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Ion-beam simulation of radiation damage produced by fast neutrons in heterophase structures

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ABSTRACT

3D Monte-Carlo algorithm and computer code have been developed that allows choosing and optimizing the conditions of ion irradiation needed for the adequate ion-beam simulation of radiation damage under fast neutron irradiation. It is established that, by the proper selection of energy and dose of Si^+ ions, it is possible to reproduce well the effect of irradiation with fission neutrons of subsurface and buried layers of silicon or Si-based 2D and 3D-heterostructures. The results can be used for testing the radiation hardness of silicon-based electronic and optoelectronic device structures.

1. Introduction

The tolerance to radiation is one of the key characteristics of solid state devices for their application in nuclear and space environments. Although this issue has been already addressed in a huge number of research works, such studies are becoming once again challenging in connection with the development of nanoelectronics [1]. This is because the response of nanostructures to radiation may be different from that for bulk materials.

One of the most important factors of radiation damage is the impact of fast neutrons. When developing new or adapting old technology of electronic devices fabrication, the task of quick evaluation of the sensitivity of parameters of the devices or their constituents to the effect of neutron fluxes can arise. Under fast neutron irradiation, defects are created by the recoil atoms, therefore one can assume that such quick evaluation can be done without the full-scale tests – by using ion beams as a source of damaging radiation, i.e. by using the ion-beam simulation. However, to check the adequacy of the simulation and to choose its correct conditions, it is necessary to perform the comparative calculations that allow determining the degree of radiation damage in electronic components for two kinds of irradiation – fast neutrons and accelerated ions.

The present article is focused on the algorithm and results of the Monte-Carlo computer calculation of concentration and distribution of point defects produced by ion beams and fast neutrons in solid-state homophase or heterophase structures of any geometry and composition, including the nanostructures. The computer calculation can be used for the prediction of the suitable conditions of ion irradiation to simulate the effect of fission neutrons.

2. Calculation approach

The objective of computer simulation was to find, using the Monte-Carlo method, the kind, doses and energies of ions, for which in a certain volume of the material (structure component, phase) there would be approximately the same degree of radiation damage, i.e. the same concentration of Frenkel pairs (for clarity, we will consider vacancies), as for the given dose of irradiation with fission neutrons.

In most semiconductor devices, the most radiation-sensitive volumes are located at some distance from the surface of the structure. Hence it is necessary to calculate the equivalent doses for the layers located at various distances from the surface. An interesting special case of heterophase structures is represented by the thin layers or islands of a material with different composition, located either on the surface or buried at some depth.

In general, under room temperature irradiation, the secondary processes should be taken into account that involve components

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of Frenkel pairs: their diffusion, recombination, aggregation into divacancies, diinterstitials or larger complexes, capture by the trap centers etc. [2]. However, for the moderate doses of neutron or ion radiation (when there is no significant overlap of displacements cascades), it may be assumed that, for the close concentrations of primary point defects, contribution of the secondary processes would only slightly break the relationship between the degrees of damage for two kinds of irradiation.

The main difference in a character of radiation damage under neutron and ion irradiation can be caused *a priori* by the following factors.

When exposed to neutron irradiation, the primary recoils start at the points uniformly distributed inside a material, whereas, under irradiation with ions, the recoils will start from the surface of a structure. The ion-induced defect formation process refers only to the near-surface layer with a thickness of the order of the mean projected ion range R_p, whereas neutrons create quasi-homogeneous distribution of defects. Certain difference occurs also in the energy spectra of moving atoms, that cross a certain part of volume and are capable to displace the atoms from the lattice sites. Nevertheless, as it is shown in Section 3, for not too large depths, it is possible to reach an approximate equivalence of the degrees of radiation damage in nanostructures under the irradiation with fission neutrons and ion beams.

The SRIM-like approach (SRIM – The Stopping and Range of Ions in Matter [3]), but taking into account the 3-dimensional nature of the problem, is taken as a basis of the developed algorithm for the calculation of spatial distribution of vacancies produced by ions or recoil atoms. The positions of all structure components (phases) of interest are set in Cartesian space. When the assigned structure contains the components, which have the lateral sizes (in the direction, parallel to surface) of the same order as the sizes of displacement cascades or smaller, the program code includes the randomization of lateral coordinates both for the ion impact points (in the case of ion irradiation) and for the starting points of the primarily recoils produced by neutrons.

For each collision of the moving ions (atoms) and neutrons with the atoms of a structure, the coordinates of this event are recorded (the vacancy coordinates). The fate of ion and all recoil atoms is traced until their energy becomes below the displacement threshold E_d. The locations of displacement cascades and vacancies relative to the structure components (or the devise constituents) are determined as a result of the calculation.

To simulate the irradiation with fission neutrons, the data on the neutron spectrum for a typical nuclear reactor and the data on neutron cross sections [4] were used. In this case the angle distribution of recoils was considered as isotropic, and their energy distribution (from E_{max} to E_d, where $E_{max} = 4M\ E_n/(1 + M)^2$, E_n – neutron energy, M – the mass number of the substance atom) was considered as uniform. Possible deviation from the isotropism will lower the number of produced vacancies by 30–50% [5].

3. Results and discussion

The developed algorithm is universal with respect to the type of nanostructure. The selection of the kind (kinds) of bombarding ion for the simulation is determined by the chemical composition of the structure components, in which it is necessary to simulate the radiation damage. If the structure or its part, which is subject to the simulation procedure, is chemically homogeneous and monatomic, then the ion kind corresponds to the kind of the atoms, of which the structure or its part consists. In the case of homogeneous but polyatomic systems with the close atomic numbers of atoms, for example GaAs, it is possible to limit the selection to only one ion kind. In the case of large difference of atomic masses, it is necessary to use ions of each chemical element of the material in the corresponding proportions. Some difficulties appear in the case of heterogeneous systems, for example Shottky barrier structures, when the atomic mass of a metal significantly differ from the mass of the semiconductor atom. In this case, the selection of the ion kinds, their energies and doses, which simulate in the best way the case of neutron irradiation, can be done by the "trial-and-error" procedure using the SRIM-calculated ion distributions as a guide. In order to reduce the degree of nonuniformity in the vacancies depth distribution under ion irradiation, it is possible to use polyenergetic irradiation instead of monoenergetic one.

Some examples of the implementation of this algorithm and computer code are given below for the silicon-based structures, subjected to irradiation with fission neutrons produced in a reactor of the GIR-2 type with the medium energy of fast neutrons about 1 MeV. The Si^+ ions were chosen as the simulating ions. The value of E_d was taken equal to 22 eV, however it does not actually influence the ratio of the vacancies concentrations for the cases of neutron and ion irradiation. The distributions of vacancy concentration in the silicon sample produced by neutron irradiation with the dose of 1×10^{15} cm^{-2} and by the sequential irradiation with Si^+ ions of two energies (140 keV, 6.3×10^9 cm^{-2} + 56 keV, 2.2×10^9 cm^{-2}) are given in Fig. 1. The energies and doses of Si^+ ions were chosen to provide the best coincidence of the calculated concentrations and distributions of vacancies. Good agreement is reached in the range of depths to 230 nm. This correspondence is reached in spite of some mismatch in the energy spectra of moving particles in the case of neutrons and ions for the region of high energies of fast atoms (Fig. 2). Such a weak effect of the energy spectra mismatch is explained by the very small fraction of high-energy particles for which this mismatch takes place (logarithmic scale for the ordinate axis in Fig. 2 should be taken into account). In the region of relatively low energies for ion and neutron irradiations, as can be seen from Fig. 2, the energy spectra are close to each other, and this provides the pointed above correspondence of the vacancy concentrations.

The picture of spatial distribution of the displacements created by ions in the surface layer with a thickness of $\sim(R_p + \Delta R_p)$ in the projection on the X–Y plane, parallel to surface (Fig. 3a), is similar to the distribution of vacancies created by neutrons, for which, due to the scattering isotropy, the form of distribution does not practically depend on the orientation of the projection plane (projection on the X–Z plane, perpendicular to surface, in the case of neutrons is given in Fig. 3b).

Let us consider further the case of irradiating the $Si/Ge_xSi_{1-x}/Si$ ($x = 0.5$) heterostructures, in which the layer of Ge_xSi_{1-x} islands

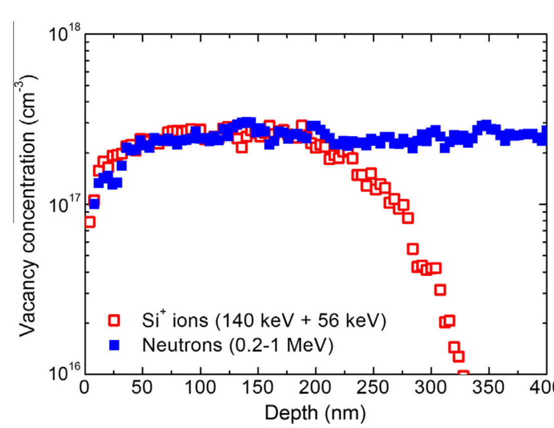

Fig. 1. Vacancy depth distributions for two kinds of irradiation of silicon: fission neutrons (0.2–1 MeV, 1×10^{15} cm^{-2}) and Si^+ ions (140 keV, 6.3×10^9 cm^{-2} + 56 keV, 2.25×10^9 cm^{-2}).