V. G. Chudinov. *Computer simulation of radiation processes.* Defects in a crystalline structure, which are formed in a solid under the action of radiation, are the main factor responsible for the loss of durability of structural and fuel materials in nuclear installations. The most important progress in the study of the characteristics of such defects has been achieved by the methods of computer simulation.[1]

In this report the atomic mechanisms for generation of some spatial defects, observed experimentally (dislocation loops of the vacancy type in the cascade region (CR),[2] pores and gas bubbles,[3] interstitial type dislocation loops,[4] depleted zones with vacancy concentrations of ~30–40% [5]) are discussed. The results discussed were obtained by the author of the report together with V. I. Protasov by the method of molecular dynamics (MMD).[6]

Metals and compounds, irradiated by fast neutrons, from the center of the periodic system are primarily studied.

It is shown that after the formation of the primary knocked-out atom (PKA) and achievement by all atoms of an energy less than the threshold energy for the formation of defects (TEFD), a radical restructuring of the defect structure of the CR, which is characterized by the following excellent features, occurs.[7,8]

First, under the conditions of significant excitation of atoms in the CR, the TEFD drops markedly. As a result of this, the number of defects generated in the CR increases substantially. Figure 1 shows the results of a calculation of a 5-keV cascade in copper. The first arrow marks the time by which all atoms in the CR had an energy less than TEFD (~25 eV). The generation of defects was completed when the energy of all atoms was less than ~5 eV (first maximum).

Second, when all atoms achieve an energy less than the acoustic energy, generation of vacancies and interstitial atoms according to a noncollisional, collective mechanism is observed, i.e., local melting according to the scheme proposed by Frenkel' occurs in the CR.[9]

Third, at the concluding stage of the subthreshold stage, due to the enormous temperature gradients (one can speak about them in the CR only conditionally) associated with the flow of heat into the surrounding medium, directed diffusion of vacancies toward the center of the CR and diffusion of interstitial atoms toward the periphery are observed. Because of diffusion the location of all atoms in the CR changes repeatedly in the crystalline lattice.

It is shown that depending on the time for completion of the processes (determined by the dimensions of the CR and, therefore, the energy of the PKA and the characteristics of the medium), clusters of vacancies of different shape can form. If $\tau \gtrsim 10^{-11}$ s, then the vacancies form an irregularly shaped pore at the center of the CR, which is transformed by the thermal pressure into a Franck vacancy type dislocation loop. A depleted zone with a high vacancy concentration is formed at $\tau \approx 10^{-12}$ s and evolution of the defect structure is absent at $\tau \approx 10^{-13}$ s (CR of the order of 10 Å). The results obtained are in excellent agreement with the experimental data[2,4,5] and are in agreement with two other presently known studies, concerning related problems.[10,11] All processes at the subthreshold stages have a distinct athermal character.[15]

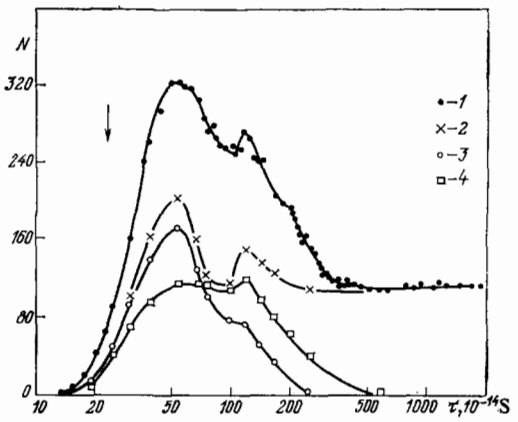

FIG. 1. Number of defects in the cascade region as a function of time. 1) Total number of vacancies, 2) number of stable vacancies, 3) number of stable interstitial atoms, 4) number of unstable Frenkel' pairs.

Simulation of the homogeneous generation of a pore[12] showed that in contrast to the generally accepted scheme for fcc metals a dendritic (10 units) cluster of vacancies, which, on reaching a certain size, spontaneously transform into a pore with a critical size, is formed at the initial stage. The pores are created according to the following general scheme: a mobile vacancy—and even more mobile divacancy—dendrite—pore with critical size—growth of the pore due to attachment of single vacancies. The presence of light gaseous impurities accelerates the processes in this scheme.

The nucleus of interstitial dislocation loops consists of a cluster of three interstitial atoms, in a dumb-bell configuration with orthogonal axes, situated at neighboring nodes of the crystalline lattice.[13] Annealing of such loops proceeds by transformation first into a tetrahedron and then into a packing-defect octahedron, which does not emit single interstitial atoms up to premelting temperatures.

The technical realization of the simulation of the processes examined above was made possible by the development of an MMD algorithm which minimized the required computational time.[14]

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Translated by M. E. Alferieff