

## DEPTH PROFILES AND CRYSTALLIZATION BEHAVIOUR OF Mg IONS IMPLANTED INTO Si

Ch. Angelov<sup>\*</sup>, Bl. Amov, A. Kinomura<sup>a</sup>, E. Goranova<sup>b</sup>, G. Beshkov<sup>c</sup>, M. Takai<sup>d</sup>

Institute for Nuclear Research and Nuclear Energy, <sup>b</sup>Central Laboratory of Solar Energy and New Energy Sources, <sup>c</sup>Institute of Solid State Physics, BAS, 72 Tzarigradsko Chaussee Blvd., Sofia 1784, Bulgaria

<sup>a</sup>National Institute of Advanced Industrial Science and Technology, Midorigaoka, Ikeda, Osaka 563-8577, Japan

<sup>d</sup>Research Center for Materials Science at Extreme Conditions, Osaka University, Toyonaka, Osaka 560-8531, Japan

The samples under investigation were prepared by implantation of  $\text{Mg}^+$  ions into high resistivity (780 – 850)  $\Omega$  cm, n-type Si wafers with (111) orientation. Two different doses of  $\text{Mg}^+$  ions were implanted:  $D1 = 2 \times 10^{17} \text{cm}^{-2}$  and  $D2 = 4 \times 10^{17} \text{cm}^{-2}$ , at an energy of 40 keV. Subsequently, the implanted samples were annealed at a temperature  $T_a = 500$  C for different times  $t_a = 30, 60$  and  $300$  s. The  $\text{Mg}^+$  ion concentration distribution was simulated by TRIDYN (dynamic computer simulation code), and the initial profiles of the implanted  $\text{Mg}^+$  were estimated. The composition and the thickness of the implanted layer, both as-implanted and annealed, were evaluated from the computer simulations of the measured Rutherford backscattering profiles, and were compared with the TRIDYN simulation.

(Received December 9, 2004; accepted January 26, 2005)

**Keywords:**  $^{24}\text{Mg}^+$  ion implantation, RBS, Computer simulation

### 1. Introduction

Recently, silicides consisting of non-toxic and abundantly spread elements, have attracted much interest as environment friendly semiconducting materials [1]. They are expected to be applied as highly efficient solar cells or infrared (IR) optoelectronic devices such as light emitting diodes and IR sensors compatible with present optical telecommunication systems [2,3].

Ion implantation is one of the most suitable techniques for obtaining polycrystalline silicides. The ion beam synthesis (IBS) method is widely employed to form them [4]. The IBS precise profile control of atoms, implanted with a high dose  $\sim 10^{17} \text{cm}^{-2}$ , is crucial for the fabrication of high quality polycrystalline layers and  $\text{Mg}_2\text{Si}$  precipitates embedded in Si matrices. The crystal growth mechanism during the IBS silicide phase formation is complicated, and depends on the implantation and the post implantation annealing conditions. Thus, implantation profile control is very important when fabricating semiconducting silicide phases. In this study, we examine the effect of annealing on the depth profiles of Mg, implanted into Si, and compare the experimental profiles of the as-implanted ions with those simulated by TRIDYN [5].

### 2. Experimental details

Ion implantation of  $^{24}\text{Mg}^+$  ions at 40 keV, into an n-type Si substrate with (111) crystal orientation and resistivity (780-850)  $\Omega\text{cm}$ , was performed using a type ILU-4 ion accelerator, allowing a high current density. The  $^{24}\text{Mg}^+$  ions were mass separated from the plasma ion source

---

<sup>\*</sup> Corresponding author: hangelov@inrne.bas.bg

using 4N pure Mg powder heated at 500 °C. The vapour pressure of Mg at this temperature is about (4-5) Pa.

During the implantation, the substrate temperature rose to about 230 °C, due to the incident ion beam with a power density of 0.48 Wcm<sup>-2</sup> (beam current density of 10-12 µA cm<sup>-2</sup>). This temperature was estimated on the basis of the model developed by Parry [6], taking into account the effects of ion beam heating, radiation cooling, conduction cooling and re-irradiation. Two types of sample were prepared by implantation of two different doses,  $2 \times 10^{17}$  cm<sup>-2</sup> and  $4 \times 10^{17}$  cm<sup>-2</sup>, at an energy of 40 keV. After the implantation, the samples were annealed at 500 °C and  $6.65 \times 10^{-3}$  Pa pressure for three different times – 30, 60 and 300 s, in order to promote coarsening and coalescence of the precipitates formed during the Mg implantation.

Rutherford backscattering spectroscopy (RBS) was used to characterize the sample composition. The samples were measured before and after annealing at random orientations, using a 1.8 MeV He<sup>+</sup> beam from a Van de Graaff accelerator and a backscattering angle geometry of 165°. In order to obtain better depth resolution, some of the samples were studied at a glancing position 100° of the detector. A silicon surface-barrier detector (SSD) was used, with an overall resolution of about 15 keV FWHM. The obtained RBS spectra were processed and simulated by the RBX computing code [7]. The experimental results were compared with the Mg concentration profiles simulated by TRIDYN.

### 3. Results and discussion

The energy and depth resolutions as a function of the target depth for RBS at 165° and 100° were calculated using Ziegler's stopping power values [8]. For depths from 0 to 80 nm, the energy resolution (15-19.5 keV) was dominated by that of the SSD (15 keV), as can be seen in Fig. 1(a). Fig. 1(b) shows the calculated depth resolution using the energy-loss factor. The effect of the glancing detecting angle (100°) is well pronounced; the depth resolution is (8.6-11.3) nm which is much higher than that at 165° (32.2-34.6 nm).

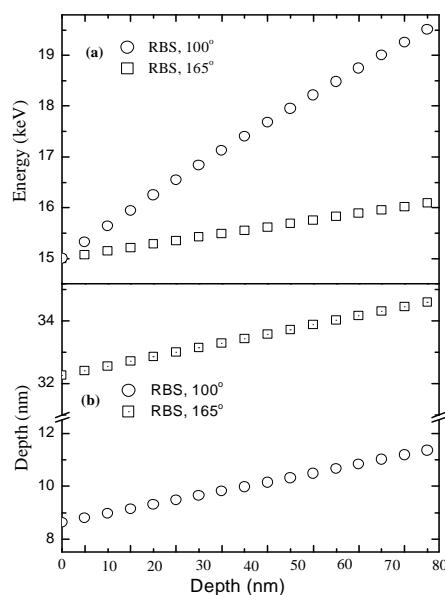


Fig. 1. Calculated energy (a) and depth (b) resolution for RBS (165° and 100°) systems, as a function of target depth

The concentration of the Mg atoms as a function of implantation depth for the different doses of implantation simulated by TRIDYN is shown in Fig. 2. As seen, the sputtering effect leads to an asymmetric distribution of the Mg concentration. This behaviour is more pronounced at higher

implantation doses, where the effect of the preferential sputtering process occurs. The difference in the sputtering yield for Si (1.22 at/ion) and Mg (2.17 at/ion) [9] leads to an increased surface roughness of the samples with increasing implanted dose.

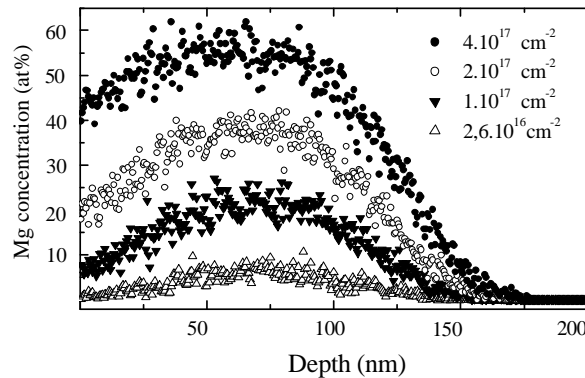
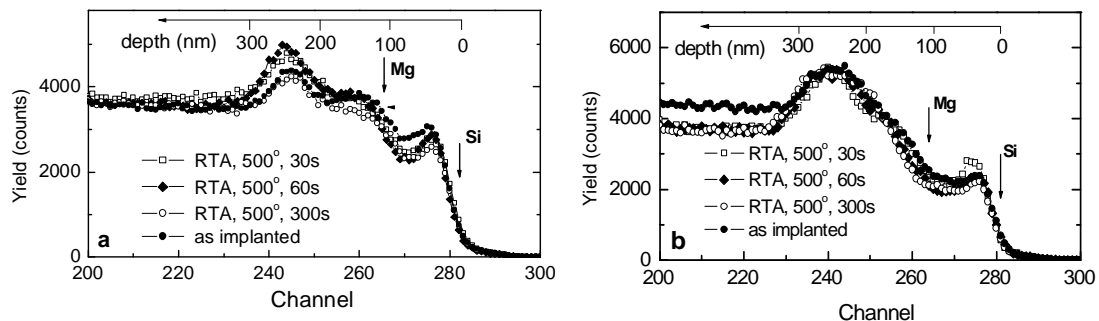


Fig. 2. Mg ion implantation profiles at four different doses:  $2.6 \times 10^{16}$ ,  $1 \times 10^{17}$ ,  $2 \times 10^{17}$  and  $4 \times 10^{17} \text{ cm}^{-2}$ , at an energy of 40 keV, simulated by TRIDYN

Figs. 3(a) and 3(b) show RBS spectra at a backward angle ( $165^\circ$ ), for samples implanted with doses  $D1$  and  $D2$ , before and after rapid thermal annealing (RTA) for 30, 60 and 300 s at  $500^\circ\text{C}$ . According to the simulations performed by RBX on the obtained RBS spectra, the profile of initially implanted Mg ions extends to 155 nm in the case of  $D1$  implantation and 167 nm in the case of  $D2$ . These results are in good agreement with those obtained by TRIDYN simulations (Fig. 2). Since Mg is a fast diffusing dopant in Si ( $3.5 \times 10^{-10} \text{ cm}^2 \text{ s}^{-1}$  at  $370^\circ\text{C}$ ), its redistribution towards the Si surface and inwards into the bulk has occurred with increased annealing time. At the same time, the peak due to the radiation defects induced by the Mg implantation at channel 258 in Fig. 3(a) and channel 257 in Fig. 3(b) decreases, clearly indicating an improvement of the crystallinity of the samples during the annealing. The difficulties in simulation of the measured spectra are due to the overlap of the RBS spectra of Si and Mg - elements with close masses. The “leading edge” of the Mg is slightly shifted from that of the Si.

Fig. 3. RBS spectra obtained at a backward angle ( $165^\circ$ ) of the as-implanted samples and those annealed for different times, with doses of  $2 \times 10^{17} \text{ cm}^{-2}$  (a) and  $4 \times 10^{17} \text{ cm}^{-2}$  (b)



In order to obtain better depth resolution, RBS spectra of the as-implanted samples ( $2 \times 10^{17} \text{ cm}^{-2}$  and  $4 \times 10^{17} \text{ cm}^{-2}$ ) at a glancing angle ( $100^\circ$ ) were obtained. The corresponding depth composition profiles obtained by fitting of the measured and simulated spectra (using RBX computer code) are shown in Figs. 4(a) and 4(b).

Thin layers of  $\text{SiO}_2$  were formed on the sample surfaces during the ion implantation. The Mg depth profiles, as simulated by TRIDYN, are in good agreement with the experimental results.

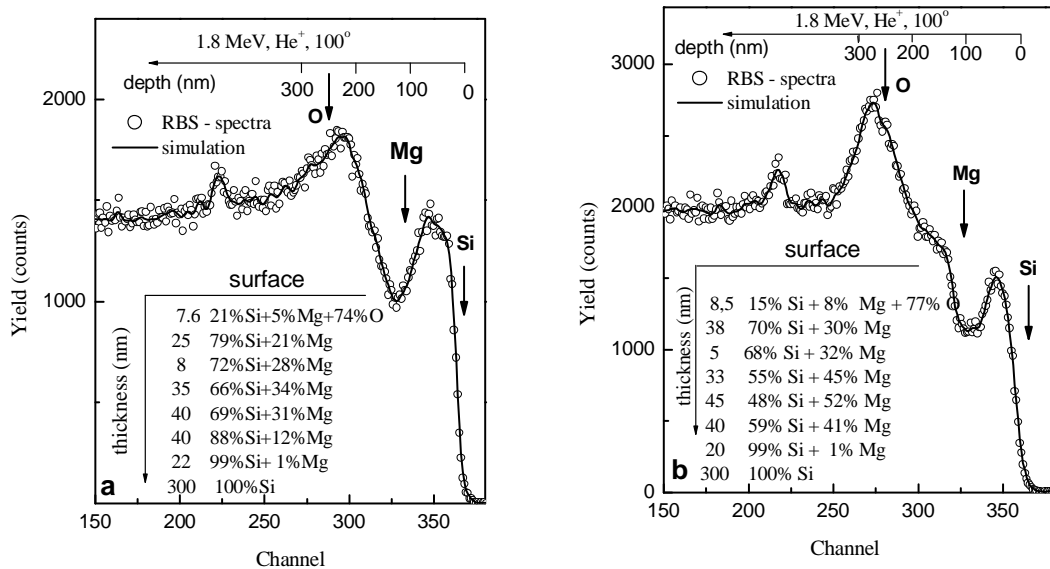


Fig. 4. Experimental RBS spectra obtained at a glancing angle ( $100^\circ$ ) with RBX simulation, for samples implanted at doses of  $2 \times 10^{17} \text{ cm}^{-2}$  (a) and  $4 \times 10^{17} \text{ cm}^{-2}$  (b).

#### 4. Conclusions

The effect of RTA on the depth profile behaviour of low energy Mg ions, implanted into Si has been investigated by RBS. By orienting the detector at a glancing angle of  $100^\circ$ , a depth resolution of approximately 9 nm was obtained. This resolution was sufficient to visualize clearly the effect of increasing annealing time on the Mg depth profile evolution. High dose ion implantation is a suitable technique for obtaining a precise and reproducible profile distribution of Mg in Si, and for synthesis of the  $\text{Mg}_2\text{Si}$  phase [10].

#### Acknowledgements

This work is supported by the National Fund for Scientific Investigations, Contract №  $\Phi$  1103/01 and by the Japan Society for the Promotion of Science (JSPS).

#### References

- [1] Y. Makyta, Proc. 1st NREL Conference "Future Generation Photovoltaic Technologies", New York: Ed. Mc. Connel, AIP, 1997. p. 3.
- [2] D. Leong, M. Harry, K. Reeson, K. P. Homewood, Nature **387**, 686-688, (1997).
- [3] H. Lange, Phys. Stat. Sol. (b) **201**, 3-65, (1997).
- [4] A. E. White, K. T. Short, R. C. Dynes, J. P. Garno, J. M. Appl. Phys. Lett. **50**, 95-97, (1987).
- [5] W. Möller, W. Eckstein, TRIDYN, Nucl. Instr. Meth. B **2**, 814-818, (1984).
- [6] P. Parry, J. Vac. Sci. Technol. **13**, 622-629, (1976).
- [7] E. Kotai, RBX, Nucl. Instr. Meth. B **85**, 588-596, (1994).
- [8] J. Ziegler, The Stopping and Range of Ions in Solids. New York: Pergamon Press, 1986.
- [9] Ch. Angelov, V. Mikli, B. Amov, E. Goranova, J. Optoelectron Adv. Mater. **7**(1), 369 (2005).
- [10] E. Goranova, B. Amov, M. Baleva, E. Trifonova, P. Yordanov, J. Mater. Sci. **39**, 1857-1859, (2004).