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RESEARCH ARTICLES

DEFECT REACTIONS OF Si IMPLANTATION IN GaAS

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ABSTRACT

We present a model of defect reactions that describes the electrical activation of Si implanted in simi - insulating GaAs. The model is fit to existing data that exhibit the dependence of carrier concentration on Si concentration, annealing temperature, and the concentration of the native mid-gap electron trap EL2. The defects present are Si_I, $Si_{Ga}V_{As}^+$, Si_{Ga}^+, Si_{As}^-, Si_{Ga}^+. Si_{As}^- *and EL2. Some defect reaction energies, dependence of optimum annealing temperature on Si dose and a restriction on the possible atomic structure of EL2 are obtained.*

INTRODUCTION

Si implantation into GaAs is a process used in FET fabrication. In this process we want the implanted Si to land on Ga site and form donor defect. After implantation the implanted region will be n-type region. Electron concentration in this region depends on the concentration of implanted Si, concentration of native defect in SI - GaAs wafer, on annealing temperature and detail in the implantation process.

In this study we are interested in the dependence of carrier concentration on annealing temperature, Si concentration and EL2 concentration, which is a mid -gap electron trap native defect.

EXPERIMENTAL DATA

From many published papers, each Si implantation study was often conducted at a constant implantation energy and a constant Si fluence. Results were often reported in the form of sheet carrier concentration as a function of annealing temperature, or carrier concentration as a function of implantation depth[1].

After implantation Si depth profile has a gaussian - like distribution form. Abromove *et al.*[2] calculated the implantation profile of each type of ion at various implantation energy in GaAs. When we use results of their calculation with the carrier profile reported in many published paper[1, 3-7], we can draw average carrier concentration as function of silicon concentration and annealing temperature as shown in figures 1 and 2.

Si activation efficiency is defined as the ratio between electron concentration in the implanted region concentration to Si concentration. From figure 1 at low Si concentration the activation efficiency is almost 100%. This activation efficiency decreases as Si concentration increases. The maximum carrier concentration is about $5x10^{18}$ cm^3 .From figure 2 the activation efficiency increases as the annealing temperature increases from about 600°C to some optimum annealing temperature, and decreases when the annealing temperature increases further. We also see from figure 2 that the optimum annealing temperature increases as Si concentration increases.

Another factor that has effect on Si activation efficiency is the concentration of native defect. The most important native defect in SI-GaAs is EL2 which is found in SI - GaAs grown under As rich condition. The maximum EL2 concentration found from experiment is about $2x10^{16}$ cm^{-3}. Brierley *et al.*[8] studied the dependence of carrier concentration on EL2 concentration. They found that the carrier concentration has some correlation with EL2 concentration. As EL2 concentration increases, carrier concentration also increases.

MODEL EFFECT OF ANNEALING TEMPERATURE ON ACTIVATION EFFICIENCY

At low Si concentration

We suppose without loss of generality that after implantation, all Si^+ land in interstitial sites as Si_I^0. After annealing for low Si concentration at annealing temperature between 600°C and 900°C, the activation efficiency is almost 100%. Defect reaction in this process must use or creat Ga sites in the same amouth as As sites. All of Si must form donor defect. A possible defect reaction is

$$Si_I^0 \rightleftharpoons Si_{Ga}V_{As}^+ + e^- . \quad \ldots\ldots (1)$$

$Si_{Ga}V_{As}^+$ is the donor defect created during the annealing process. The corresponding mass action law is

$$K_1(T)N_{SI} = N_{SV}N_H , \quad \ldots\ldots (2)$$

where $K_1(T)$ is the equilibrium constant, depends only on temperature,

N_{SI}, N_{SV}, and N_H are the concentrations of Si_I^0, $Si_{Ga}V_{As}^+$, and electron at annealing temperature, respectively,

and $$Ki(T) = Ki^0 e^{-Ei/kT}, \quad \ldots\ldots (3)$$

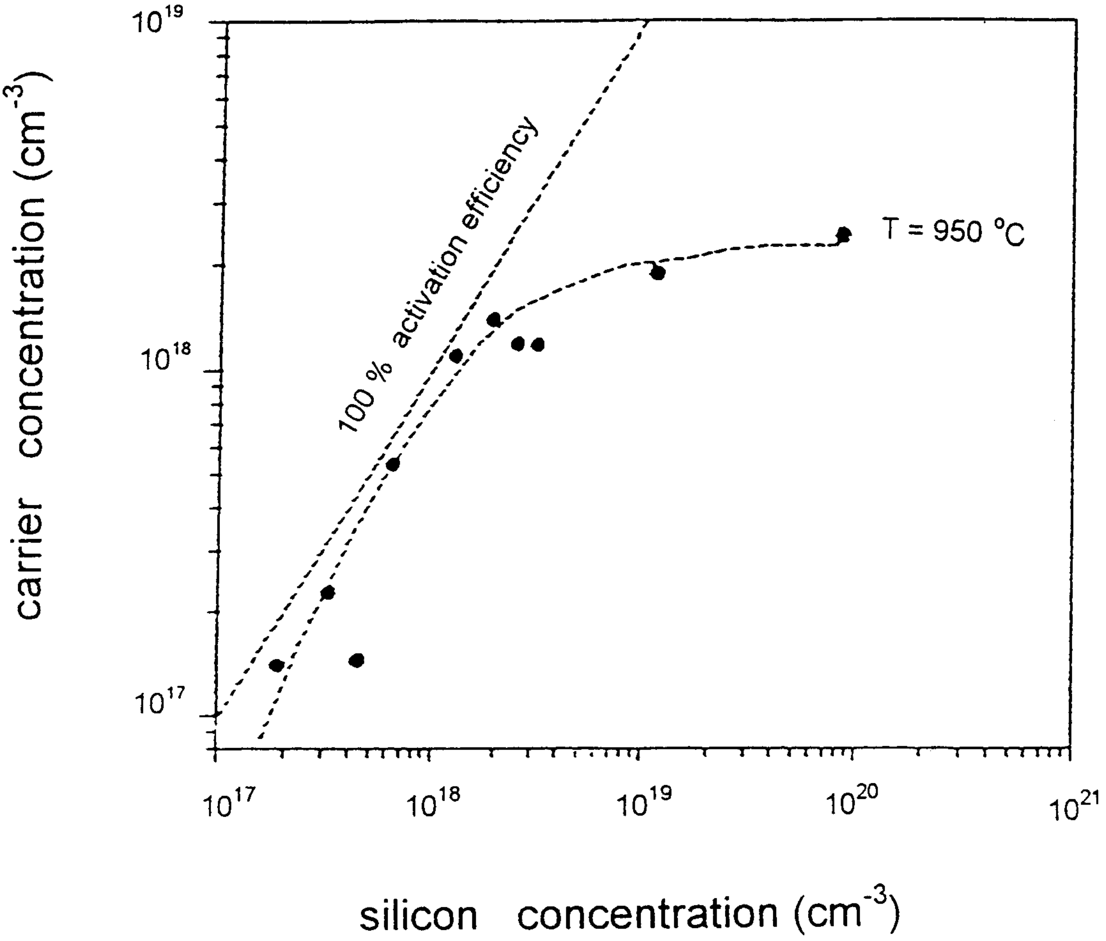

Fig. 1. Carrier concentration as a function of implanted silicon concentration compared with experimental results from many published papers (1, 3-7)

●●●●●●● from experiments

- - - - - - - - average

at an annealing temperature of 950°C.

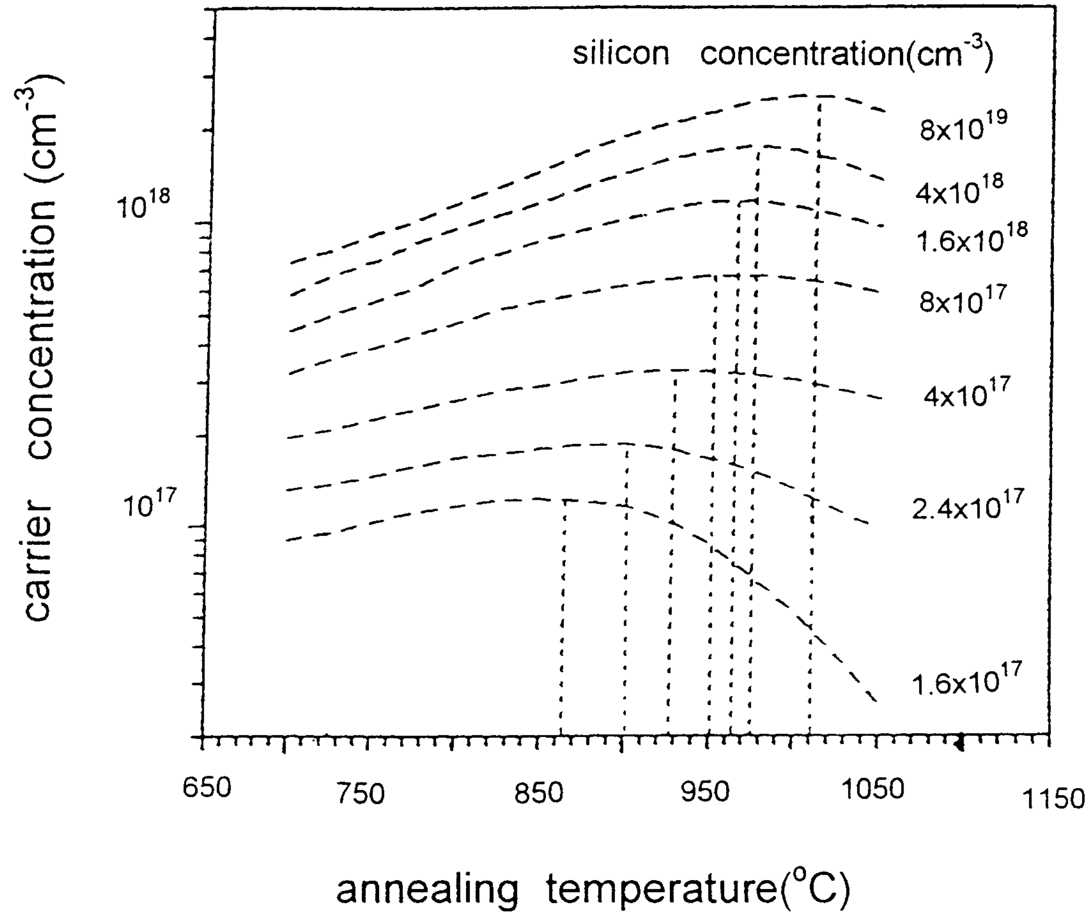

Fig. 2. The dependence of carrier concentration on annealing temperature for constant Si doses. The vertical dashed lines show the optimum annealing temperature for each dose.

K_i^0 and E_i are the constant and the energy of the ith reaction.

At very high annealing temperature, the activation efficiency decreases as the annealing temperature increases. Si-related acceptor defect should be created as well as Si-related donor defect. A possible defect reaction is

$$2\ Si_I^0 \rightleftharpoons Si_{Ga}^+ + Si_{As}^- . \qquad (4)$$

Its corresponding mass action law is

$$K_2(T)N_{SI}^2 = N_{SG}\, N_{SA}\ , \qquad (5)$$

where N_{SG} and N_{SA} is the concentration of Si_{Ga}^+ and Si_{As}^- respectively.

At high Si concentration

At a constant annealing temperature, as shown in figure 1, the activation efficiency decreases as Si concentration increases. Many published papers[9-13] suggest that the neutral $Si_{Ga}^+ . Si_{As}^-$ may become important. A defect reaction that might occur is

$$2\ Si_I^0 \rightleftharpoons Si_{Ga}^+ . Si_{As}^- . \qquad (6)$$

Its corresponding mass action law is

$$K_3(T)N_{SI}^2 = N_{SGA}\ , \qquad (7)$$

where N_{SGA} is the concentration of $Si_{Ga}^+ . Si_{As}^-$.

At very low Si concentration

Since EL2 is an As rich defect, arsenic vacancy-related defect should be its favor. A possible defect reaction is

$$EL2 + \delta_E\ Si_{Ga}V_{As}^+ \rightleftharpoons \delta_E Si_{Ga}^+ , \qquad (8)$$

$$\text{and } K_4(T)N_E N_{SV}^{\delta E} = N_{SG}^{\delta E} \qquad (9)$$

is its mass action law,

where N_E is the concentration of EL2,

δ_E is the stoichiometry deviation signature of EL2.

δ_E is defined as the difference between numbers of As atoms and Ga atoms in EL2. After annealing all EL2 must be used in this reaction. It has a remark that $Si_{Ga}V_{As}^+$ defect has stoichiometry deviation signature the same as Si_I^+ presented in ref. 14.

Constraints in modeling

In order to calculate carrier concentration at room temperature as a function of Si concentration and annealing temperature from above reactions, we have to have other constraints. The first constraint in our modeling is the conservation of Si; The concentration of Si before annealing must equal to the summation of Si concentrations in all Si-related defects after annealing. The second constraint is that the number of Ga sites and As sites used or created must be equal. Sometimes this constraint is called the conservation of stoichiometric deviation[15]. The third constraint is the neutrality of the sample; The net local charge of sample must be zero. The last constraint shows the important of intrinsic carrier concentration at annealing temperature n_i and also shows the relation between the carrier concentration at annealing temperature N_H and room temperature N_L;

$$NH - \frac{n_i^2}{N_H} = N_L. \quad \text{..} \quad (10)$$

RESULTS

At low Si concentration of $8x10^{17}$ cm^{-3}, we use only reactions in eqs.(1) and (4). The best values of E1 and E2 are 1.1 eV and 5.5 eV respectively, and the best values of K_1^0 and $ln(K_2^0)$ are $1.2x10^{23}$ cm^{-3} and 48.5 respectively. Graphs of carrier concentration versus annealing temperature and versus Si concentration are shown in figures 3, 4 and 5. From figures 3 and 4, when only reactions in eqs.(1) and (4) are used with a set of E_1, E_2, K_1^0 and K_2^0, carrier concentration increases as annealing temperature increases from about 600°C to 950°C. Then the carrier concentration decreases as the annealing temperature increases further. This is the same as general feature observed from experiments. By using these two reactions, the optimum annealing temperature is constant, at about 950°C, but from experiments, it depends on Si concentration. From figure 5 at low Si concentration, the result from our modeling is close to the experimental results, but at high Si concentration, the model gives higher carrier concentration.

Including reaction in eq. (6) in our calculation, the appropriate K_3^0 and E_3 are $3.1x10^{-16}$ cm^3 and 0.4 eV. The results are shown in figure 6, 7 and 8. From these figures we can see that when $Si_{Ga}^+.Si_{As}^-$ defect is added in our model, it does not only reduce the activation efficiency at high Si concentration but also shifts the optimum annealing temperature to the higher value as Si concentration increases.

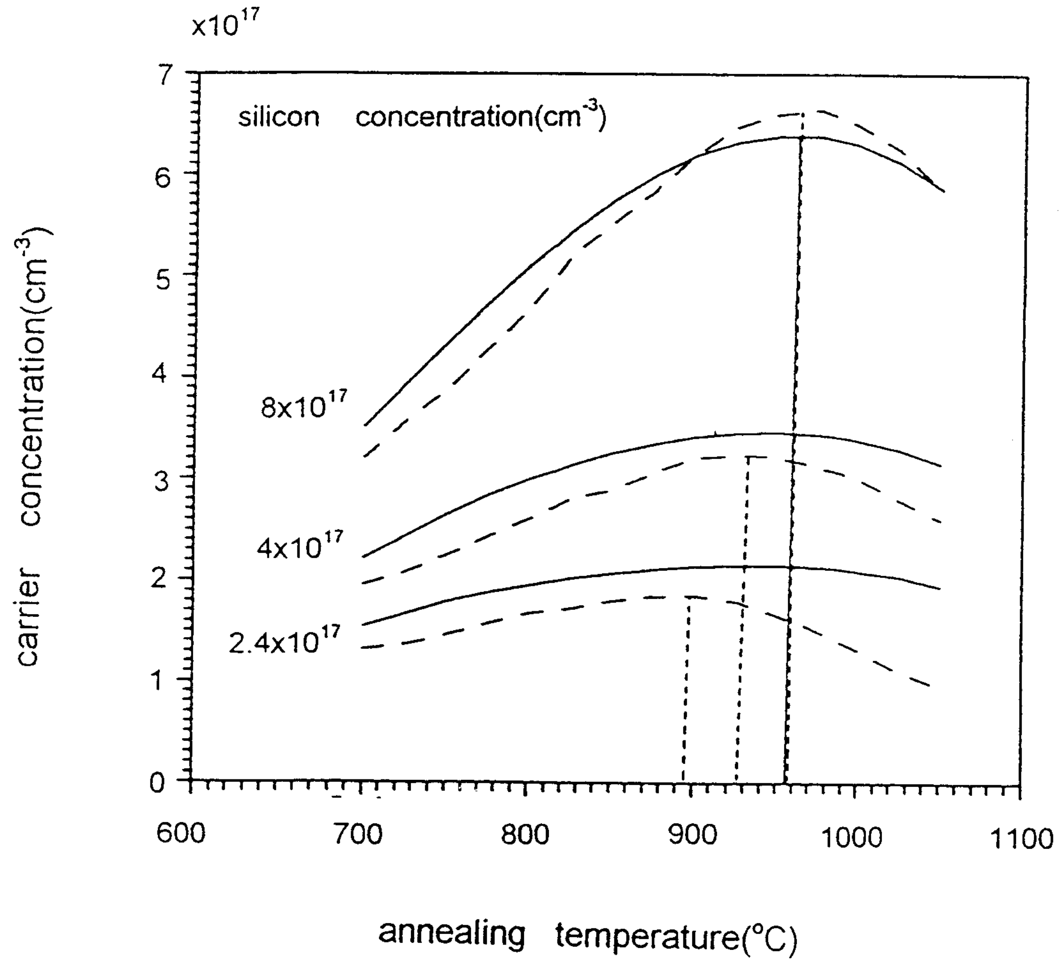

Fig. 3. Room temperature carrier concentration as a function of annealing temperature at Si concentration equal to and less than 8x10^{17} cm^{-3}.

- - - - - average from many experiments

——— calculated by using only two reactions in eqs. (1) and (4).

Vertical lines show the optimum annealing temperatures.

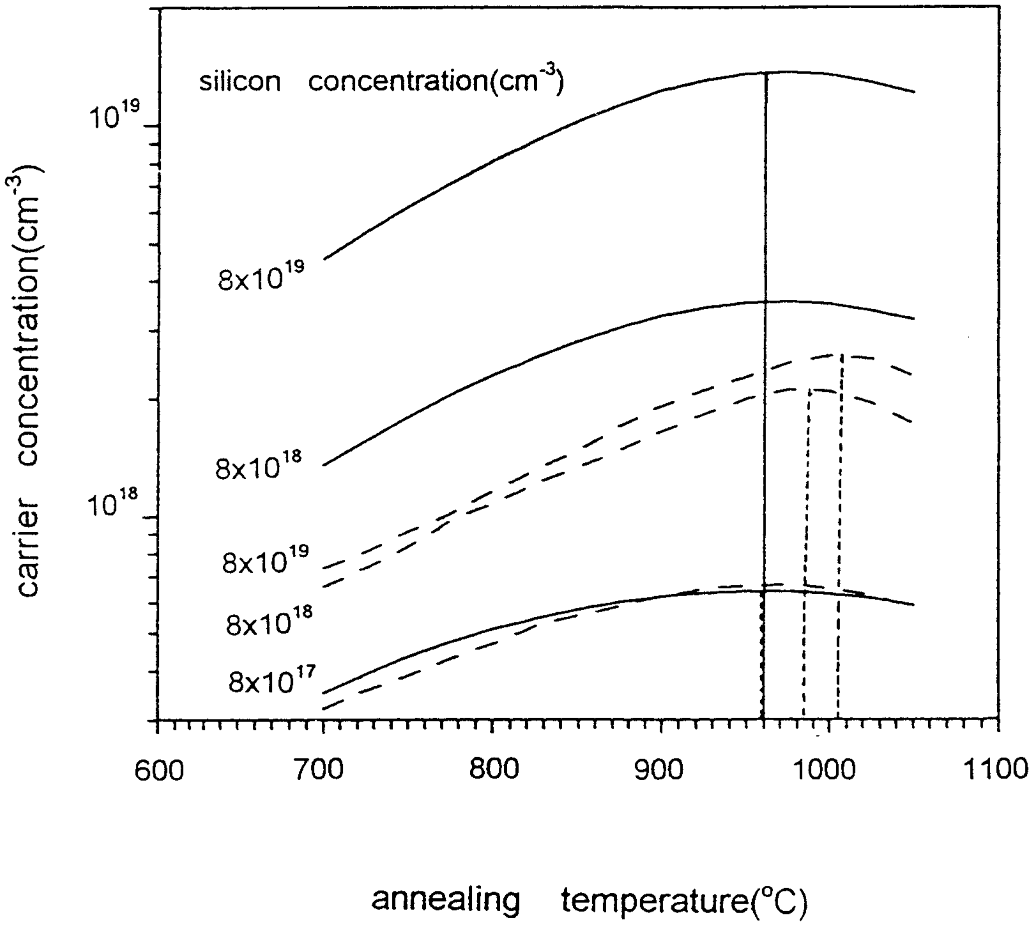

Fig. 4. Room temperature carrier concentration as a function of annealing temperature at Si concentrations equal to and greater than 8x10^{17} cm^{-3}.

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——— calculated by using only the two reactions in eqs.(1) and (4).

Vertical lines show the optimum annealing temperatures.

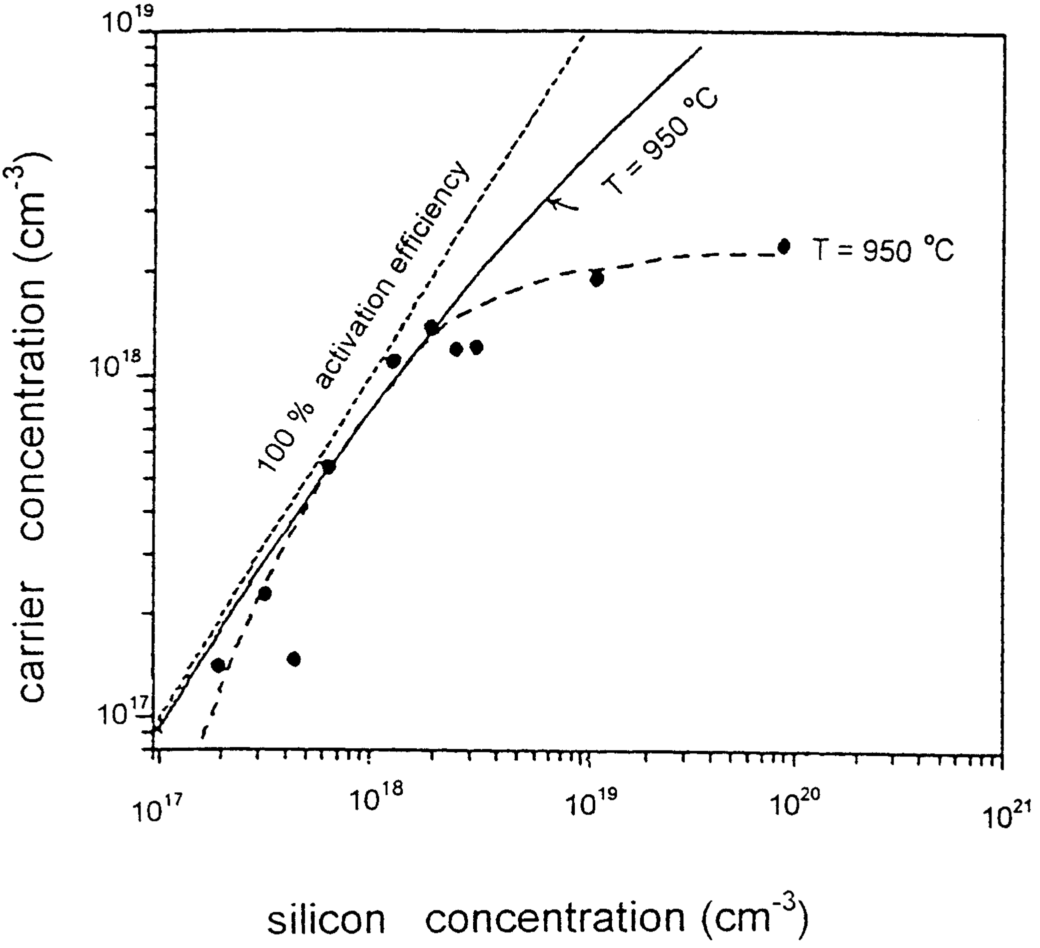

Fig. 5. Room temperature carrier concentration as a function of Si concentration

●●●●●●● experimental data

- - - - - - - average from many experimental results

——————— result from modeling by using only two defect reactions in eqs. (1) and (4)

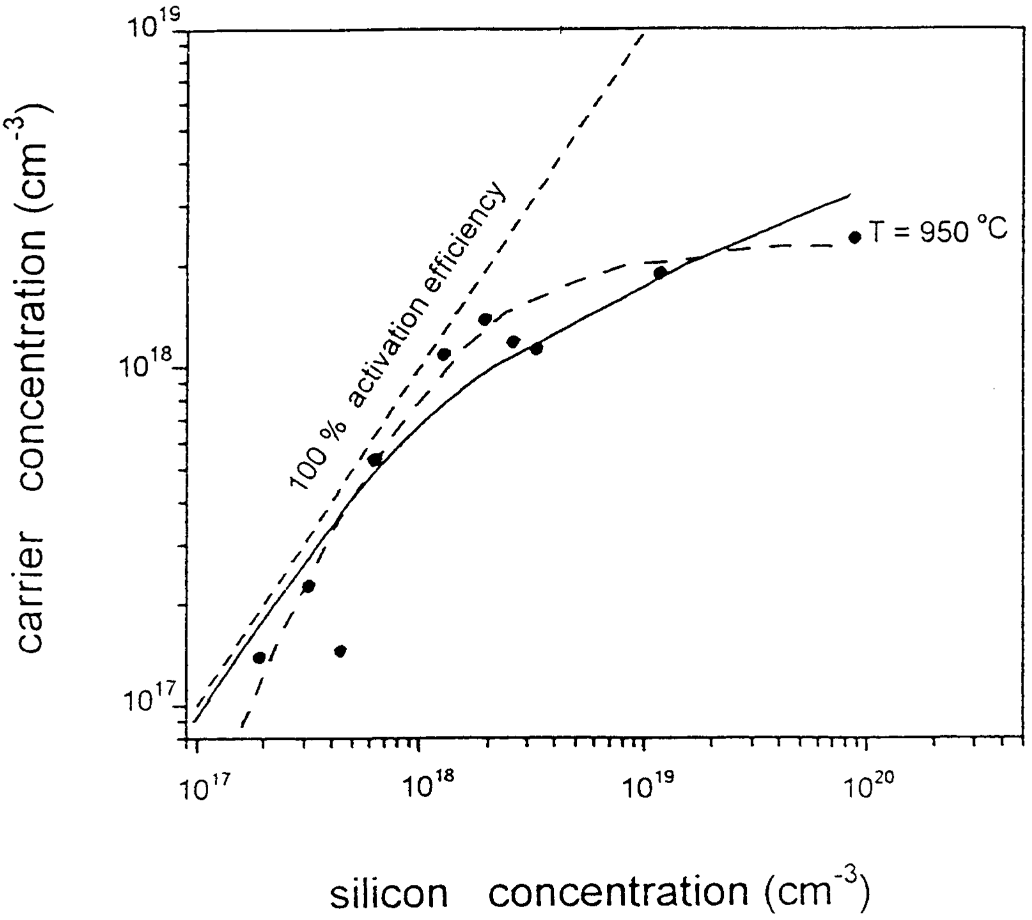

Fig. 6. Room temperature carrier concentration as a function of silicon concentration at annealing temperature T= 950° C

●●●●●●● original experimental results

- - - - - - - - average from many experimental results

———— from model which includes the Si_{Ga}^{+} . Si_{As} defect.

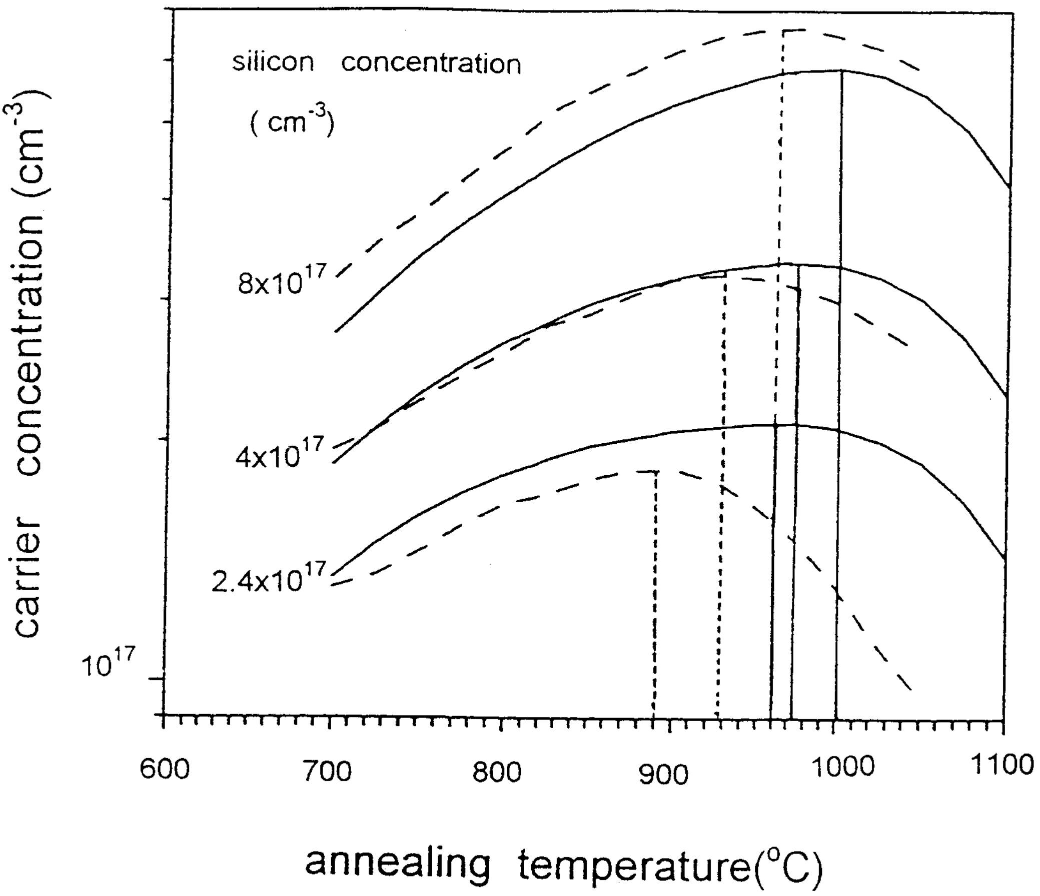

Fig. 7. Room temperature carrier concentration as a function of annealing temperature for silicon concentrations equal to and less than 8x10^{17} cm^{-3}.

- - - - - - - average from many experimental results

———— result from model which includes the Si_{Ga}^{+} . Si_{As}^{-} defect.

The vertical lines are optimum annealing temperatures.

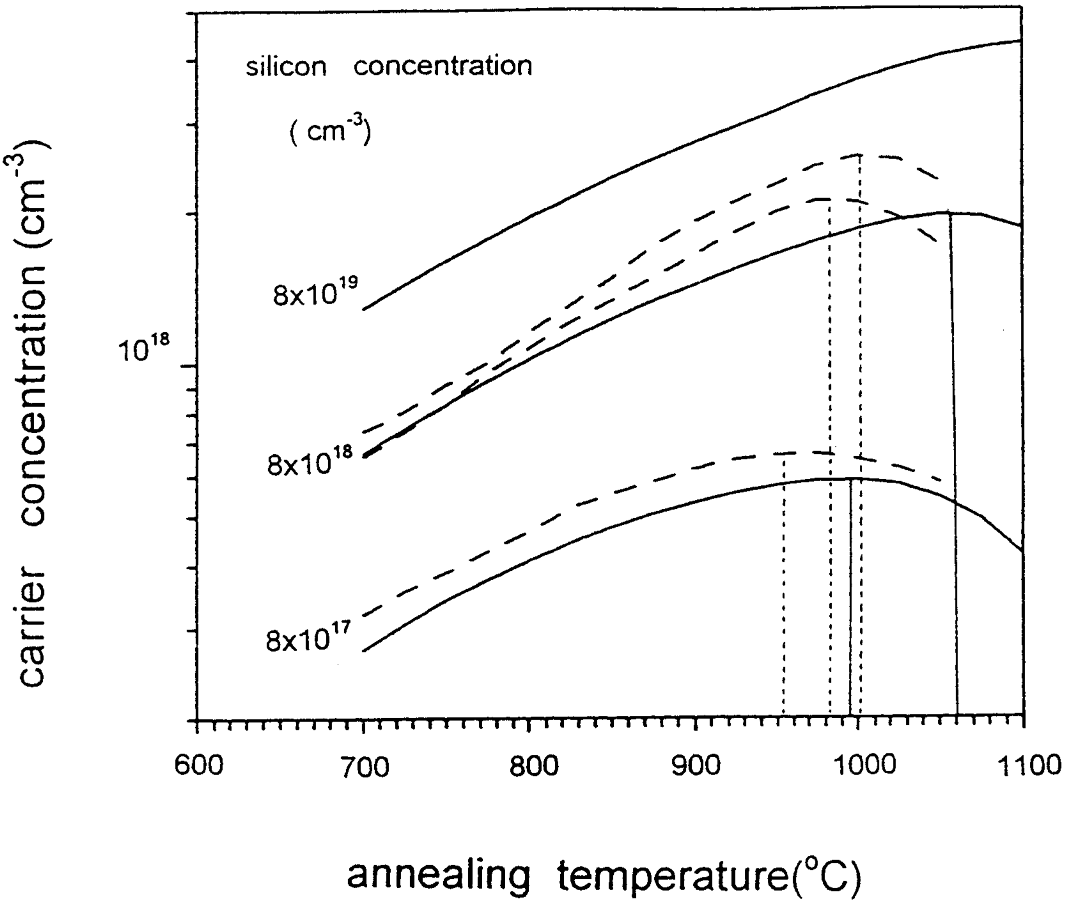

Fig. 8. Room temperature carrier concentration as a function of annealing temperature for silicon concentrations equal to and greater than 8x10^{17} cm^{-3}.

- - - - - - - average from many experimental results.

———— result from model which includes the Si_{Ga}^{+} . Si_{As} defect.

The vertical lines are optimum annealing temperatures.

At low Si concentration, effect of EL2 in eq. (8) is added. Since $Si_{Ga}V_{As}^+$ has the same stoichiometric deviation signature the same as Si_I^+ presented in ref.14, this result fits well to Brierley's data and give the same appropriate values of δE.

CONCLUSION

In this paper we consider Si activation in GaAs from many published papers and present some possible defect reactions during post annealing. The model shows effect of annealing temperature and Si concentration on activation efficiency. In this model effect of EL2 is also included. From experimental data we calculate reaction energy for each reaction. We can use these values to calculate carrier concentration at various annealing temperature and various Si concentration.

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