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Analysis of Individual Collision Cascade Parameters during Irradiation of Ga_2O_3 by Atomic and Molecular Ions

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Abstract—Collision cascade density is one of the most important parameters that determine radiation damage accumulation in semiconductors under ion bombardment. We perform calculation of collision cascade parameters formed in β-Ga_2O_3 by irradiation with 1.3 keV/amu atomic F, P, and molecular PF_4 ions using two different methods: the method considering sub-cascade formation, and by calculation an average number of vacancies in spheres of fixed radius. The calculated results are compared with experimental data on damage accumulation in β-Ga_2O_3 under irradiation with aforementioned ions. It is shown that both methods qualitatively predict the effect of collision cascade density on radiation damage accumulation in gallium oxide. Fractal nature of cascades formed in β-Ga_2O_3 is established, corresponding fractal dimension is calculated.

Keywords: Gallium oxide, β-Ga_2O_3 ion irradiation, defect engineering, collision cascade density

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1. INTRODUCTION

Ion implantation is one of the main methods used in the production of semiconductor devices to introduce doping impurities, create electrically insulating regions, etc. It is well known that ion bombardment of semiconductors is always accompanied by the accumulation of radiation damage [1]. The nature and rate of such damage accumulation depend on many parameters, such as ion energy, flux, and ion mass, as well as substrate temperature [1, 2]. These dependencies are quite well known for the majority of conventional semiconductors.

However, there is an additional parameter that can also dramatically affect the effectiveness of radiation damage accumulation, enhancing the concentration of structural defects growth as it increases. Such a parameter is the average density of individual displacement cascades f_c, i.e., the density of displaced target atoms averaged over all cascades at a given depth. Already in early works it was experimentally shown (see, for example, in [3–5]) that, keeping all other parameters the same, an increase in f_c leads to an increase in the amount of structure damage formed. At the same time, it has long been calculated for the case of atomic ion bombardment, that heavy ions (large Z) create denser cascades than light ones.

The task is complicated if the irradiation is performed by molecular ions, when the atomic components of the molecules create their own cascades, which in turn form the final total collision cascade. Thus, prediction of the effect of cascade density for each such a specific case becomes significantly more difficult. In the general case, to solve such a problem it is necessary to have a calculation methodology that would allow, at least in arbitrary units, to compare this density for different specific cases. This will make it possible to predict how much more effective the structure disorder formation will be during the implantation with two types of ions under the same other bombardment conditions.

Thus, one of the main objectives of this publication is to compare different methods for estimating the density of collision cascades. These estimations are quite simplified due to the significant complexity of cascade geometry. At the same time, not the determination of the absolute cascade density, which is not well developed yet, but the relative values are important from the point of view of predicting the effect of this density on radiation damage accumulation. The potential and importance of such an assessment can be demonstrated, for example, by the results described in the work [6]. It was shown there that under ion irradiation, the cascade density influence has a threshold character in the formation of the structure damage: an increase in density above a certain critical value leads to a rapid increase in the planar surface amorphization rate and an increased efficiency of damage accumulation in the crystal bulk.

Previously, it was also experimentally shown that the density of collision cascades dramatically affects the resulting radiation damage in many semiconductors, including, for example, Si [7–9], SiC [10–12],

ZnO [13, 14], GaN [6, 15, 16], α-Ga_2O_3 [17] and β-Ga_2O_3 [18]. Thus, the determination of cascade parameters for a specific irradiation conditions is an important problem, the solution of which can make it possible to predict the accumulation rate and the final value of radiation damage.

For the last time, there has been a strong interest in materials suitable for the production of high-power electronic and new generation optoelectronic devices. Some wide-band gap semiconductors like GaN, InGaN, SiC have already been successfully used in production for these purposes. Nevertheless, there is a need for materials with an even wider band gap ($\gtrsim$4 eV). A promising semiconductor in this regard is beta-gallium oxide (β-Ga_2O_3), which has such characteristics as a wide band gap (4.85 eV), high breakdown voltage (~8 MV/cm), thermal conductivity and electron mobility [19–21]. Thus, all calculations and experiments were carried out specifically for this semiconductor.

2. CASCADE DENSITY CALCULATION METHODS

Three-dimensional initial distributions of primary atomic displacements (more precisely—vacancies) were calculated for the target and ions under consideration using the Monte Carlo simulation method used by well-known code TRIM [22]. The calculation in this program is performed on the base of the binary collision approximation, i.e., without taking into account the nonlinear effects that take place inside dense cascades, which could in turn lead to an increased defect formation (the subject of this article). Cascades formed under molecular ion irradiation are modelled as the sum of randomly selected cascades for each atomic component that is constituent of the molecule. Resulting distributions of displacements in the average collision cascade were obtained as by averaging (for more details, see [6]).

The 3D coordinate distributions of all displacements (vacancies) obtained in the above manner were used later to estimate the density of displacement cascades. We know about two algorithms developed for calculating this density, excluding MD simulation and early estimation methods (see reviews [5, 6]). We will consider them sequentially.

In the first algorithm (described in detail in [6]), the entire cascade is divided into successive layers of some small thickness ΔX parallel to the target surface.

It is assumed that subcascades consisting of a sufficiently large number of closely spaced vacancies will be formed [6, 9]. The point of entry of the ion into the target was taken as the origin of the Cartesian coordinate system, the axis X was directed perpendicular to the surface, and the axes Y and Z along the surface. Subcascades were determined based on the lateral distribution of vacancies in each layer according to the following criterion: vacancies located closer than 2 nm from each other were considered to belong to one subcascade. Subcascades with fewer than 4 vacancies were excluded from consideration. The standard deviation of vacancies from the center of their distribution within one subcascade was calculated:

$$R_{i,j} = \frac{1}{N_{i,j}^{\text{vacancy}}} \sum_{k=1}^{N_{i,j}^{\text{vacancy}}} \left\{ \left(Y_{i,j,k} - \frac{1}{N_{i,j}^{\text{vacancy}}} \sum_{k=1}^{N_{i,j}^{\text{vacancy}}} Y_{i,j,k} \right)^2 + \left(Z_{i,j,k} - \frac{1}{N_{i,j}^{\text{vacancy}}} \sum_{k=1}^{N_{i,j}^{\text{vacancy}}} Y_{i,j,k} \right)^2 \right\}^{1/2}, \quad (1)$$

where i, j, k—the number of the cascade, subcascade and vacancies, respectively; $N_{i,j}^{\text{vacancy}}$—the number of vacancies in the subcascade i, j.

Since the main part of the vacancies of the subcascade is concentrated within $R_{i,j}$, this value can be considered its radius. The subcascade has a cylindrical shape with a radius of $R_{i,j}$ and a height of ΔX. The average density of the individual collision cascade f_{av} can then be calculated using the obvious formula:

$$f_{av} = \frac{1}{n^{at}} \frac{\sum_{i=1}^{N^{\text{cascade}}} \sum_{j=1}^{N_i^{\text{subcascade}}} N_{R_{i,j}}^{\text{vacancy}}}{\sum_{i=1}^{N^{\text{cascade}}} \sum_{j=1}^{N_i^{\text{subcascade}}} \pi R_{i,j}^2 \Delta X}, \quad (2)$$

where N^{cascade}—the total number of cascades considered, $N_i^{\text{subcascade}}$—the number of subcascades in the cascade i, $N_{R_{i,j}}^{\text{vacancy}}$—the number of vacancies in the cylinder of radius $R_{i,j}$ inside the subcascade i, j; $\pi R_{i,j}^2 \Delta X$—cylinder volume.

The second approach was described in [23], where it was used. In this case, the number of adjacent vacancies N_v was calculated for each vacancy in the cascade, i.e., vacancies situated within a sphere of radius R_c centered at this vacancy. For each depth, the number of adjacent vacancies was averaged first over all vacancies located in the vicinity of 2.5 nm along the axis X, and then over all cascades. The collision cascade density at a certain depth was calculated as the total average number of neighboring vacancies at a given depth divided by the volume of the sphere $(4/3)\pi R_c^3$.

Back in the 1980s, it was shown that the distribution of atomic displacements in the collision cascade can be described within the framework of fractal geometry [24, 25]. This approach to calculating the density of cascades allows calculating the fractal dimension of cascades if the geometry of the cascade has a fractal nature. This method showed for SiC the relationship of fractal parameters of cascades with experimental data on damage accumulation in case of

Table 1. Radiation parameters β-Ga_2O_3

Ion	Energy		Dose per 1 *DPA* 10^{14} cm^{-2}	Flux	
	keV	keV/amu		10^{11} cm^{-2} s^{-1}	10^{-3} DPA/s
F	25	1.3	11.4	27.6	2.41
P	40	1.3	6.28	15.1	2.41
PF_4	140	1.3	1.97	4.7	2.41

irradiation with pulsed beams of atomic ions [23]. Nevertheless, in the general case, such a relationship has not been studied at the moment.

It is possible to determine whether the cascade has a fractal nature by varying the parameter R_c. If the vacancy distribution is a fractal structure, then the number of neighboring vacancies N_v should depend on the radius of the sphere R_c according to the law $N_v \sim (R_c)^D$, where D—fractal dimension, and $D < 3$. Accordingly, when plotting the dependence of the average value N_v on R_c on a logarithmic scale, it can be expected that the dependence will be linear, and the slope will determine the value of D.

Experimental data on the accumulation of radiation damage were obtained by irradiation of monoclinic β-Ga_2O_3 crystals grown by the HVPE and irradiated with F^+, P^+, PF_4^+ ions using 500 kV HVEE implanter. All implantations were performed at room temperature 7°C off the normal to the surface to avoid channeling effects. The irradiation parameters are presented in Table 1. Doses and flux expressed in displacements per atom (DPA) and DPA/s, respectively, remained the same for all ions used. This ensures a correct comparison of radiation damage generated by atomic and cluster ions, since the only difference between all irradiation cases is the different density of collision cascades [9]. The resulting disorder was measured using the RBS/C method on the same implanter. The RBS/C spectra were processed using one of well accepted algorithms [26] to obtain depth profiles of relative disorder.

3. RESULTS AND DISCUSSION

Figure 1 shows the cascade densities calculated using both methods as a function of the distance from the surface. As noted above, for predicting the effectiveness of radiation damage, it makes sense to talk only about the relative difference in density for different ions within the framework of a single calculation method. In addition, one should take into account the fact that, as can be clearly seen from Fig. 1b, the probability of generation at a given depth of the cascade (η) may be less than unity. Then the cascade simply does not form there and the concentration of stable defects does not increase.

A higher cascade density in the near-surface region for cluster ions PF_4 compared with atomic ions is obtained by both methods. This is naturally explained

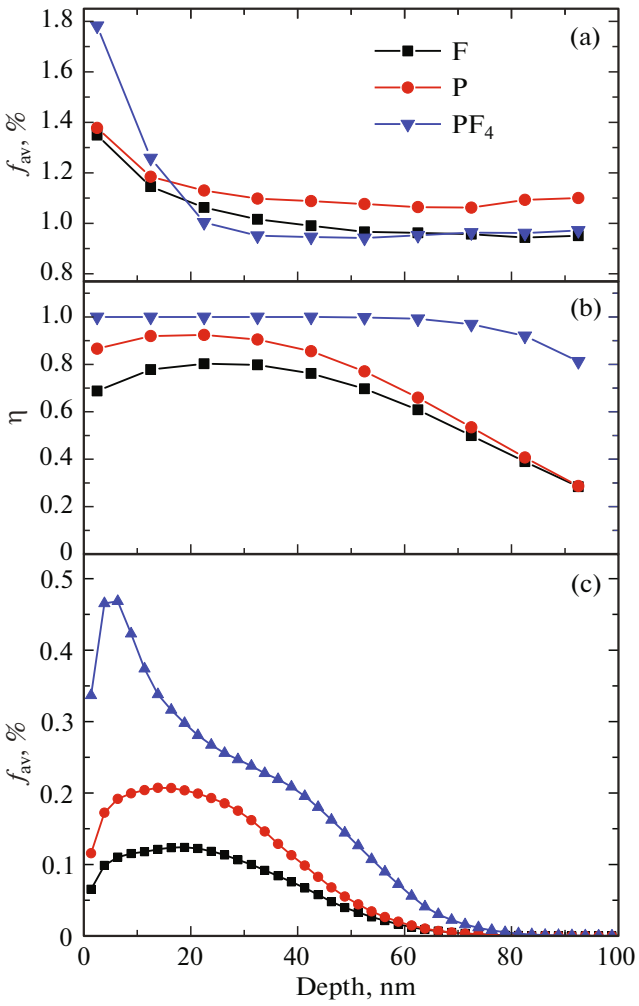

Fig. 1. The depth dependences of the density of the collision cascades, calculated (a) according to the [6] method, which considers the formation of subcascades (b) the proportion of ions forming at least one subcascade in the layer corresponding to a given depth (c) cascade densities calculated using the [23] method, considering neighboring vacancies in a sphere of fixed radius (here $R_c = 8$ nm).

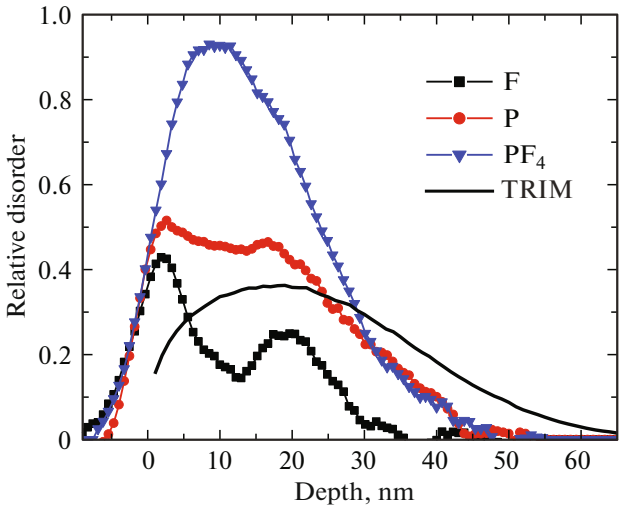

Fig. 2. Profiles of relative disorder in β-Ga_2O_3 after irradiation with 25 keV F, 40 keV P, 140 keV PF_4 ions to a dose of 0.441 DPA, as well as the profile of vacancy generation (TRIM) for P 40 keV (at an arbitrary scale along the axis *Y*).

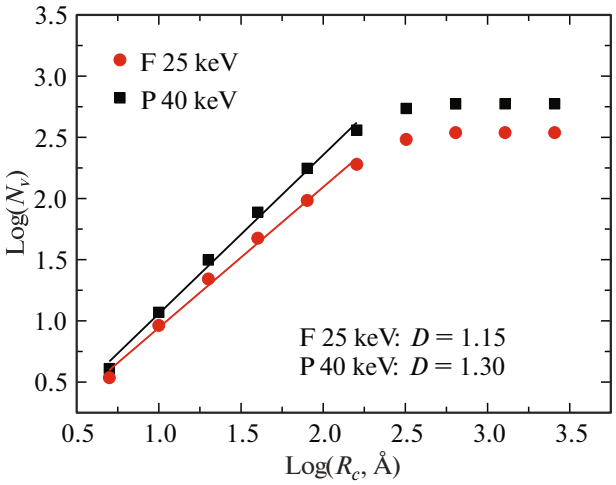

Fig. 3. Dependence of the average number of adjacent vacancies on the value of the parameter R_c at the depth of 16 nm.

by the effective overlap of individual cascades of molecular ion components near the surface. These calculations are consistent with the relative disorder profiles based on experimental data shown in Fig. 2. These profiles, formed by irradiation with β-Ga_2O_3 equivalent doses F, P, PF_4, have two disorder maxima—surface and bulk. While the first maximum is formed as a result of diffusion of mobile point defects generated by stopping ions to the surface, which takes place at the stage of formation of stable disorder. The depth of the bulk maximum formation corresponds to the maximum of vacancy generation. The so-called "molecular effect" is observed in case of near-surface peak, i.e., an increase in the rate of accumulation of radiation damage during irradiation of the material with molecular ions compared to irradiation with atomic [17, 18]. Since, the number of primary point defects generated within the framework of the binary collision approximation remained the same for both irradiations, the observed differences are due to nonlinear effects caused by differences in the density of individual cascades.

The difference in damage accumulation under irradiation with atomic ions of different masses (F and P) in the framework of the subcascade approach is due to two factors: (1) a higher density of cascades created by heavier P ion; (2) a larger fraction of ions forming at least one subcascade, in the case of P ion. Both of the considered methods make it possible to predict the resulting radiation damage to a certain extent by calculating the parameters of individual cascades.

It is possible to check whether the geometry of the displacement distributions under consideration has a fractal nature by drawing the dependence of the logarithm of the average number of vacancies on the logarithm of the parameter R_c (Fig. 3). As shown above, the linearity of such a dependence suggests the possibility of considering cascades as having fractal geometry, and the slope of the lines corresponds to fractal dimension *D*. Figure 4 shows the dependences of the calculated fractal dimensions of the cascades for the ions under consideration at different depths. Interestingly, similar to the density of cascades, the value of the fractal dimension under irradiation by molecular ions turns out to be higher at the surface compared to irradiation by atomic ions. This indicates the possibility to use the fractal dimension of individual collision cascades as a parameter that allows predicting the amount of damage accumulation in semiconductors.

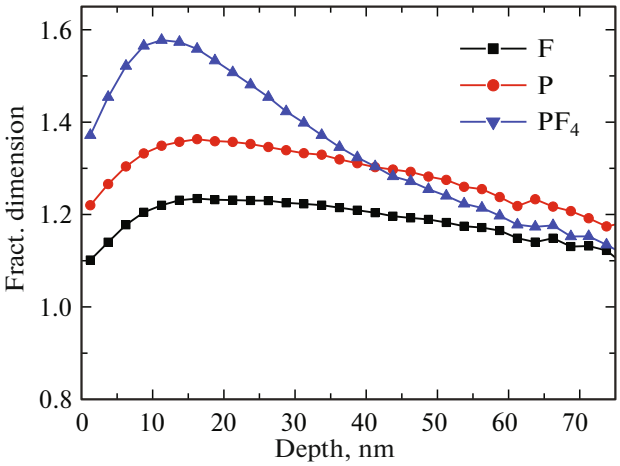

Fig. 4. The depth dependence of the fractal dimension of collision cascades.

4. CONCLUSIONS

The parameters and geometry of the collision cascades in β-Ga_2O_3 irradiated by 1.3 keV/amu atomic F and P, and molecular PF_4 ions were analyzed. The comparison of two methods for calculating cascade parameters showed that both represent experimental data on the effect of collision cascade density on the defect accumulation in gallium oxide and make it possible to estimate the amount of accumulated damage in case of irradiation by various ion types. The strong impact of the density of collision cascades on the effectiveness of the stable damage formation in β-Ga_2O_3 was confirmed. The fractality of the collision cascades was established for all the considered cases and their fractal dimensions have been calculated.

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CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest.

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