Radiation-Stimulated Self-Diffusion into Semiconductors

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Abstract – In this paper the kinetic coefficients of long-lived isotopes of arsenic, gallium and selenium into germanium were determined. From this data the defect migration enthalpy was calculated.

1. Introduction

The study radiation-stimulated diffusion of isotopes created in solids by charged particles irradiation is currently essential. A lot of experimental papers have been published on this topic in the last years (see the review in [1]). In this paper, the model [2], based on physical and chemical kinetics, is applied for the interpretation of the experiment [3] results. As a result, the important physical information is obtained.

2. Theoretical Model

The modified V.V. Beloshitsky [4] description of process radiation-stimulated diffusion of isotopes, created at sufficiently long and intensive irradiation of solids by the charged particles has been presented in paper [2]. Along with diffusion transfer, the capture of an active impurity (index a) by vacancies (v) in a condition (c) and its activation by defects (d) is assumed. The important issue of the model is that diffusion occurs in the presence of intensive creating and disappear of (d-v) pairs. These processes are described by the following system of the connected equations:

$$\partial n_a/\partial t = D_a\,\partial^2 n_a/\partial x^2 - n_a\,n_v\,k_{cap} + n_c\,n_d\,k_{act} + $$
$$+ j\,N_i\sigma_i(E_p(x))\Theta(R_p - x + x_0),$$
$$\partial n_c/\partial t = n_a n_v k_{cap} - n_c n_d k_{act},$$
$$\partial n_d/\partial t = D_{dv}\partial^2 n_d/\partial x^2 - n_c n_d k_{act} - n_v n_d k_{ann} +$$
$$+ jN\sigma_d\Theta(R_p - x + x_0),$$
$$\partial n_v/\partial t = D_{dv}\partial^2 n_v/\partial x^2 - n_a n_v k_{cap} - n_v n_d k_{ann} +$$
$$+ jN\sigma_d\Theta(R_p - x + x_0),$$

$x_0 = -v_b t$, $E_p(x) = E_0(1 - x/R_p)$, $\sigma_d = 3.52\cdot10^{-16}$ cm^2, where $\Theta(x)$ – unit function, N and N_i – density of nucleuses only substance and element, making an isotope, R_p – range of energy E_o ion from [5], j – current of ions, at last, D_a, D_{dv}, K_{cap}, K_{act}, K_{ann} – free parameters of model. For defects and vacancies the condition was, that the (d–v) flow would cause displacement of border of substance with speed V_b, determined using a doze of an irradiation. The initial conditions were assumed to be zero. The boundary conditions were chosen from the experimental data. The system of the equations under the above described initial and boundary conditions was solved numerically by a method of final differences. The values of model variables were selected by a method of the least squares so that in the best way to fit experimental (Na + Nc) depth profile structures. The minimization was spent by a simplex-method.

3. Results of the Calculations

The calculations of the experiment data [3] on activation definition of depth profile structures 71-As, 72-As, 74-As, 76-As and 67-Ga, arising in Ge at irradiation 10 MeV protons current 0.1 μA/cm^2 during 0.5 hour have been carried out. Depth profile structures 73-As, 73-Se and 75-Se, arising in Ge under the irradiation by α-particles 20 MeV by a current 0.1 μA/cm^2 during 0.5 hours were also processed. The published data on the reactions cross sections σ_i (Ep) from library of the appreciated data EXFOR [6] and book [7] was used in the model. For an isotope 71-As the maximal cross section (p, γ) reaction as 14.31 mbarn is estimated as well. The rough unfolding of cross section (α,p) reaction for an isotope 73-As is shown in Fig. 1. It should be noted, that width of a resonance approximately twice is less, than in cross section Zr-92 (p, n) Nb-92m reaction on the rest sample [8, 9], although the dipole sums are almost the same (see Table 1).

Table 1. Dipole sums (MeV*barn)

Nuclear reaction	Rest sample	Shake sample	Ref.
Zr-92(p,n)Nb-92m	5	2.5	[8, 9]
Pb-206(p,n)Bi-206	–	0.47	[9]
Ge-70(α,p)As-73	5	–	This paper

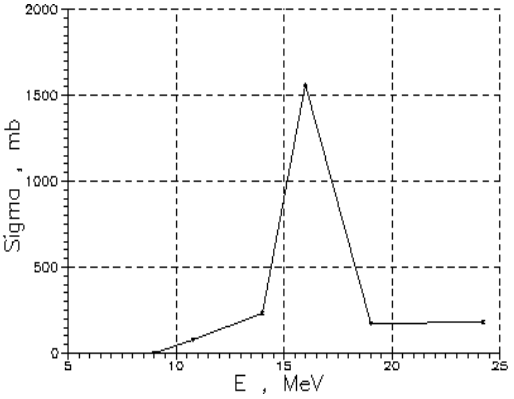

Fig. 1. Unfolding Ge-70(α,p)As-73 nuclear reaction cross section

The points at 10.8 and 24.2 MeV are extracted from EXFOR. The calculations results are given in Table 2. The enthalpy of defects migration in Ge H_{dv} = = 14896 cal/mol (T_{eff} = 528 K) and H_{dv} = 37756 cal/mol (T_{eff} = 621 K) were estimated using the absolute values of self-diffusion coefficients. A comparison of these enthalpy with the similar data for silicon [10] shows a good agreement at 621 K, but demonstrates the much smaller value at 528 K. However, value at 528 K agree well with our data [2] for GaAs and GaP. In our paper [9] the equation $H_{dv} = H_{dvo} + N\,R\,T_{eff}/2$, where $N = 45$ for semiconductors and Hdvo=5393 cal/mol for silicon, R = 1.98584 cal/mol/K is obtained.

Table 2. Calculated diffusion coefficients

Isotope	$D_{a,}\ 10^{-11}$ cm^2/s	$D_{dv,}\ 10^{-11}$ cm^2/s	Threshold	Reaction
Ga^{67} **	6395.147	6288.1	4.577	(p,α)
As^{71} **	9127.133 *	6288.1	1.654	(p,γ)
As^{72}	9810.129	6288.1	5.133	(p,n)
As^{74}	10712.11	6288.1	3.345	(p,x)
As^{76} **	12620.77	6288.1	3.630	(p,n)
Se^{73}	2823.848	0.00046	7.567	(α,n)
As^{73} **	2823.848 *	0.00046	9.0	(α,p)
Se^{75}	633.854	0.00046	6.309	(α,x)

* Is obtained by interpolation.
** The Coulomb barrier (is obtained by fit).

The contradiction in enthalpy for Ge can be overcome, assuming jump in N from 45 up to 9 somewhere between 621 and 528 K. In Table 3 the values H_{dvo} for a set of semiconductors are given. The data of Table 3 can be described by the formula $H_{dvo} = k\,(M)^{1/2}$,

Table 3. H_{dvo} values for set of semiconductors

Semiconductor	H_{dvo}, cal/mol	Molecular weight	N	Ref.
Si	5393	28.0855	45	[10]
SiC	6177	40.0965	45	[11, 13]
Ge	10020	72.59	45 9	This paper
GaP	12677	100.6938	9	[2]
GaAs	13803	144.6416	9	[2]
$Hg_{0.76}Cd_{0.24}Te$	4801	307.0271	43	[14]

where k = 1126.55 cal/mol, that coincides with factor at Z in the formula $H = H_o - k\,Z$ from [12]. However, our handling of results from [14] on low-temperature (167−218 K) self-diffusion in HCT, resulted in N = 43 and H_{dvo} = 4801 cal/mol. This shows existence of limiting weight M_o = 288.8668 of the period on molecular weight. Also, this results suggests an absence of jump in enthalpy.

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References

[1] V.A. Didik, R.Sh. Malkovich, E.A. Skoryatina, V.V. Kozlovski, Nucl. Instr. Meth. Phys. Res. B **160**, 387 (2000).
[2] V.A.Starostin, Phys. and Chem. of Mater. Treat. **2**, 83–85 (2000) (in Russian).
[3] V.A. Didik, V.V. Kozlovski, R.Sh. Malkovich, E.A. Skoryatina, Solid State Phys. **45**, No. 9, 1576–1578 (2003) (in Russian).
[4] P.A. Aleksandrov, E.K. Baranova, V.V. Beloshitsky, K.D. Demakov, V.A. Starostin, Rad. Eff. **88**, 249–255 (1986).
[5] O.F. Nemetz,Yu.V. Gofman, *Handbook on Nuclear Physics*, Kiev, 1975, 414 pp. (in Russian).
[6] http://depni.npi.msu.su/cdfe/exfor/index.php
[7] V.N. Levkovsky, *Activation Cross Sections for average mass nucleus (A = 40–100) by average energy range (E = 10–50 MeV) protons and alfa-particles (experiment and systematic)*, Moscow, 1991, 215 pp. (in Russian).
[8] V.A. Starostin, Surface and Coatings Technology **158–159**, 234–237 (2002).
[9] V.A. Starostin, *in: Proc. of VI Inter. Conf. on Modification of Materials with Particle Beams and Plasma Flows*, Tomsk, Russia, 23–28 September 2002, pp. 263–266 (in Russian).
[10] K.D. Demakov, V.A. Starostin, S.G. Shemardov, Technical Physics **47**, No. 10, 1333–1336 (2002).
[11] V.A. Starostin, Phys. and Chem. of Mater. Treat. **5**, 104–105 (1999) (in Russian).
[12] C.T. Tomizuka, L. Slifkin, Phys. Rev. **96**, 610–615 (1954).
[13] P.A. Aleksandrov, E.K. Baranova, K.D. Demakov et. al., Phys. and Techn. of Semiconductors **21**, No. 5, 920–922 (1987) (in Russian).
[14] V. Richter, R. Kalish, J. Appl. Phys. **67**, No. 10, 6578–6580 (1990).