MODELING OF TEMPERATURE FIELDS AND TRACK FORMATION IN INDIUM ANTIMONIDE DURING IRRADIATION WITH HIGH-ENERGY KRYPTON IONS

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The paper focuses on the radiation heating of crystal structure and track formation in indium antimonide to radiation of high-energy krypton ions. The simulation performed showed a significant radiation heating of the electronic and, as a consequence, of the atomic subsystem. It has been shown that for short time the substance recrystallizes with the relaxation of point defects and the formation of an ion track.

Keywords: indium antimonide; ion irradiation; radiation heating; molecular dynamics.

Introduction

Miniature Hall elements based on indium antimonide heteroepitaxial films are used to manufacture a wide range of sensors. It is promising to use such sensors for space instrumentation, since their properties are stable at ultralow temperatures. The impact of high-energy space ions (hundreds of MeV) can lead to various types of radiation damage to sensors. The strongest influence is exerted by the formation of bulk defects in the crystalline film of the sensor in the form of “tracks”, which is determined by strong radiation heating and accompanying defect formation processes. As a result, macrostresses arise, the mobility of charge carriers decreases, the resistance of the films increases, and the properties of the sensors change.

Thus, the actual goal of this work is the modeling of temperature fields and sizes of track formation in films of indium antimonide upon irradiation with krypton ions with an energy of 145 MeV.

Materials and methods

The theoretical object was the InSb subjected to irradiation with high-energy Kr ions. The irradiation parameters were: bombarding ion energy – 145 MeV, irradiation temperature – 300 K. Simulation in the SRIM program was used to quantify the magnitude of ionization and nuclear losses. The ion track size was estimated using the LAMMPS software package.

Results and discussion

Modeling in SRIM showed that the value of ionization losses exceeds the value of nuclear losses by a factor of ~ 125. Consequently, the dissipation of ion energy occurs predominantly on the electronic subsystem, due to which, during irradiation, significant radiation heating is observed and, as a result, intensive formation of defects, melting, and sublimation of the material near the track [1].

Since the SRIM code does not take into account the heating of the electronic subsystem in the framework of the two-temperature model and, therefore, does not take into account a significant part of the defects generated in the region of radiation heating, the following formula was used to estimate the temperature in the region near the track surface:

$$T(r,x,t) = T_0 + \frac{\frac{dE(x)}{dx_e} + \frac{dE}{dx_n}}{4\pi\chi} \frac{e^{-\frac{r^2}{4\pi Dt}}}{t}, \quad (1)$$

where r – distance from track surface, x – depth, t – time, T_0 – ambient temperature, $\frac{dE}{dx_n}$ and $\frac{dE}{dx_e}$ – nuclear and ionization losses respectively, χ – coefficient of thermal conductivity, D – heat diffusion coefficient [1].

In contrast to nuclear losses, the value of ionization losses depends on the energy and, consequently, on the depth x. To take this into account, the model proposed by the authors of [2] was used. In particular, it is assumed that the value of ionization losses is proportional to the root of the particle energy:

$$\frac{dE}{dx_e} = \lambda E^{\frac{1}{2}}, \qquad (2)$$

The coefficient λ is determined using a linear approximation of the data obtained from the TRIM program. The numerical values of the coefficients included in the equation 1 and 2 are presented in table 1.

Table 1. Numerical values of coefficients for equations 1 and 2

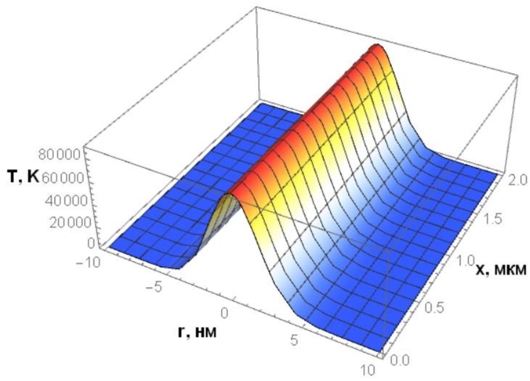
$\frac{dE}{dx_n}$, $J \cdot m^{-1}$	$5.67 \cdot 10^{-9}$
D, $m^2 s^{-1}$	$0.16 \cdot 10^{-4}$
χ, $W \cdot m^{-1} \cdot K^{-1}$	18
λ, $J^{1/2} m^{-1}$	0.16
E_0, J	$2.32 \cdot 10^{-11}$
T_0, K	300

Figure 1 shows the temperature distributions near the ion track depending on the depth and distance from the track surface. It can be seen from the data in Figure 1a that the temperature near the track surface can reach $9 \cdot 10^4$ K, which can lead not only to the melting of the material, but also to the transition to a gaseous state [1]. When passing 10^{-10} s, the temperature near the track is almost equal to the ambient temperature (Fig. 1b). At this stage, the substance recrystallizes inside the track [1], as a result of which transverse and longitudinal mechanical stresses arise along the boundary with the damaged layer [3].

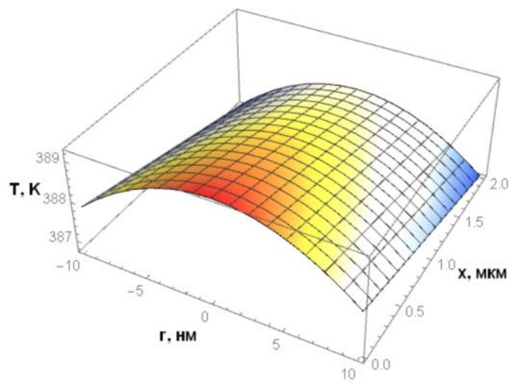
Figure 2 shows the simulation results in the LAMMPS program. The simulation used a 16.2×16.2×1.3 nm cell with periodic boundary conditions.

The modeling took place in 2 stages. At the first stage, the cell is thermalized at a temperature of 300 K for $2 \cdot 10^{-11}$ s. The next step is cell annealing: the atoms in the center of the cell are given a temperature distribution corresponding to the distribution near the track surface (Fig. 1a).

It can be seen from the obtained data (Fig. 2) that recrystallization of the substance took place in 10^{-10} s with the relaxation of 92% of point defects and the formation of an ion track with a size of 7.2×4.8 nm. At the same time, the temperature near the track became equal to the ambient temperature (Fig. 2d).



(a)



(b)

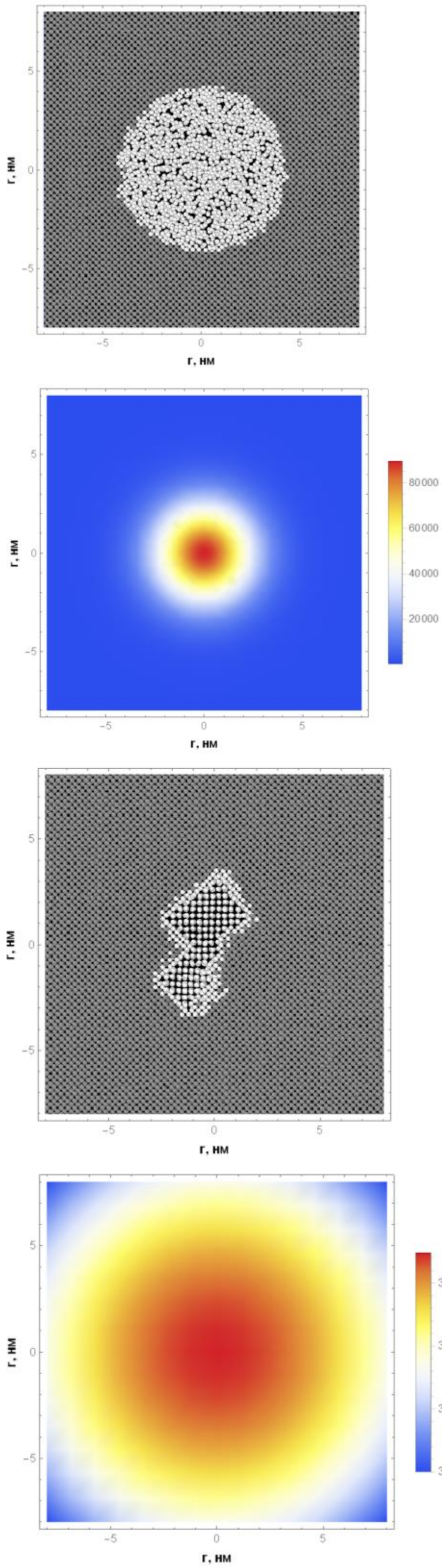
Fig. 1. Temperature distribution near the ion track as a function of depth (x) and distance from the track surface (r) at time (t): (a) – 10^{-13} s; (b) – 10^{-10} s

Note that during experimental irradiation of InSb heteroepitaxial films on GaAs substrates with krypton ions with an energy of 145 MeV and fluences of 10^{12} and $5 \cdot 10^{12}$ cm^{-2}, a significant increase in macrostresses was found [4]. It is assumed that this is due to an increase in volumetric defects in the form of "tracks" with an increase in the dose of irradiation with krypton ions.

Conclusion

Modeling of temperature fields and sizes of ion tracks during irradiation with krypton ions with an energy of 145 MeV in indium antimonide films was carried out using an analytical solution of the heat equation in the framework of a two-temperature model and the SRIM and LAMMPS programs.

As a result, it was shown that at a time after irradiation t = 10^{-13} s, the temperature near the track is $9 \cdot 10^4$ K. It was also found that within



(a) (b) (c) (d)

Fig. 2. A cell of atoms (a, c) and the corresponding temperature distribution (b, d) at time: (a, b) – $2{\cdot}10^{-13}$ s; (c, d) – 10^{-10} s

10^{-10} s, the substance recrystallization occurs with relaxation of 92% of point defects and the formation of an ion track with a size of 7.2×4.8 nm.

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