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**Diffusion of Phosphorus and Arsenic Ions Implanted  
into Mono- and Polycrystalline-Si**

Dyfuzja jonów fosforu i arsenu implantowanych do mono- i polikrystalicznego krzemu

Диффузия ионов Р и As имплантированных в моно- и поликристаллический кремний

ABSTRACT

The temperature dependences of the diffusion coefficient of phosphorus and arsenic ions implanted in mono- and polycrystalline silicon have been measured. The measurements were carried out in a temperature range of 600–1200° C. The implantation energy for the ions was about 50 keV. The residual activity method combined with the ion etching removal technique was used for measuring the diffusion profiles.

INTRODUCTION

Polycrystalline silicon films are important for various applications in the semiconductor device technology [1, 2]. Polycrystalline silicon layers are useful in the field of planar structures as dielectrically isolating structures and as gate electrodes in silicon gate MOS integrated circuits. Heavily doped polycrystalline-Si is used as a diffusion source in shallow emitter bipolar integrated circuits. In all cases the doping by ion implantation method is possible. This method simplifies the processes of obtaining poly-silicon by separating the polycrystalline layers formation, and doping and heat treatment [3]. For this reason the knowledge of projected ranges and the diffusion coefficient of

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## SPUTTERING SYSTEM

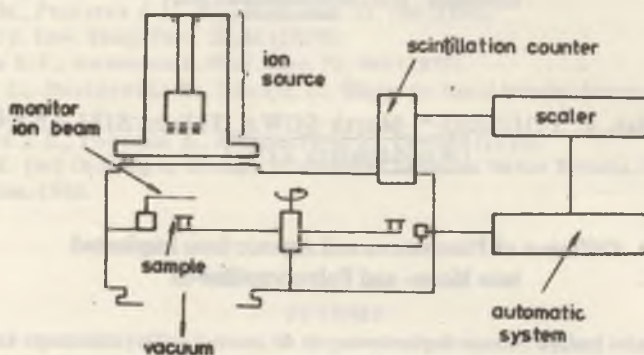


Fig. 1. A block diagram of the sputtering system

implanted impurities in poly-silicon is needed. The purpose of the present work is to investigate the diffusion of arsenic and phosphorus ions from implanted layer in polycrystalline-Si. For comparison the temperature dependences of the diffusion coefficient for single crystal Si are also presented.

## EXPERIMENTAL

The poly-Si layers were prepared in the Institute of Electron Technology, — CEMI Warsaw. The polycrystalline silicon 500–600 nm thick was deposited by the thermal decomposition of silane at 600° C. The decomposition was carried out in nitrogen as a carrier gas. The flow rate was equal to 51.1 l/min and the deposition rate was 50 nm/min. The grain size was about 30 nm with  $\langle 110 \rangle$  preferred orientation. The poly-Si layers were deposited on the thermally grown silicon dioxide film with thickness of  $1350 \text{ \AA} \pm 50 \text{ \AA}$ . The n-type, phosphorus-doped silicon wafers of  $3\text{--}6 \text{ } \Omega \cdot \text{cm}$  resistivity and  $\langle 111 \rangle$  orientation were used.

To investigate the concentration profile of P and As ions, the residual activity method combined with the ion etching technique was used. The block diagram of the apparatus is shown in Fig. 1. The ion source of the Kaufmann type is used in the sputtering apparatus. The residual activity of the sputtered samples were measured by the scintillator detector.

## RESULTS AND DISCUSSIONS

## Thermal diffusion of phosphorus

To investigate the thermal diffusion of phosphorus, the samples implanted with about  $1 \times 10^{11} \text{ }^{32}\text{P}/\text{cm}^2$  were heat-treated at temperatures of 800–1200° C. The implantation energy was 45 keV and 50 keV. The heat treatment was carried out in argon atmosphere with the time ranged from 15 to 60 min.

The effective diffusion coefficient can be evaluated by comparing the profiles before and after the heat treatment. If the diffusion coefficient  $D$  is independent of the concentration and the surface boundary effect can be neglected the diffusion profile is expressed by the Gaussian distribution

$$N(x, t) = \frac{N_D}{2\pi(\Delta R_p^2 + 2Dt)^{1/2}} \exp\left[-\frac{(x - R_p)^2}{2\Delta R_p^2 + 4Dt}\right] \quad (1)$$

Where  $N(x, t)$  is the concentration of the implanted ions,  $N_D$  is the total number of the implanted ions per  $\text{cm}^2$ ,  $x$  is the distance from the surface,  $R_p$  and  $\Delta R_p$  are the mean projected range and standard deviation respectively and  $t$  is the diffusion time.

For  $x = R_p$  a simple relation describing the ratio relative average concentrations at  $t = 0$  and  $t = t$  is given by

$$\frac{N(R_p, t)}{N(R_p, 0)} = \left(1 + \frac{2Dt}{\Delta R_p^2}\right)^{1/2} \quad (2)$$

This equation allows a simple fit of  $D$ -values for well buried layers.

For a surface acting as a perfect sink one can impose condition that the concentration is zero at  $x = 0$  for all values of  $t > 0$ . The solution of the diffusion equation for this boundary condition was obtained by Meyer et al. [4]. For a surface acting as mirror barrier, the solution of the diffusion equation is given by:

$$N(x, t) = \frac{N_D}{[2\pi(\Delta R_p^2 + 2Dt)]^{1/2}} \left\{ \exp\left[-\frac{(x - R_p)^2}{2\Delta R_p^2 + 4Dt}\right] + \exp\left[-\frac{(x + R_p)^2}{2\Delta R_p^2 + 4Dt}\right] \right\} \quad (3)$$

In the present work the implantation energy was 50 keV, then the  $R_p$  is about a few hundred angstroms and we cannot neglect surface boundary effect.

We can assume for the phosphorus as well as for arsenic atoms that the surface is an impenetrable barrier so it can act as a 'mirror' and the diffusion profiles can be represented by the equation(3)

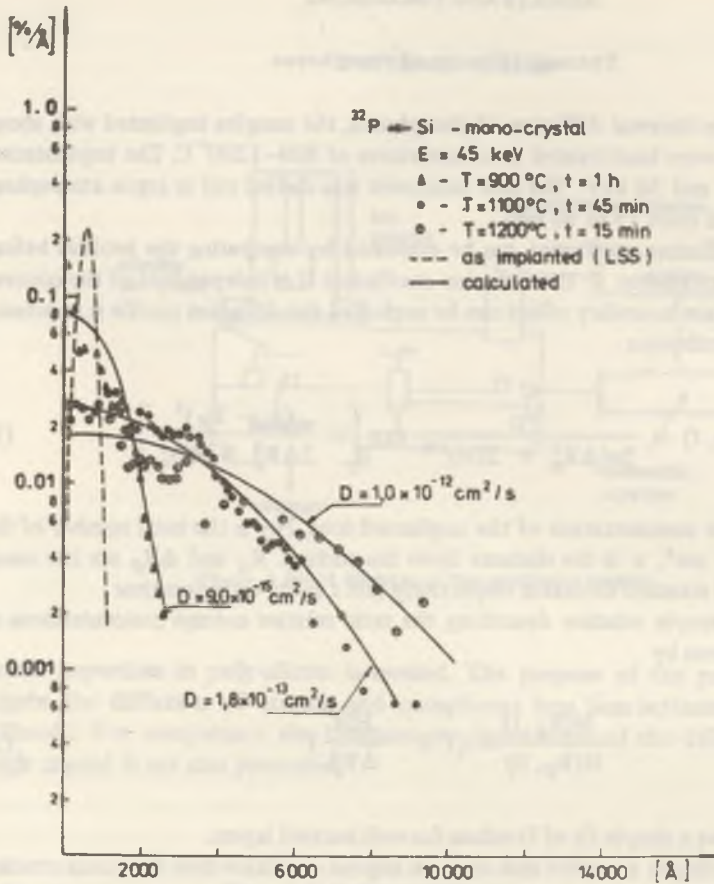


Fig. 2. The concentration profiles of  $^{32}\text{P}$  implanted into mono-crystalline-Si

Tab. 1. Diffusion coefficients of phosphorus implanted into mono- and poly-crystalline silicon

T°C		t(min)		D cm <sup>2</sup> /sec	
mono	poly	mono	poly	mono	poly
900	800	60	30	$9.0 \cdot 10^{-15}$	$3.5 \cdot 10^{-15}$
1100	840	45	30	$1.8 \cdot 10^{-13}$	$7.0 \cdot 10^{-14}$
1200	900	15	15	$1.0 \cdot 10^{-12}$	$2.8 \cdot 10^{-13}$
	1000		30		$8.8 \cdot 10^{-13}$

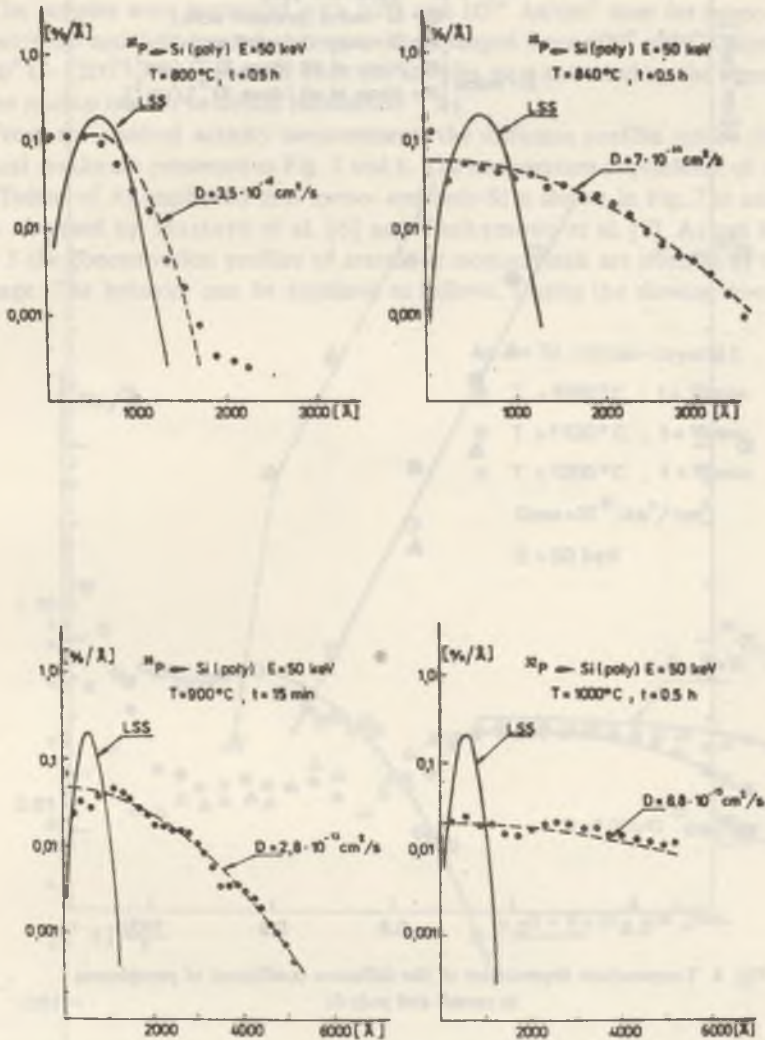


Fig. 3. The diffusion profiles of  $^{32}\text{P}$  implanted into poly-crystalline-Si

Figures 2 and 3 represented the concentration profiles as a function of the depth  $x$  and temperature for the mono- and polycrystalline-Si, respectively. For comparison, the implan-

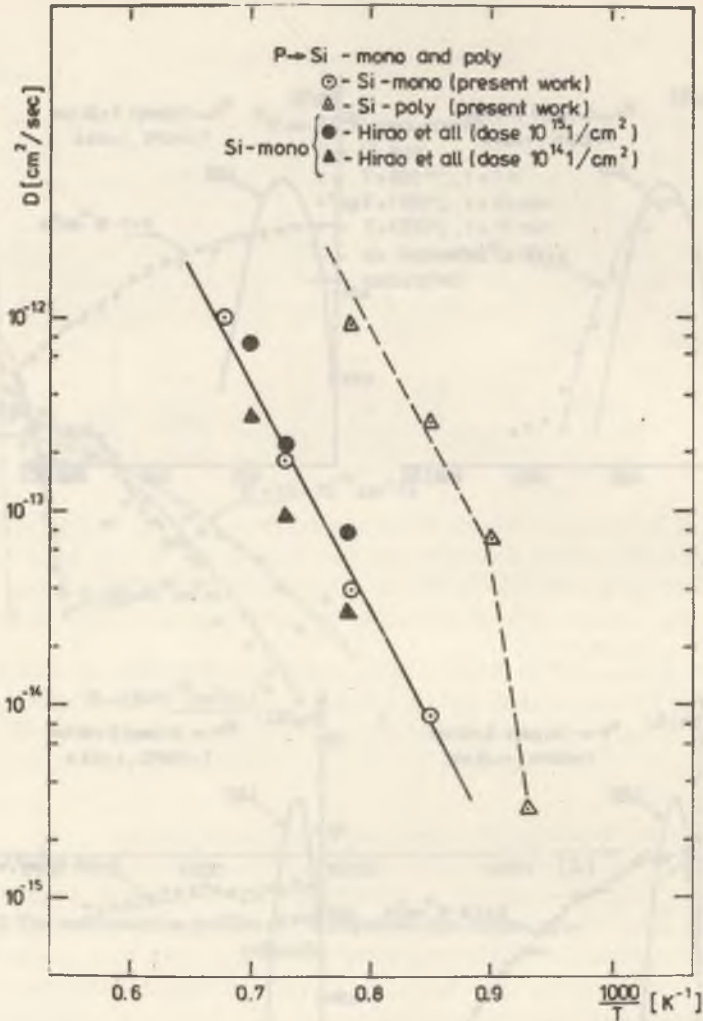


Fig. 4. Temperature dependence of the diffusion coefficient of phosphorus in mono- and poly-Si

tation profiles before heating are also included in the figures. The solid lines represent the Gaussian distribution according to equation (3). The calculated values of the diffusion coefficient are tabulated in Tab. 1. The temperature dependence of the diffusion coefficient of P ions in the mono- and polycrystalline-Si is shown in Fig. 4 with the data obtained by Hirao et al [5].

It can be seen from Fig. 4 that the diffusion coefficient of  $^{32}\text{P}$  in polycrystalline-Si rapidly increases between  $800^\circ\text{C}$  to  $840^\circ\text{C}$  and this can be due to the migration of the implanted ions from inside the grain to grain boundary areas. For the monocrystalline Si, our data are in good agreement with the data obtained by Hirao et al. [5].

## Thermal diffusion of arsenic

The samples were implanted with  $10^{15}$  and  $10^{16}$  As/cm<sup>2</sup> dose for mono- and poly-Si respectively and heat-treated at temperatures ranged from 600°–900° C for poly-Si and 1000° C–1200° C for mono-Si. Then the samples were activated by the thermal neutrons in the nuclear reactor to obtain radioactive <sup>76</sup>As.

From the residual activity measurements the diffusion profiles can be obtained. The typical results are presented in Fig. 5 and 6. The temperature dependence of the diffusion coefficient of As implanted into mono- and poly-Si is shown in Fig. 7 in addition to the data obtained by Masters et al. [6] and Tsukamoto et al. [7]. As can be seen from Fig. 5 the concentration profiles of arsenic in monocrystals are affected by the radiation damage. The behavior can be explained as follows. During the slowing down process of

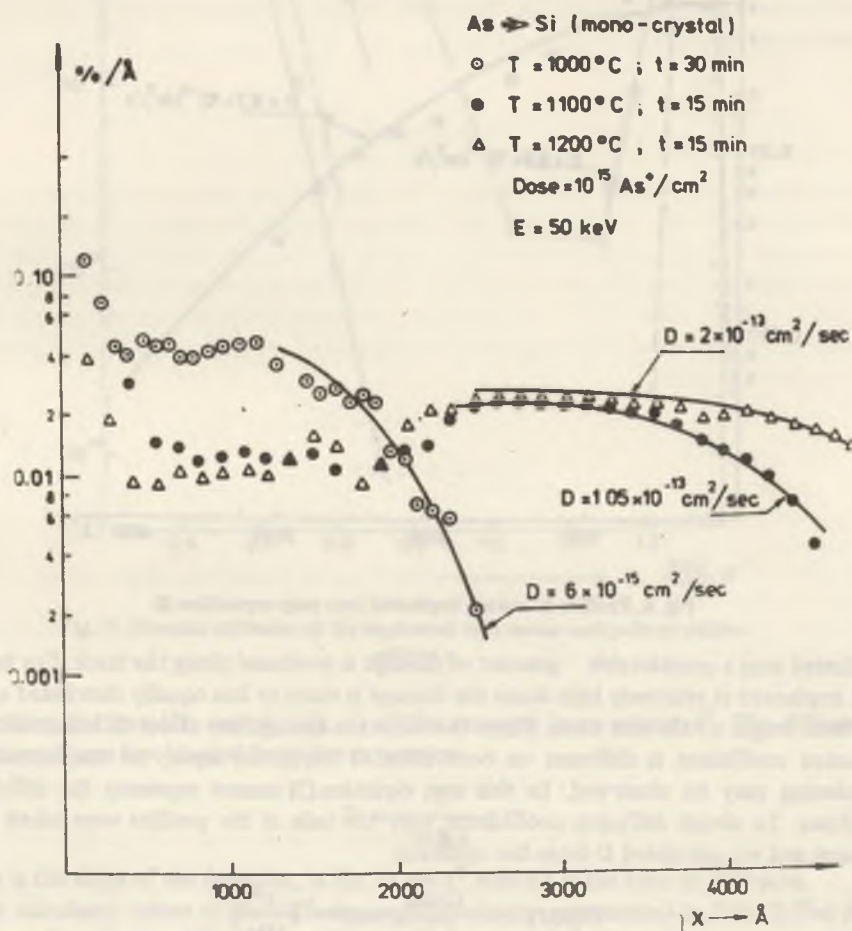


Fig. 5. Diffusion profiles of arsenic in mono-crystalline-Si

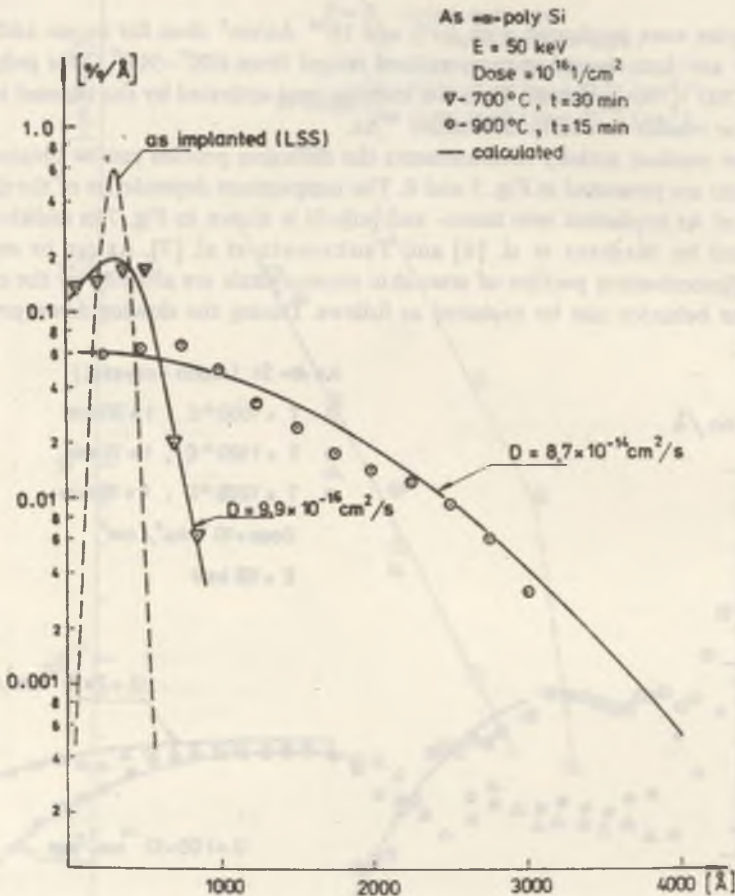


Fig. 6. Profiles of arsenic implanted into poly-crystalline-Si

implanted ions a considerable amount of damage is produced along the track. For heavy ions implanted at relatively high doses the damage is more or less equally distributed along the total length of the ion track. Since the radiation damage can affect diffusion and the diffusion coefficient is different on both sides of implanted layer, the unsymmetrical broadening may be observed. In this case equation (3) cannot represent the diffusion processes. To obtain diffusion coefficients, only the tails of the profiles were taken into account and we calculated  $D$  from the equation:

$$N(x, t) = \frac{\text{Const}}{\sqrt{\pi D t}} \exp - \left( \frac{x^2}{4 D t} \right) \quad (4)$$



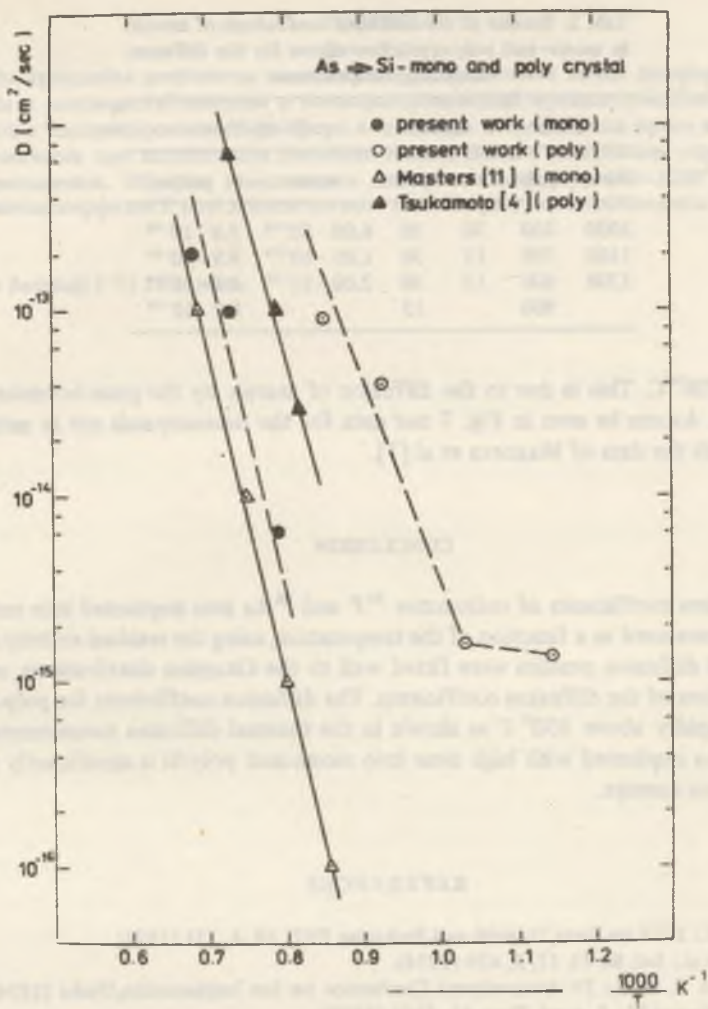


Fig. 7. Thermal diffusion of As implanted into mono- and polycrystalline-silicon

by plotting the specific activity  $i(x, t)$  of the removed layer against  $x^2$ . The diffusion coefficient  $D$  can be obtained from the expression

$$D = \frac{1}{4t\alpha} \quad (5)$$

where  $\alpha$  is the slope of the function,  $\ln i(x, t)$  vis  $x^2$  where  $t$  is the time of diffusion.

The calculated values of the diffusion coefficients are summarized in Tab. 2. For the polycrystalline-Si, the diffusion coefficient of arsenic atoms is nearly constant between

Tab. 2. Results of the diffusion coefficients of arsenic in mono- and poly-crystalline-silicon for the different annealing temperatures

T°C		t(min)		D cm <sup>2</sup> /sec	
mono	poly	mono	poly	mono	poly
1000	600	30	30	$6.00 \cdot 10^{-15}$	$8.8 \cdot 10^{-16}$
1100	700	15	30	$1.05 \cdot 10^{-13}$	$9.9 \cdot 10^{-16}$
1200	800	15	30	$2.00 \cdot 10^{-13}$	$4.4 \cdot 10^{-14}$
	900		15		$8.7 \cdot 10^{-14}$

600° C and 700° C. This is due to the diffusion of arsenic by the grain boundary at low temperatures. As can be seen in Fig. 7 our data for the monocrystals are in satisfactory agreement with the data of Masters et al [7].

### CONCLUSION

The diffusion coefficients of radioactive <sup>32</sup>P and <sup>76</sup>As ions implanted into mono- and poly-Si were measured as a function of the temperature, using the residual activity method. The measured diffusion profiles were fitted well to the Gaussian distributions, using the calculated values of the diffusion coefficients. The diffusion coefficients for poly-Si starts to increase rapidly above 850° C as shown in the thermal diffusion measurements. The diffusion of As implanted with high dose into mono- and poly-Si is significantly affected by the radiation damage.

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### STRESZCZENIE

W pracy zbadano rozkład zasięgów jonów fosforu i arsenu implantowanych do monokrystalicznego i polikrystalicznego krzemu. Energia implantowanych jonów wynosiła 45 i 50 keV. Rozkłady uzyskano metodą pomiaru aktywności pozostałościowej połączonej z jonowym trawieniem kolejnych warstw próbki. Pomiar wykonano dla temperatur wygrzewania z przedziału 600°-1200° C. Z wyników doświadczeń określono współczynniki dyfuzji i znaleziono ich temperaturową zależność.

## РЕЗЮМЕ

В работе приведены результаты исследований распределения ионов фосфора и мышьяка внедренных в монокристаллический и поликристаллический кремний с энергией 45 и 50 кев. Распределение имплантированного фосфора и мышьяка исследовалось путем измерения остаточной активности при постепенном снятии тонких слоев с поверхности образца методом ионного распыления. Образцы отжигались в диапазоне температур 600–1200° Ц. Получены коэффициенты диффузии Р и As и исследованно их температурную зависимость.

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