow Be_s^- + I_m^+$. We could note that the Be diffusion depth in InGaAs grown by GSMBE is small in comparaison with the depth in InGaAs grown by CBE. This shows the necessity to include growth parameters in the p-type dopant diffusion models in III-V compounds.
A beryllium diffusion profile in InGaAsP grown by GSMBE is presented on figure 8. The Be diffusion depth is higher in InGaAsP grown by GSMBE in comparaison with the diffusion depth in InGaAs grown by GSMBE. A detailed study of Be diffusion in InGaAs and in InGaAsP grown by GSMBE will be presented in a forthcoming paper.

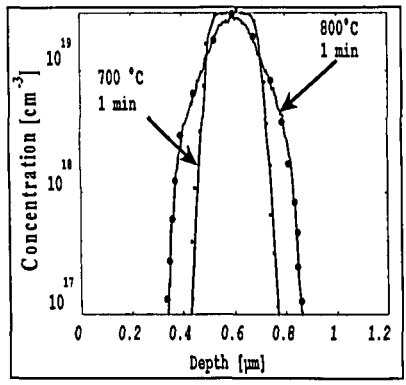

Figure 7 : SIMS Be diffusion profiles in InGaAs grown by GSMBE and calculated curves

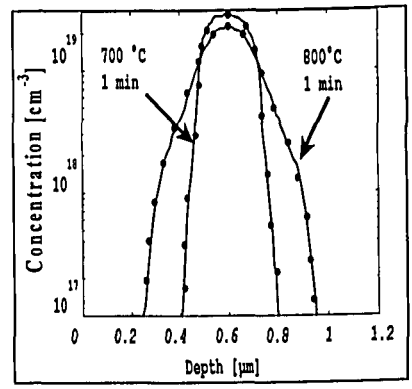

Figure 8 : SIMS Be diffusion profiles in InGaAsP grown by GSMBE and calculated curves

4. Conclusions

From our experiments (InGaAs grown by CBE, $C_0 = 3x10^{19}\,cm^{-3}$ and V/III=2), we have deduced $D = (7,7-9)x10^{-13}\,cm^2s^{-1}$ for T=700°C and $D = (1,4-1,5)x10^{-11}\,cm^2s^{-1}$ for T=800°C. In order to improve the process simulators, our work shows the necessity to include growth parameters in the p-type dopant diffusion models in III-V compounds. Accurate determination of coefficients C_i^{eq}, D_i, $C_I^{eq}(n_i)$, D_I and K_I and theoritical analysis of species charges in III-V compounds would be the most significant developpment of future research.

References

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