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Critical Exponents in Percolation Model of Track Region

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Numerous experiments on defect formation in insulators, metals, alloys, and amorphous semiconductors have shown that these materials are sensitive to track formation when they are bombarded by swift heavy ions (SHI).

Detail understanding of the basic processes of materials modification by SHI will help to construct materials with preassigned properties.

Tracks were examined like a chain of deal spherical regions; it was assumed that each incident ion creates one such chain. In this model, we assume that the track is formed randomly, but in that place of the ion path, where the energy value, which loses each ion to the unity of the way, is above some threshold value.

As a result of irradiation the number of tracks will continue to grow, areas of the single tracks modified substance continue to overlap, form of modified matter becomes more complicated, creating branched structure.

Based on the scaling hypothesis large-scale curve were constructed, critical exponents for this percolation model was established. Two such curves were evaluated: in the case of non-equiprobable distribution of tracks regions in depth with ratio of critical exponents $(\beta/\theta)_s = 0.68$ and in the case with equiprobable distribution of tracks regions in depth, so-called model of continuous percolation with ratio of critical exponents $(\beta/\theta)_e = 0.41$.

Differences between critical exponents of this model and the continuous percolation model indicate that the dependence of the modified structure area on the dose and the angle related with the correlation between individual tracks. It results in next effect: angular dependence of the surface area of the branched structure has maximum value at certain «critical» angle of ions incidence.

Keywords: Track, Branched structures, Swift heavy ions, The Monte Carlo method, Critical exponents, Percolation threshold, Percolation.

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1. INTRODUCTION

Numerous experiments on defect formation in insulators, metals, alloys, and amorphous semiconductors have shown that these materials are sensitive to track formation when they are bombarded by swift heavy ions (SHI).

Detail understanding of the basic processes of materials modification by SHI will help to construct materials with preassigned properties.

Areas of individual tracks with modified substance start to overlap with the irradiation, as a result modified form of matter becomes more complicated, forming a branched structure.

Formation of branched structures from separate tracks depending on the characteristics of the projectile beam and on parameters of the SHI induced tracks were theoretically modeled in this work.

Study of changes in material properties as a result of electronic excitation upon irradiation by SHI and the creation of latent tracks in these materials is an exciting and promising field for new research and development. However, despite the relevance of the topic and practical significance of the expected results, the formation of branched structures of the individual tracks has been insufficiently studied.

2. MODELLING

2.1 Theoretical & experimental prerequisites

Tracks of various shapes and lengths, filled with a modified (with respect to the material of the sample) material, are formed in solids under SHI irradiation along its trajectory. They have diffraction pattern of tracks differ from diffraction pattern of whole sample. They are generated as a result of the strong relaxation of electronic excitations and formed along the trajectory of the ion. Tracks are beginning both from the irradiated surface and at some distance from it. Continuous and discontinuous cylindrical and spherical track field were found.

Elongated defects, similar to the "chain of pearls" that are placed along the trajectory of the ions at depths ranging from 35 to 100 nm and from 7 to 10 microns, were found after irradiation by xenon ions with $E = 250$ MeV in InP at room temperature [1]. Also in the iron garnet irradiated by ions with energies around 12 MeV in a mode of high speed [2] with the energy loss in the range of 4.5-7 keV·nm^{-1} the appearance of spherical domains of the modified material were observed. Discrete tracks point-shaped and oblong dark spots with a diameter equal to an average of about 3-10 nm along the trajectories of incoming ions in the form of a "chain of pearls" with a number of

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"pearls" in the track of two to five pieces were observed on the bright-field pictures in the paper [3].

Physical mechanisms of track formation, probability distribution of their formation along the trajectory and in the chain have not been yet fully clarified. The distribution of the tracks in the depth of the sample did not correlate with either the distribution of implanted ions, or the distribution of point defects formed by the ions. The experimental results do not uniquely determine the distribution of tracks.

However, it is widely recognized that the track is formed as a result of redistribution of the energy transmitted by one ion in the electron subsystem. Also it is known that the track is formed randomly in that place of the ion path, where the value of missing energy per unit of ion path is above a certain threshold, in a place where the rush of energy release is presented. It was noted that the simulation results of energy spectra using the SRIM 2008, shows that the maximum energy during the passage of high-energy ions are also located in an average of 25-40 nm. From the experimental data it is known that the tracks in the form of a chain of spheres are created at different depths (between 0 and 50 nm, between 0 and 500 nm) for different materials and conditions of exposure. For example, for InP irradiated by xenon ions, the average distance between tracks spherical averages of 25-40 nm, length of the chain is in the range from 50 nm to 150 nm.

2.2 Formulation of problem

We simulated sample in the form of plane-parallel plate with a thickness of 50 to 300 nm. For the calculations was chosen fragment of the plate in the shape of the box size from 50 to 300 nm. The case where the ion energy is sufficient to create a chain of spheres modified substances, energy is 20-40 MeV/amu around was modeled. Each incident ion creates a track in a sequence of a certain number of spherical regions. The trajectories of all ions are parallel to each other. In this model, we simulate different distribution areas in depth, such as: a) one sphere in the chain, b) one sphere in a chain or two spheres in the chain, c) one sphere or two spheres or three. And so on up to six spheres in the chain.

The first spherical region is equally likely to appear anywhere in the segment of the ion trajectory from its point of penetration into the sample to the point of 2ρ, where ρ - the average distance between the spheres. In the calculations ρ is equal to 40 nm. The distance from the first sphere to the second is chosen randomly from range of values between 0 and 2ρ, the form of distribution doesn't depend on the «history» (it is the same as for the preliminary scope, only shifted along the ion path in the appearance point of the previous sphere). Some specific distribution of tracking areas in depth was obtained as a result, distribution for the case when there are maximum three spheres in the chain is shown in Fig. 1.

Consecutively, two surfaces were exposed to radiation.

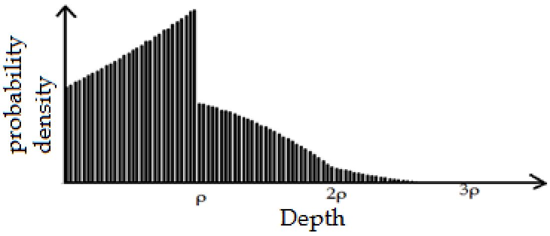

Fig. 1 – Distribution for a chain with one, two or three spheres

3. RESULTS AND DISCUSSION

With the irradiation modified substance areas of individual tracks start to overlap, as a result modified form of matter becomes more complicated, forming a branched structure. Some part of this branched structure is bordered on one surface of the sample, while others lie on the boundary with the opposite surface. When these parts connect one to another, they will create so-called "spanning cluster," which percolates from one surface to another (Fig. 2).

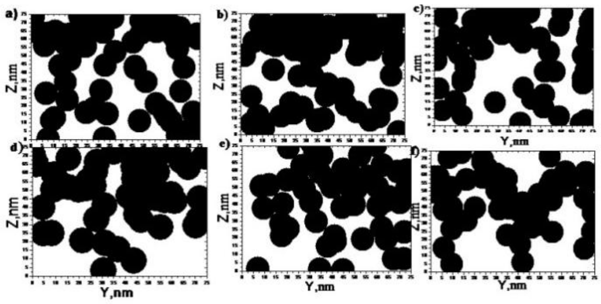

Fig. 2 – Percolation clusters induced by irradiation at different angles: a) 25 °, b) 30 °, c) 45 ° d) 60 ° e) 70 ° f) 90 °

On Fig. 2 percolation clusters induced by irradiation at different angles are shown. Percolation clusters will have different appearance, length and location in space.

Percolation threshold, fraction of spanning cluster with modified material for different doses and different distributions of track areas in depth for different scales of the sample were evaluated. Based on the scaling hypothesis large-scale curves were constructed (Fig.3), critical exponents for percolation model was established.

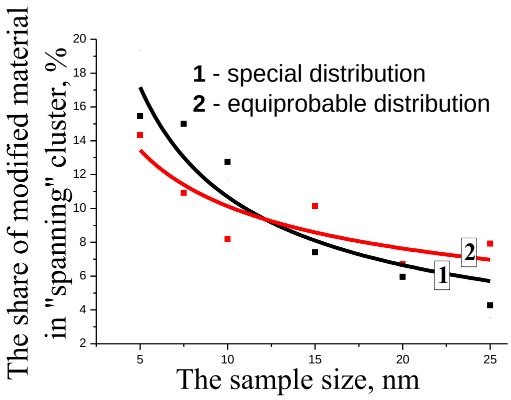

Fig. 3 – Dependence of share of modified material in «spanning» cluster in case with the biggest apparance frequency of first «spanning» cluster on the sample size.

Scale was changed in the following way: the sample size was increased in two times, irradiation dose – in four times, the number of spheres in the chain in two times (to make modified structure density and percolation effects didn't change).

For each scale dependence of the appearance frequency of first spanning cluster (percolation) on the number of spheres was obtained, in each case deal number of areas, where percolation is most frequent, was defined. This value corresponds to a value of modified material share, which is the percolation threshold for corresponding finite size of sample and will approach the percolation threshold of the infinite cluster. Using the percolation threshold dependence on the number of track regions in the sample the percolation threshold of the infinite cluster was determine.

$$P_\infty(p = p_c) \sim L^{-\beta/\theta} \quad (L \to \infty) \tag{1}$$

Formula 1 describes dependence of modified matter share in «spanning» cluster P_∞ in case with the biggest appearance frequency of first «spanning» cluster ($p = p_c$) on the sample size L. Using this equation ratio of critical exponents β/θ was evaluated. Two such curves were evaluated: in the case of non-equiprobable distribution of tracks regions in depth described in the section 2.2 with ratio of critical exponents $(\beta/\theta)_s = 0.68$ and in the case with equiprobable distribution of tracks regions in depth, so-called model of continuous percolation, with ratio of critical exponents $(\beta/\theta)_e = 0.41$.

Higher ratio of the critical exponents in case with special non-equiprobable distribution than in case with equiprobable distribution talks about higher connectivity of the track regions structure in the first case.

This higher connectivity gives us interesting effects and influences on angle and dose dependences of different tracks structure parameters. Dependence of the branched structure surface area on the dose and angle in the cases of one surface irradiation and consequently two surfaces irradiation is shown on Fig. 4 and on Fig. 5.

With the increasing of irradiation angle dose curve convex most strongly varies (Fig. 4).

Angular dependence of the surface area of the branched structure has maximum value at certain «critical» angle of ions incidence (Fig. 5 and Fig. 6).

Tracks region begin more weakly to overlap With angles more than critical, because they start to appear on greater depth.

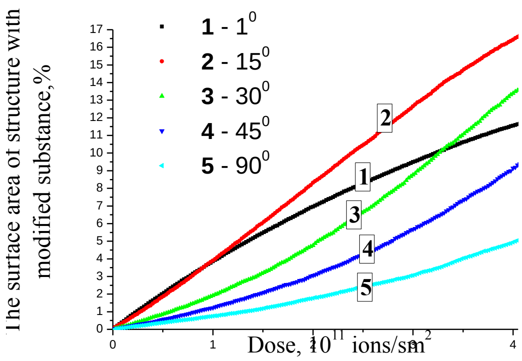

Fig. 4 – Dependence of the branched structure surface area on the dose and from different angles, irradiation of one surface

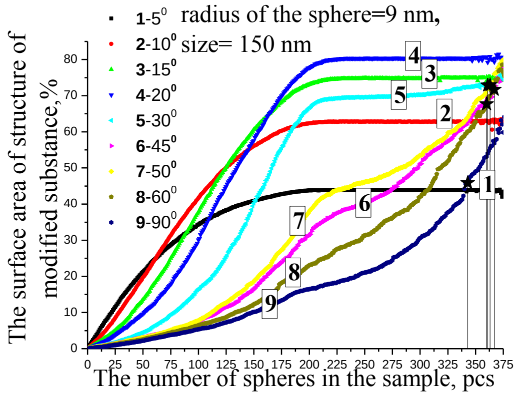

Fig. 5 – Dependence of the branched structure surface area on the dose and from different angles, irradiation of two surfaces

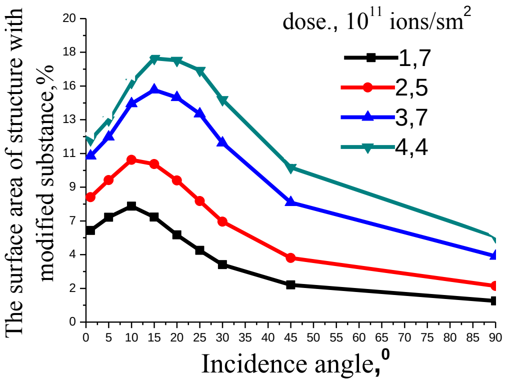

Fig. 6 – Dependence of the branched structure surface area on incidence angles (at fixed doses)

4. CONCLUSIONS

Differences between critical exponents of this model and the continuous percolation model indicate that the dependence of the modified structure area on the dose and the angle related with the correlation between individual tracks. Also it causes fact that percolation threshold in this case of specific non-equiprobable distribution is below the percolation threshold of continuous percolation.

Dose dependence of surface area changes its convexity at certain "critical" angle. Surface area of branched structure reaches its maximum value at this "critical" angle of ions incidence (at fixed dose), which increases with dose increasing.

Created model based on experiments has vivid scaling properties, that allows to predict different parameters of the modified structure at different scales of the sample.

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