Available online at www.sciencedirect.com
ScienceDirect
Computational Materials Science 43 (2008) 902–908
COMPUTATIONAL MATERIALS SCIENCE
www.elsevier.com/locate/commatsci

A computational study of ion-implanted beryllium diffusion in gallium arsenide

S.D. Koumetz [a,*], J.-C. Pesant [b], C. Dubois [c]

[a] GPM, UMR CNRS 6634, Technopôle du Madrillet, 76800 Saint Etienne du Rouvray, France
[b] IEMN, UMR CNRS 8520, Cité Scientifique, 59652 Villeneuve d'Ascq, France
[c] LPM, UMR CNRS 5511, 7 Avenue Jean Capelle, 69621 Villeurbanne, France

Received 21 August 2007; accepted 5 February 2008
Available online 19 March 2008

Abstract

The diffusion of implanted beryllium in gallium arsenide at 100 keV for doses of 1×10^{13} and 1×10^{14} cm^{-2} during post-implant RTA were studied and simulated at temperatures of 700–900 °C for 1–4 min. The observed Be diffusion profiles, obtained by the SIMS technique, can be satisfactorily explained in terms of a "kick-out" model of the substitutional-interstitial diffusion mechanism, involving singly ionized Be and doubly ionized Ga interstitial species. The generation of the excess Ga interstitials, according to the "plus-one" approach, and its annihilation in the local Ga interstitial sink region were taken into account. The corresponding coupled partial differential equations of the relevant diffusion model were solved numerically with proper initial and boundary conditions using the computational algorithms based on finite-difference approximations.

PACS: 66.30.J−; 61.72.U−; 61.72.uj; 68.49.Sf; 82.80.Ms; 61.72.Cc

Keywords: Diffusion; Be; GaAs; Ion implantation; RTA; SIMS

1. Introduction

Gallium arsenide is a high-mobility, direct band-gap III–V semiconductor which is useful for a large variety of applications.

Due to its strong penetrating power [1] and high electrical activation [2] ion-implanted beryllium is one of the commonly used p-type dopants in gallium arsenide.

It has been observed that Be implanted in GaAs exhibits an important diffusion behavior during post-implanted annealing [3–6] which need be clearly understood to improve GaAs device fabrication process.

In comparison with the diffusion studies of grown-in Be in GaAs [7–11], investigations on the diffusion mechanisms of implanted Be in GaAs are still limited [5,6]. In these last works, Be diffusion in GaAs is considered to proceed under the kick-out form of the substitutional-interstitial diffusion (SID) mechanism [12] in consistency with the impurity-induced superlattice disordering [13]:

$$\mathrm{Be_i^{+j}} \underset{k_b}{\overset{k_f}{\Longleftrightarrow}} \mathrm{Be_s^-} + \mathrm{I_{Ga}^{+n}} + (1+j-n)\mathrm{h^+} \tag{1}$$

where $\mathrm{Be_i^{+j}}$ represents an ionized Be interstitial with charge $+j$, $\mathrm{Be_s^-}$ stands for an active substitutional Be acceptor with charge -1 on a Ga site, $\mathrm{I_{Ga}^{+n}}$ indicates an ionized Ga interstitial with charge $+n$, $\mathrm{h^+}$ is a free hole, k_f and k_b denote the forward and backward reaction rate coefficients, respectively. The thermodynamic equilibrium constant associated with diffusion reaction (1) is given by

$$K = \frac{k_b}{k_f} \tag{2}$$

2. Experiment

For this experiment, undoped semi-insulating ⟨1 0 0⟩ oriented liquid-encapsulated Czochralski-grown (LEC) GaAs

* Corresponding author. Tel.: +33 232 955152.
E-mail address: Serge.Koumetz@univ-rouen.fr (S.D. Koumetz).

0927-0256/$ - see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.commatsci.2008.02.003

wafers from Freiberger were implanted at room temperature with Be^+ ions at an energy of 100 keV and doses of 1×10^{13} and $1 \times 10^{14}\ cm^{-2}$ in an Eaton 3204 system.

The post-implant rapid thermal annealing (RTA) of the samples was performed under $N_2 + 15\%H_2$ flowing forming gas at temperatures of 700, 750, 800, 850 and 900 °C for 1, 2, 3 and 4 min in a halogen-lamp furnace Jetstar 100S from Jipelec. The implanted capless samples covered a virgin GaAs wafer to create an overpressure of As between the contact surfaces according to the close contact method [14].

The Be atomic profiles were measured by secondary ion mass spectrometry (SIMS) using a Cameca IMS-4F system. An oxygen-ion primary sputtering beam at an energy of 8 keV and an intensity of 300 nA was rastered over a flat 250 μm × 250 μm area, and $^{9}Be^+$, $^{69}Ga^+$ and $^{75}As^+$ secondary ions were collected from an inner area of 60 μm in diameter with a mass resolving power of 300.

The depth of the SIMS craters were determined by means of a P10 KLA-Tencor surface profilometer with an accuracy of about 5%.

3. Results and discussion

3.1. Transient enhanced diffusion

The observed transient enhanced diffusion (TED) of ion-implanted Be in GaAs during the early stages of RTA treatments, has been essentially attributed in our study to the strong excess of Ga interstitial point defects generated by the implanted Be interstitial ions moving onto substitutional lattice sites via kick-out process as soon as the annealing begins according to the plus-one model [15]. This approach assumes that during the anneal one additional self-interstitial without vacancy is created by kick-out process for each implanted dopant ion in addition to the self-interstitials of Frenkel pairs which are generated by knock-on process in course of ion implantation. Since the self-interstitial excess predicted by the plus-one model is much larger then that due to the implanted process [6], the distribution of additional self-interstitials matches the implanted dopant distribution [15].

It has been assumed in this work that the implantation process involves the formation of a heavily damaged region [16], extending from the surface to just beyond the mean projected range distance R_p inside the sample [6]. The extended defects of this region, such as primarily interstitial-type dislocation loops [17] act as sinks for Ga interstitials [18], absorbing their excess with a rate linearly proportional to the deviation of its concentration from thermal equilibrium value [19]. It was supposed also that after certain saturation time, depending on damage and annealing temperature, the dislocation loops stopped to grow and consequently acted as inefficient sinks [6,18]. On the other hand, we assumed that the annihilation of the excess self-interstitials at climbing dislocations [20] outside the damage region was negligibly small.

3.2. Diffusion model

In this paper, to explain the observed Be diffusion, we propose a kick-out model based on singly positively charged Be interstitials [6,7,10,21] and doubly positively charged Ga interstitials [8,9,22–26] in accordance with theoretical and experimental studies of Be and Ga mobile charge states:

$$\mathrm{Be_i^+} \underset{k_b}{\overset{k_f}{\Longleftrightarrow}} \mathrm{Be_s^-} + \mathrm{I_{Ga}^{+2}} \tag{3}$$

Using the second law of Fick adapted for SID mechanism and the law of mass action [27], the mathematical form of Be diffusion in GaAs, based on the reaction (3), can be given by the following set of three coupled partial differential equations (PDE) [15,28]:

$$\frac{\partial C_{\mathrm{Be_s^-}}}{\partial t} = k_f C_{\mathrm{Be_i^+}} - k_b C_{\mathrm{Be_s^-}} C_{\mathrm{I_{Ga}^{+2}}} \tag{4}$$

$$\frac{\partial C_{\mathrm{Be_i^+}}}{\partial t} = D_{\mathrm{Be_i^+}} \frac{\partial^2 C_{\mathrm{Be_i^+}}}{\partial x^2} - D_{\mathrm{Be_i^+}} \frac{\partial}{\partial x}\left(\frac{C_{\mathrm{Be_i^+}}}{p}\frac{\partial p}{\partial x}\right) - (k_f C_{\mathrm{Be_i^+}} - k_b C_{\mathrm{Be_s^-}} C_{\mathrm{I_{Ga}^{+2}}}) \tag{5}$$

$$\frac{\partial C_{\mathrm{I_{Ga}^{+2}}}}{\partial t} = D_{\mathrm{I_{Ga}^{+2}}} \frac{\partial^2 C_{\mathrm{I_{Ga}^{+2}}}}{\partial x^2} - 2D_{\mathrm{I_{Ga}^{+2}}} \frac{\partial}{\partial x}\left(\frac{C_{\mathrm{I_{Ga}^{+2}}}}{p}\frac{\partial p}{\partial x}\right) + (k_f C_{\mathrm{Be_i^+}} - k_b C_{\mathrm{Be_s^-}} C_{\mathrm{I_{Ga}^{+2}}}) - k_{\mathrm{I_{Ga}^{+2}}}(C_{\mathrm{I_{Ga}^{+2}}} - C^{eq}_{\mathrm{I_{Ga}^{+2}}}) \tag{6}$$

Here $C_{\mathrm{Be_i^+}}$, $C_{\mathrm{I_{Ga}^{+2}}}$ and $D_{\mathrm{Be_i^+}}$, $D_{\mathrm{I_{Ga}^{+2}}}$ represent concentrations and diffusion coefficients of $\mathrm{Be_i^+}$ and $\mathrm{I_{Ga}^{+2}}$ species, respectively. $C_{\mathrm{Be_s^-}}$ and p denote $\mathrm{Be_s^-}$ and h^+ concentrations, respectively. The second terms on the right-hand sides of Eqs. (5) and (6) account for the built-in electric field action on $\mathrm{Be_i^+}$ and $\mathrm{I_{Ga}^{+2}}$ charged mobile species [29]. The last term of Eq. (6) with the Ga interstitial annihilation rate coefficient $k_{\mathrm{I_{Ga}^{+2}}}$ is due to the local sinks of the heavily damaged region [6,19].

It can be seen from Eqs. (5) and (6) that we considered space and time independent diffusion coefficients of involved mobile species [8,30].

The local thermal equilibrium concentration of the doubly positively ionized Ga interstitials is determined by the local hole thermal equilibrium concentration via Fermi-level effect [31]:

$$C^{eq}_{\mathrm{I_{Ga}^{+2}}} = C^{eq}_{\mathrm{I_{Ga}^{+2}}}(n_i)\frac{(p^{eq})^2}{n_i^2} \tag{7}$$

where $C^{eq}_{\mathrm{I_{Ga}^{+2}}}(n_i)$ stands for $\mathrm{I_{Ga}^{+2}}$ thermal equilibrium concentration under intrinsic conditions.

The forward rate coefficient of the reaction (3) can be substituted in Eqs. (4)–(6) using the principle of detailed balance for this reaction at dynamical equilibrium [28,32]:

$$k_f = k_b \frac{C^{eq}_{\mathrm{Be_s^-}} C^{eq}_{\mathrm{I_{Ga}^{+2}}}}{C^{eq}_{\mathrm{Be_i^+}}} \quad \text{at } x = R_p \quad \text{for } t = 0 \tag{8}$$