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Peculiarities of neutron interaction with boron containing semiconductors

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Abstract. The results of point defect creation calculation in B_4C, BN and BP semiconductor single crystals irradiated in the fast neutron reactor IBR-2 are presented. It has been shown that during the thermal neutron interaction with light isotope boron atoms (^{10}B) the damage creation by means of fission nuclear reaction fragments (α-particles and ^7Li recoil nuclei) exceeds the damage created by fast neutrons ($E_n > 0.1$ MeV) by more than two orders of value. It has been concluded that such irradiation can create a well developed radiation defect structure in boron-containing crystals with nearly homogeneous vacancy depth distribution. This may be used in technological applications for more effective diffusion of impurities implanted at low energies or deposited onto the semiconductor surface. The developed homogeneous vacancy structure is very suitable for the radiation enhanced diffusion of electrically charged or neutral impurities from the surface into the technological depth of semiconductor devices under post irradiation treatment.

Key words: semiconductors • thermal neutrons • point defects • vacancies • damage concentration • thermal neutron fluence • cross-section of damage creation • fission fragments • lithium • helium • α-particles • diffusion of impurities • homogeneity of damage and active impurities

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Introduction

Studies of different types of irradiation and a comparison of its action in semiconductors is an object of interest for radiation physics [3, 10–12, 17] and for its potential applications in novel nanotechnologies. Radiation destruction, surface sputtering, changes of phase composition structure in solid solutions [17], amorphous phase production in initially crystalline structures, recrystallization and adhesion processes, atomic ion-beam mixing [3] in immiscible systems [10], heavy ion track creation [3, 10–12] have attracted steady attention during few last decades because of possible application of the observed effects for creation of new advanced materials.

At the same time, the problem of impurity doping of semiconductors is very important. Sometimes it is impossible to obtain the required concentrations and depth distribution of doping impurities during the semiconductor growth processes. Impurity doping of semiconductors is provided by direct low energy ion implantation (ions energy of the order of a few hundred keV) or the formation of thin impurity layer on the semiconductor surface followed by a long-time annealing.

Boron containing semiconductors like B_4C, BN and BP and some other compounds are seldom studied by experimentalists because of poor purification methods and difficulty in exploiting their semiconductor properties [6, 8, 9]. However, most of such semiconductors has radiation resistant properties and consequently can be used in strong radiation conditions as in nuclear reactors (see [6, 8, 9, 15] and references therein).

Creation of well developed vacancy structure with homogeneous vacancy depth distribution is a good possibility for the following diffusion redistribution of impurities into some semiconductors during post-annealing processes.

The purpose of this article is to demonstrate a possibility of creation of homogeneous vacancy distribution into boron-containing semiconductors (B_4C (AIII-BIV), BN and BP (AIII-BV)), with enhanced concentration of light isotope boron atoms (${}^{10}B$) under irradiation with thermal neutrons in the fast neutron reactor IBR-2.

Consideration of the influence of nuclear fission fragments on the damage creation in boron--containing semiconductors

Nuclear reactions of thermal neutron capture by light ${}^{10}B$ isotopes with subsequent decays to fission fragments (α-particles and ${}^{7}Li$ recoil nuclei) can be written as [2]:

$$(1.1)\quad n + {}^{10}B \rightarrow {}^{7}Li + \alpha,\ \text{at}\ p_1 = 0.93,\ Q_1 = 2.78\ \text{MeV}$$

$$(1.2)\quad n + {}^{10}B \rightarrow {}^{7}Li^{*} + \alpha,\ \text{at}\ p_2 = 0.07,\ Q_2 = 2.39\ \text{MeV}$$

where Q_1, Q_2 are the energies of reactions and p_1, p_2 are the probabilities of nuclear decay. The value $Q_1 =$ 2.78 MeV corresponds to a decay of the composed nuclei (n + ${}^{10}B$) up to the ground states of ${}^{7}Li$ recoil nuclei, and the value $Q_2 = 2.3$ MeV corresponds to a decay of the composed nuclei (n + ${}^{10}B$) up to the excited states of ${}^{7}Li^{*}$ recoil nuclei [2].

Parameters of interactions of α-particles and ${}^{7}Li$ recoil nuclei with semiconductors (BN, BP and B_4C) at high concentrations of ${}^{10}B$ atoms are presented in Tables 1a and 1b. In these tables the values ρ, N and T_{melt} are the density, number of ${}^{10}B$ atoms per volume unit and melting temperature of semiconductors, respectively; R_p^{α} and R_p^{Li}, N_V^{α} and N_V^{Li}, S_{inel}^{α} and S_{inel}^{Li}, σ_{α}^{max} and σ_{Li}^{max} are the projected ranges, number of vacancies per one particle (α-particle or ${}^{7}Li$ recoil nucleus), inelastic energy loss and damage creation cross-section for α-particles and ${}^{7}Li$ recoil nuclei in semiconductors, respectively. All parameters have been calculated using a computer code TRIM-2000 [1].

The thickness of boron-containing semiconductors has been taken into account as being the same and equal to $Z_{max} = 50$ μm. The threshold energy for displacement is assumed as $E_d = 20$ eV. The first value in the column for S_{inel}^{α} (see Table 1a) corresponds to the value of inelastic energy loss near the decay places of the composed nuclei (n + ${}^{10}B$) and the second one corresponds to the value of inelastic energy loss at the maximum of ionizing energy loss of α-particles. $\sigma_{\alpha,Li}^{max}$ is damage creation cross-section at the maximum of elastic energy loss (Bragg peak) of α-particles and ${}^{7}Li$ recoil nuclei.

Point defect creation in amorphous $Fe_{77}Ni_2Si_{14}B_7$ metallic alloy under the influence of fission fragments from nuclear reaction (1.1) was discussed in Ref. [7]. The alloy was irradiated with fission neutrons [16] in the fast neutron reactor IBR-2 using a "REGATA" channel of the so-called pneumatic post for transportation of samples to the reactor active zone of Frank Laboratory of Neutron Physics (FLNP) [5, 13, 14]. Calculations of damage creation were carried out under elastic scattering of fast neutrons at $E_n > 0.1$ MeV and thermal neutrons at $0.01\ \text{eV} < E_n < 0.45$ eV.

The relations between full neutron fluencies Φ_n for different neutron energies are presented in Table 2 for the experimental conditions of amorphous alloy irradiation [7].

The calculated values of full numbers of light boron isotope atoms per cubic centimeter (N_{B10}) and the numbers of α-particles (N_{α}) and ${}^{7}Li$ recoil nuclei (N_{Li}) produced by nuclear reaction (1.1) in semiconductors (BP, B_4C and BN crystals) were obtained using the expression:

$$(2)\qquad N_{\alpha} \equiv N_{Li} = N_{B^{10}} \times \sigma_{capture} \times \Phi_n^{thermal}$$

These values are presented in Table 3. The damage doses produced by α-particles (D_{α}) and by ${}^{7}Li$ recoil nuclei (D_{Li}) at the layer with a thickness $Z_{max} = 50$ μm with a square of $S = 1$ μm² were obtained using the expression:

$$(3)\qquad D_{\alpha,Li} = N_V^{\alpha,Li} \times N_{\alpha,Li} / N_{Z_{max}}$$

Then, full damage dose can be presented as:

Table 1a. Characteristic parameters of interaction of α-particles produced during nuclear reaction (1.1) with energy $E_{\alpha} = 1.77$ MeV

Semiconductor	ρ (g/cm³)	N (atom/cm³)	T_{melt} (K)	R_p^{α} (μm)	N_V^{α} (vac/α)	S_{inel}^{α} (keV/nm)	σ_{α}^{max} (dpa × cm²/α)
BP	2.89	0.833×10^{23}	1400	4.72 ± 0.10	142.9	0.34/0.43	3.40×10^{-17}
B_4C	2.52	1.373×10^{23}	2723	4.26 ± 0.07	106.4	0.36/0.53	2.37×10^{-17}
BN	2.34	1.135×10^{23}	3000	4.87 ± 0.10	130.4	0.34/0.46	2.70×10^{-17}

Table 1b. Characteristic parameters of interaction of ${}^{7}Li$ recoil nuclei produced during nuclear reaction (1.1) with energy $E_{Li} = 1.01$ MeV

Semiconductor	ρ (g/cm³)	N (atom/cm³)	T_{melt} (K)	R_p^{Li} (μm)	N_V^{Li} (vac/Li)	S_{inel}^{Li} (keV/nm)	σ_{Li}^{max} (dpa × cm²/Li)
BP	2.89	0.833×10^{23}	1400	2.13 ± 0.14	316.8	0.71	6.80×10^{-17}
B_4C	2.52	1.373×10^{23}	2723	1.88 ± 0.07	244.4	0.79	5.60×10^{-17}
BN	2.34	1.135×10^{23}	3000	2.27 ± 0.10	292.7	0.91	5.85×10^{-17}

Table 2. Characteristics of neutron fluencies for different energies under irradiation of $Fe_{77}Ni_2Si_{14}B_7$ amorphous alloy [7]. σ_n^{fast} is the approximate cross-section of damage creation for fast neutrons (at E_n > 0.1 MeV), $\sigma_{capture}$ is the cross-section of thermal neutron capture by ^{10}B atoms [2]

Type of neutrons	E_n (eV)	Φ_n (neutron/cm^2)	σ_d^{fast} (dpa × cm^2/n)	$\sigma_{capture}$ (barn)
Thermal	$0.01 \div 0.45$	$\Phi_n^{thermal} = 2.1 \times 10^{17}$	no	3838 [9]
Resonance	$0.45 \div 10^5$	$\Phi_n^{reson} = 4.7 \times 10^{17}$	no	–
Fast	$10^5 \div 2 \times 10^7$	$\Phi_n^{fast} = 1.8 \times 10^{17}$	$\approx (2 \div 4) \times 10^{-22}$	–

Table 3. Calculated values of full numbers $N_{Z_{max}}$ and N_{B10} atoms in BP, B_4C and BN semiconductors, numbers of produced α-particles (N_α) and ^{7}Li recoil nuclei (N_{Li}), damage doses D_α and D_{Li}, full dose $D_{\alpha,Li}^{total} = D_\alpha + D_{Li}$ at a thermal neutron fluence of $\Phi_n^{thermal} = 2.1 \times 10^{17}$ n/cm^2, $Z_{max} = 50$ μm

Semi-coductor	$N_{Z_{max}}$ at volume $V = 0.005$ cm^3	N_{B10} at volume $V = 0.005$ cm^3	$\Phi_n^{thermal}$ (n/cm^2)	$\sigma_{capture}$ (barn)	N_α and N_{Li} × 10^{16}	D_α and $D_{Li} \times 10^{-2}$ (dpa)	$D_{\alpha,Li}^{total} \times 10^{-2}$ (dpa)
BP	4.165×10^{20}	4.12×10^{19}	2.1×10^{17}	3838	3.32	1.13/2.53	3.66
B_4C	6.865×10^{21}	1.09×10^{20}	2.1×10^{17}	3838	8.79	1.36/3.13	4.49
BN	5.675×10^{20}	5.62×10^{19}	2.1×10^{17}	3838	4.53	1.04/2.33	3.37

$$D_{\alpha,Li}^{total} = D_\alpha + D_{Li} \tag{4}$$

The damage doses produced by α-particles and by ^{7}Li recoil nuclei and full damage dose are presented in Table 3.

The value $N_{Z_{max}}$ in expression (3) is the full number of atoms in a thin layer of thickness Z_{max} = 50 μm of semiconductors sample.

As it is known, the concentration of light ^{10}B isotope atoms in natural elementary boron is 19.8%.

Damage dose under irradiation by fast neutrons of semiconductors (BN, BP and B_4C) up to the fluence of $\Phi_n^{fast} = 1.8 \times 10^{17}$ n/cm^2 with approximate cross-section $\sigma_d^{fast} \approx (2 \div 4) \times 10^{-22}$ dpa × cm^2/n should be:

$$D_n^{fast} = \sigma_d^{fast} \times \Phi_n^{fast} \approx (3.6 - 7.2) \times 10^{-5} \text{ dpa} \tag{5}$$

or less. Fast neutron fluence was taken from Ref. [7].

One can compare two values: $D_{\alpha,Li}^{total} > 10^{-2}$ dpa (see Table 3) and $D_n^{fast} \approx (3.6 \pm 7.2) \times 10^{-5}$ dpa (5). It should be concluded that the damage creation in boron-contained semiconductors under irradiation with thermal neutrons takes place predominantly by means of fission fragments of nuclear reaction (1.1). Moreover, the radiation defects are distributed in the volume of semiconductors nearly uniformly. The corresponding calculations will be carried out below.

Calculations of damage depth distributions of thermal neutron absorption processes during passing through semiconductor flat-parallel samples with flight of fission fragments from lateral surfaces taken into account

During passage of thermal neutrons (in an energy range of 0.01 eV < $E_n^{thermal}$ < 0.45 eV) through flat parallel samples of boron-containing semiconductors their flux should decrease under the capture process by ^{10}B light isotope atoms (see nuclear reactions (1.1) and (1.2)). This process and the process of radioactive decay can be written by the differential equation:

$$\frac{d\Phi_n(Z)}{dZ} = -\lambda_Z \times \Phi_n(Z) \tag{6}$$

One can obtain the dependence of the number of thermal neutrons on the depth Z from the left flat side of semiconductor samples, i.e. flux vs. the depth:

$$\Phi_n^{thermal}(Z) = \Phi_{n,0}^{thermal} \times \exp(-\lambda_Z \times Z), \quad \text{at } 0 \le Z \le Z_{max} \tag{7}$$

λ_Z is described by the equation:

$$\lambda_Z \equiv \sigma_{capture} \times \rho_{B^{10}} \tag{8}$$

where ρ_{B10} is the number of ^{10}B atom per cubic centimeter and $\Phi_{n,0}^{thermal} \equiv \Phi_n^{thermal}(Z = 0)$ is the initial thermal neutron flux.

We suppose $\Phi_{n,0}^{thermal} = 2.1 \times 10^{17}$ n/cm^2 as in the case of irradiation in the fast neutron reactor IBR-2 [1, 2, 7, 15] of amorphous alloys using a pneumatic "post" of transportation channel "REGATA" [8]. Among boron-containing semiconductors, the maximum thermal neutron absorption should been in the case of B_4C, where there are four boron atoms per each carbon atom. For this reason, we carried out all calculations for the small thickness Z_{max} = 50 μm. Let us introduce a new parameter using the expression:

$$k_j \equiv \Phi_n^{thermal}(Z = Z_j) / \Phi_{n,0}^{thermal} \tag{9}$$

This parameter k_j is the attenuation parameter of neutron flux vs. the depth $Z = Z_j$. The value of depth $Z = Z_{1/2}$ at $k = 0.5$ can be considered as the depth of the semi absorption. The depths Z_j whose corresponding values k_j can be written as:

$$Z_j = -\frac{\ln(k_j)}{\sigma_{capture} \times \rho_{B^{10}}} \tag{10}$$

The depths Z_j for parameter k_j = 0.9; 0.7; 0.5; 0.3 and 0.1 are presented in Table 4 for three kinds of boron-containing semiconductor single crystals.

The densities of thermal neutrons after traveling through flat parallel samples with Z_{max} = 50 μm should be (see expression (7) and Table 4):

Table 4. Atomic density of ^{10}B atoms (ρ_{B10}), parameters λ_Z (Eq. (7)), depths Z_j with coefficients k_j for BP, B_4C and BN. Thickness of all semiconductor samples $Z_{\max} = 50$ μm, $k_j \equiv \Phi_{n}^{\text{thermal}}(Z = Z_j)/\Phi_{n,0}^{\text{thermal}}$

Type	ρ_{B10} (atom/cm^3)	$\lambda_Z \equiv \sigma_{\text{capture}} \times \rho_{B10}$ (μm^{-1})	Z_1 (μm) $k_1 = 0.9$	Z_2 (μm) $k_2 = 0.7$	Z_3 (μm) $k_3 = 0.5$	Z_4 (μm) $k_4 = 0.3$	Z_5 (μm) $k_5 = 0.1$
BP	0.82×10^{22}	3.15×10^{-3}	33	113	220	359	731
B_4C	2.17×10^{22}	8.33×10^{-3}	13	43	83	136	276
BN	1.12×10^{22}	4.30×10^{-3}	24	83	161	263	535

$$(11)\begin{cases} \text{BP} - \Phi_{n,\text{BP}}^{\text{thermal}}(Z_{\max} = 50\ \mu\text{m}) = 1.79\times10^{17}\ \text{n/cm}^2\ (85\%) \\ \text{B}_4\text{C} - \Phi_{n,\text{B}_4\text{C}}^{\text{thermal}}(Z_{\max} = 50\ \mu\text{m}) = 1.38\times10^{17}\ \text{n/cm}^2\ (66\%) \\ \text{BN} - \Phi_{n,\text{BN}}^{\text{thermal}}(Z_{\max} = 50\ \mu\text{m}) = 1.69\times10^{17}\ \text{n/cm}^2\ (80\%) \end{cases}$$

The percentage marked in round brackets was calculated under the assumption of initial neutron flux $\Phi_{n,0}^{\text{melt}}$ $(Z = 0) \equiv 2.1 \times 10^{17}$ n/cm^2. So, one can conclude that the absorption of thermal neutrons is not high if the thickness of samples is not very large, i.e. it is possible to take necessary thickness of boron containing semiconductors with homogeneous damage distribution.

Let us note that α-particles and ^{7}Li recoil nuclei can escape from lateral flat parallel surfaces of semiconductors if the captures of thermal neutrons by ^{10}B atoms (see nuclear reaction (1)) will take place near these parallel surfaces. In that case the flights of fission fragments should be in 4ϖ geometry. The corresponding scheme of such behavior is presented in Fig. 1.

If the depths from both flat parallel lateral sides of samples will be such that the following inequalities will take place $Z < R_p^{\alpha}$ and $Z < R_p^{\text{Li}}$ (for the left side of samples) or $Z_{\max} - R_p^{\alpha} < Z < Z_{\max}$ and (for the right side of samples), respectively, and the direction of fission fragment flights will be to the surfaces then such fragments can leave sample and decrease the damage creation rate.

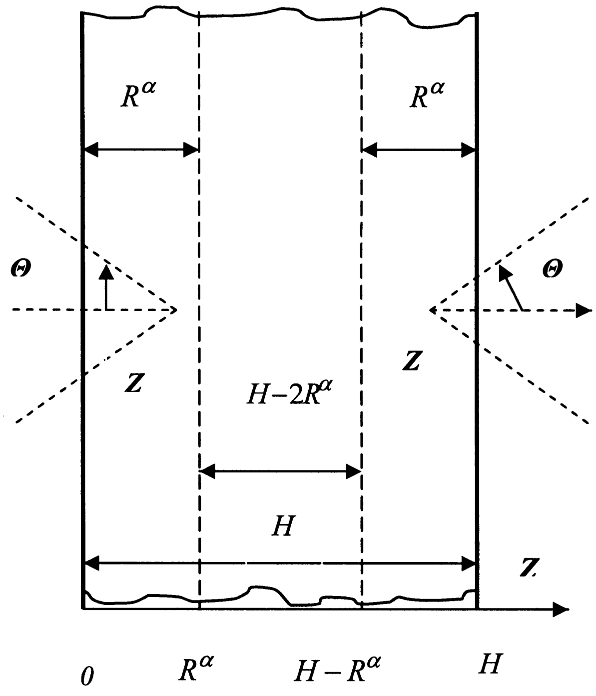

Fig. 1. Scheme of cross-section of thin semiconductor specimen of thickness greater than $H \geq 50$ μm with the directions of α-particles and ^{7}Li recoil nuclei flights to the both lateral surfaces of specimen.

One can calculate, using a computer code TRIM-2000 [1], that nearly 60–70% of point defects are created in the Bragg-peak area – a maximum damage creation zone. Thus the escaped α-particles and ^{7}Li recoil nuclei decrease the total damage level in the region within the projected ranges from both surfaces of the samples. The corresponding calculations of damage distribution have been carried out in Ref. [7]. Here, we present the results of these calculations. The damage distribution dependence $D_{\alpha,\text{Li}}^{\text{total}}(Z)$ vs. the depth Z between the flat parallel surfaces of boron-contained semiconductors under the influence of elastic scattering of α-particles and ^{7}Li recoil nuclei can be presented in the form:

$$(12.1)\quad D_{\alpha,\text{Li}}^{\text{total}}(Z) = 0.5\times D_{\alpha}\times\left[1+\frac{Z}{R^{\alpha}}\right]+0.5\times D_{\text{Li}} \times\left[1+\frac{Z}{R^{\text{Li}}}\right],\ \text{at}\ 0 \leq Z \leq R^{\text{Li}}$$

$$(12.2)\quad D_{\alpha,\text{Li}}^{\text{total}}(Z) = D_{\text{Li}}+0.5\times D_{\alpha}\times\left[1+\frac{Z}{R^{\alpha}}\right],\ \text{at}\ R^{\text{Li}} \leq Z \leq R^{\alpha}$$

$$(12.3)\quad D_{\alpha,\text{Li}}^{\text{total}}(Z) = D_{\alpha}+D_{\text{Li}},\ \text{at}\ R^{\alpha} \leq Z \leq H-R^{\alpha}$$

$$(12.4)\quad D_{\alpha,\text{Li}}^{\text{total}}(Z) = D_{\text{Li}}+0.5\times D_{\alpha}\times\left[1+\frac{Z^*}{R^{\alpha}}\right],\ \text{at}\ H-R^{\alpha} \leq Z \leq H-R^{\text{Li}}, Z^* \subseteq \left[R^{\alpha}, R^{\text{Li}}\right]$$

$$(12.5)\ D_{\alpha,\text{Li}}^{\text{total}}(Z) = 0.5\times D_{\alpha}\times\left[1+\frac{Z^*}{R^{\alpha}}\right]+0.5\times D_{\text{Li}}\times\left[1+\frac{Z^*}{R^{\text{Li}}}\right],\ \text{at}\ H-R^{\text{Li}} \leq Z \leq H, Z^* \subseteq \left[R^{\text{Li}}, 0\right]$$

Here, the parameters $R^{\alpha,\text{Li}} = R_p^{\alpha,\text{Li}} + \Delta R_p^{\alpha,\text{Li}}$, where $R_p^{\alpha,\text{Li}}$ are the projected ranges and $\Delta R_p^{\alpha,\text{Li}}$ are the half of widths of Bragg peaks for α-particles and ^{7}Li recoil nuclei in boron containing semiconductors. This means that we take into account in our calculations only the particles that do not leave the samples irradiated by neutrons ($0 \leq Z \leq R^{\text{Li}}$ and $H - R^{\text{Li}} \leq Z \leq H$).

For calculation of the whole damage, it is necessary to multiply the values of $D_{\alpha,\text{Li}}^{\text{total}}(Z)$, Eqs. (12), by thermal neutron absorption coefficients $k_{\text{absorption}} = \exp(-\lambda_Z \times Z)$. Then, we can write the final expression:

$$(13)\quad D_{\alpha,\text{Li}}^{\text{final}}(Z) = D_{\alpha,\text{Li}}^{\text{total}}(Z)\times\exp(-\lambda_Z\times Z),\ \text{at}\ 0 \leq Z \leq H$$

Relation (13) is an approximate one, because we did not take into account the correct integration of damage cross-section dependences vs. the depths and angles for some α-particles and ^{7}Li recoil nuclei at boron containing semiconductors that left the samples. The

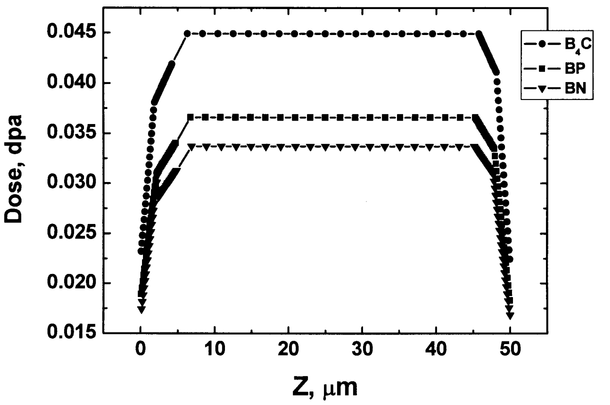

Fig. 2. The distributions of vacancy concentrations in irradiated BP, B$_4$C and BN semiconductors by thermal neutrons vs. the depth without absorption of thermal neutrons (see expressions (12.1)–(12.5)).

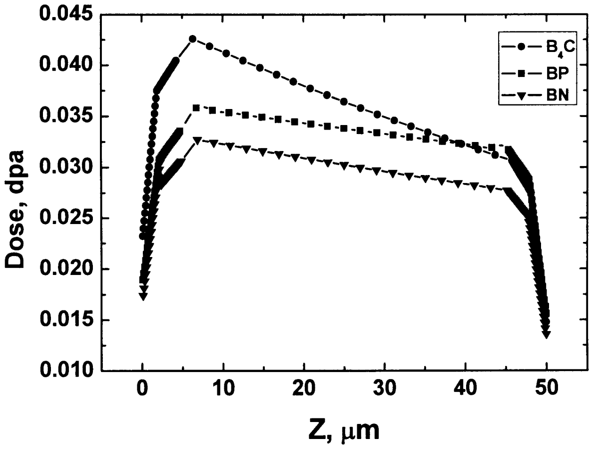

Fig. 3. The distributions of vacancy concentrations in irradiated BP, B$_4$C and BN semiconductors by thermal neutrons vs. the depth with thermal neutrons absorption (see expression (13)).

associated inaccuracies in our calculations are negligibly small (see also [8]). The depth distributions of vacancies without absorption (see expressions (12.1)–(12.5)) and with absorption (see expression (13)) are presented for three semiconductors in Figs. 2 and 3. As one can see, the difference between the left and right sides of foil is very small, so it is possible to increase the thickness of samples.

And the homogeneity of vacancies should not be bad.

Some estimations and comparisons

It is sometimes impossible to obtain the necessary type of semiconductor conductivity or complex form of surface nanostructures by introduction of impurities during a semiconductor crystal growth. In this case the implantation of electrically active impurities (energy of ions is about a few hundred keV) is used. Sometimes it is also necessary to carry out a long time annealing processes to obtain homogeneous impurity distributions. Well developed homogeneous vacancy structures are very suitable for radiation enhanced diffusion of impurities deposited or implanted in the subsurface region of crystal towards the bulk of semiconductor under post irradiation annealing.

The diffusion coefficient of electrically active impurities is proportional to point defect concentrations and equal [15, 17] to:

$$D_{\text{imp}} = \alpha \times [d_{\text{imp},V} C_V + d_{\text{imp},I} C_I] \tag{14}$$

here α is the thermodynamical factor, $d_{imp,v}$ and $d_{imp,I}$ are spatial diffusion coefficients in vacancies (V) and interstitial sites (I), C_V and C_I are vacancy and interstitial sites concentrations, respectively. So, creation of the point radiation defects by neutron leads to an increase of impurity diffusion.

As one can see, the total quantities of α-particles and ^{7}Li recoils at thermal neutron fluence $\Phi_{n,0}^{\text{thermal}}$ = 2.1 × 10^{17} n/cm^2 are:

$$N^{\text{Li}}(\text{BP}) \cong 3.32\times10^{16};\ N^{\text{Li}}(\text{BN}) \cong 4.53\times10^{16};$$
$$N^{\text{Li}}(\text{B}_4\text{C}) \cong 8.79\times10^{16} \tag{15}$$

in a relatively thick layer (volume is equal to V = 1 cm^2 × 0.005 cm, see Table 3). The average volume concentrations of ^{7}Li atoms in all these semiconductors at this neutron fluence should be:

$$\text{n}^{\text{Li}}(\text{BP}) = 6.64\times10^{18}\,\text{cm}^{-3};\ \text{n}^{\text{Li}}(\text{BN}) = 9.06\times10^{18}\,\text{cm}^{-3};$$
$$\text{n}^{\text{Li}}(\text{B}_4\text{C}) = 1.758\times10^{18}\,\text{cm}^{-3}.$$

As it is well known, helium atoms are not electrically active, only ^{7}Li impurities are electrically active in all the considered semiconductors. Let us calculate the volume concentrations of ^{7}Li impurities vs. thermal neutron fluences. It is clear that the following dependences for average volume concentrations vs. thermal neutron fluences can be written:

$$\text{n}_{\text{Li}}(\Phi_{\text{n}}^{\text{thermal}}) = \frac{\text{n}_{\text{Li}}(\Phi_{\text{n},0}^{\text{thermal}})}{\Phi_{\text{n},0}^{\text{thermal}}} \times \Phi_{\text{n}}^{\text{thermal}} \tag{16}$$

Consequently, the absolute concentrations of ^{7}Li impurities created after neutron transmutations can be changed very easy by variation of thermal neutron fluences. And also the damage dose of point defects (see Table 3) for the neutron fluence $\Phi_{\text{n}}^{\text{thermal}}$ = 2.1 × 10^{17} n/cm^2 are equal to:

$$D_{\alpha,\text{Li}}^{\text{total}}(\text{BP}) \cong 3.66\times10^{-2}\,\text{dpa};$$
$$D_{\alpha,\text{Li}}^{\text{total}}(\text{BN}) \cong 3.37\times10^{-2}\,\text{dpa};$$
$$D_{\alpha,\text{Li}}^{\text{total}}(\text{B}_4\text{C}) \cong 4.49\times10^{-2}\,\text{dpa}. \tag{17}$$

A similar dependence of damage dose vs. thermal neutron fluences can be written as for the average concentrations [14].

Let consider some characteristics of BN, BP and B$_4$C semiconductors which we used for calculations in this article, these parameters are presented in Table 5.

Top symbols '*' and '**' for BP semiconductor mean a single crystal or a thin film [9], respectively. Top symbol '+' for BN$_{\text{cub}}$ semiconductor corresponds to a polycrystalline material and type of carriers not determined [9].

One can conclude using the comparison of calculated values of ^{7}Li atom average concentrations in the

Table 5. Some characteristic parameters of BN, BP and B_4C semiconductors [6, 9]

Type of semiconductor		BN_{cub} [9]	BP [6]	B_4C [6]
Density, g/cm^3		3.487	2.89	2.52
Lattice parameter, nm		0.36157	0.4538	0.56(a); 1.212(c)
Energy gap, eV		5.8÷6.2	2.0	1.64
Melting point, K		3246	1400	2723
Carrier concentration, cm^{-3}	n^-	10^{15} (500 K)$^+$ 10^{14} (900 K)$^+$	$7 \times 10^{16} \div 4 \times 10^{19}$ (300 K)* $8 \times 10^{17} \div 2 \times 10^{21}$ (300 K)**	Unknown
	p^+		$2 \times 10^{16} \div 5 \times 10^{18}$ (300 K)* $1 \times 10^{19} \div 1 \times 10^{20}$ (300 K)**	Unknown

considered semiconductors and its carrier concentrations, that at this thermal neutron fluences such values are very close.

It is necessary to note that, as a rule, lithium atoms have very big mobility (high diffusivity) at room temperatures too and try to be absorbed by the surface layers of materials. This is the reason why it is necessary to keep germanium semiconductor detectors at liquid nitrogen temperature and why there exist the so-called sweating alloys with high concentration of lithium atoms. So, it is necessary to study the diffusivity of lithium in all the discussed semiconductors because Li can leave bulk semiconductors and may be absorbed by their surfaces.

Conclusion

The main consequence of our calculations is that the irradiation of natural boron containing semiconductor single crystals by thermal neutrons provides a good opportunity for the creation of well developed damage structures with high concentration of point defects and their complexes at medium neutron fluences. In our case the final damage concentrations in BN, BP and B_4C single crystals irradiated up to a relatively low thermal neutron fluence of $\Phi_{n,0}^{thermal} = 2.1 \times 10^{17}$ n/cm^2 are $D_{\alpha,Li}^{final} > 10^{-2}$ dpa (see Table 3). The homogeneity of damage distribution vs. the distance between the flat parallel sample sides is determined by the thickness of semiconductor (see expressions (12), (13)).

The long-lived nuclear fission fragments of all semiconductors are absent after thermal neutron irradiation as it was shown in Ref. [4].

The variation of thermal neutron fluence allows one to change the active ^7Li impurity and vacancy concentrations and the vacancies in all the considered semiconductors in wide value intervals at a relatively low level of neutron fluences (see expression (16)).

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