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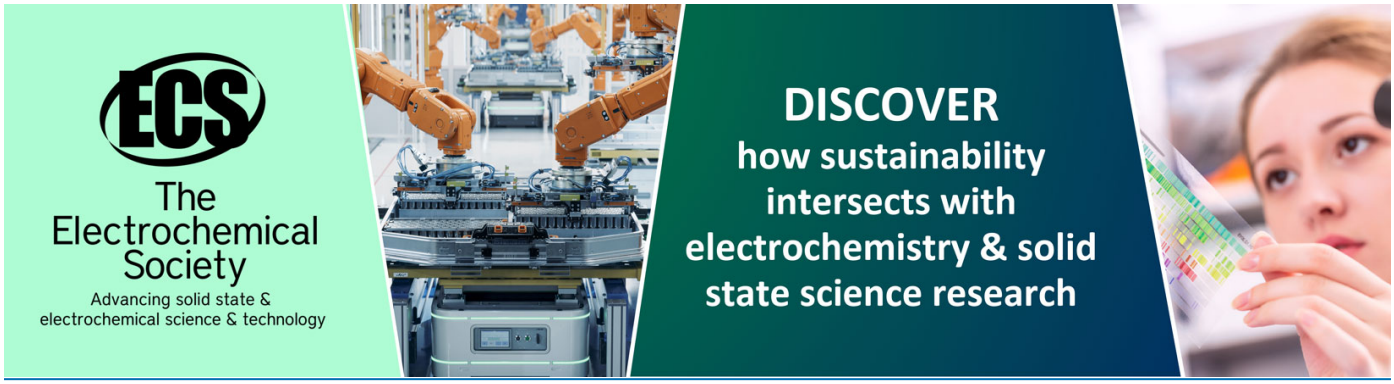

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Modeling structural defect formation in cadmium telluride during electron irradiation

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Abstract. We have conducted the formation of interstitial atoms and vacancies and made their clusters in the form of dislocation loops and voids in cadmium telluride under irradiation by electrons. We have calculated dependences of the radii of dislocation loops and voids depending on the irradiation time. We have compared the results of the simulation with the experimental data on the irradiation of CdTe in a transmission electron microscope as well.

1. Introduction

Modern technologies make it possible to produce semiconductor materials of very high quality with low content of structural defects, but the structural defects that remain in them can make serious changes in the physico-chemical properties, and, subsequently, affect the operation of devices based on them. Reliable operation of modern semiconductor devices of ultra-small sizes requires the control of the presence and density of not only traditional structural defects such as dislocations, stacking faults and micro-twins, but also defects of ≤ 10 nm in size. Devices have to work in unfavorable conditions, for example, under the influence of radiation with different energy. Such an impact on semiconductor materials causes the transformation and development of a defective network.

Cadmium telluride (CdTe) relating to compounds A_2B_6 is one of the main materials of semiconductor microelectronics. Cadmium telluride has a band gap of 1.5 eV, which provides an excellent match to the solar spectrum, a relatively high average atomic number, and the ability to achieve high resistivity values; it makes these materials ideal for gamma and x-ray detector devices [1]. However, the CdTe material is sensitive to effects of ionizing radiation because of the low value of stacking fault energy (SFE) (~11±2 mJ/m^2). Irradiation of CdTe by electrons in a transmission electron microscope causes similar evolution of defects [2]. We have studied the influence of electrons with sub-threshold energy on the processes of structural transformations in semiconductors in [3-7] where we have reported about the possibility of formation of point defects (vacancies and interstitials) in these materials under such irradiation. In relation to this, we have conducted a simulation of the processes of defect formation in CdTe under electron irradiation. Previously, we have developed chemical reaction rate in CdTe in order to describe the dynamics of electron irradiation damage in CdTe [8]. Taking into account the experimental studies reported in [7], we know that in addition to the formation of interstitial clusters, vacancy clusters are observed in CdTe, so the model is modified taking into account the formation of vacancy clusters and the results of the simulation are compared with the previously obtained experimental data.

2. Results and Discussion

Using effective values of activation energy and effective concentrations of interstitial atoms c_I and vacancies c_V, we have recorded equations simulating changes in concentrations c_I and c_V, as well as the growth of interstitial loops and pores with radii r_I and r_V and concentrations c_{bI} and c_{bv} in the following form:

$$\begin{cases} \frac{dc_I}{dt} = c_0 G - K c_I c_V - 2K_{1I} c_I^2 - K_{1I} \frac{2\pi r_1}{b} c_I c_{bI} - K_{SI} c_I c_S, \\ \frac{dc_V}{dt} = c_0 G - K c_I c_V - 2K_{1V} c_V^2 - K_{1V} \frac{4\pi r_V^2}{b^2} c_V c_{bV} - K_{SV} c_V c_S, \\ \frac{dc_{bI}}{dt} = c_0 K_{1I} c_I^2, \\ \frac{dc_{bV}}{dt} = c_0 K_{1V} c_V^2, \\ \frac{dr_I}{dt} = c_0 K_{1I} c_I b, \\ \frac{dr_V}{dt} = c_0 K_{1V} c_V b. \end{cases} \quad (1)$$

Here $c_0 = 1{,}5 \cdot 10^{22}$ cm^{-3} is the concentration of the nodes of the unirradiated crystal, $G = \sigma \cdot j$, $\sigma = 3 \cdot 10^{-22}$ cm^{2}is the electron scattering cross section at the lattice sites, $j = 10^{19}$ cm^{-2}c^{-1} is the electron flux density, $K_i = \nu \cdot \exp(-E_i / kT)$ is the reaction constant, $\nu$is - the frequency of vibration of atoms in the lattice, k is the Boltzmann constant, T is the temperature, E_i is the activation energy of processes, c_s is the concentration of "sinks" on the surface, $2\pi r_I / b$ and $4\pi r_V^2 / b^2$ is the number of seats joining point defects (PD) on the perimeter of the loop and on the void surface respectively, b is a parameter of the order of magnitude of the interatomic distance (Burgers vector). The value of $c_0 G$ is the generation rate of Frenkel pairs.

The recombination of the PD with the surface is performed as a result of the diffusion of the PD on the surface, the change in the concentration of the PD as a result of their displacement to the surface can be represented using the following formula:

$$\left(\frac{\partial c_{I,V}}{\partial t}\right)_{surface} = K_S c_{I,V} c_S = -D_{I,V} \frac{\partial^2 c_{I,V}}{\partial z^2}, \quad (2)$$

where z is the coordinate perpendicular to the sample surface and $D_{I,V} = b^2 \nu \cdot \exp(-E_{mI,mV} / kT)$ is the diffusion coefficient of interstitial atoms and vacancies. Taking (2) into account, it can be transformed (1) into a system of partial differential equations in the following way:

$$\begin{cases} \dot{u}_1 - D_I u_1'' - G = -c_0 K u_1 u_2 - 2c_0 K_I u_1^2 - \\ - 2\pi c_0 K_I u_1 u_3 u_5, \\ \dot{u}_2 - D_V u_2'' - G = -c_0 K u_1 u_2 - 2c_0 K_V u_2^2 - \\ - 4\pi c_0 K_V u_2 u_4 u_6^2, \\ \dot{u}_3 = c_0^2 K_I u_1^2, \\ \dot{u}_4 = c_0^2 K_V u_2^2, \\ \dot{u}_5 = c_0^2 K_I b u_1, \\ \dot{u}_6 = c_0^2 K_V b u_2, \end{cases} \quad (3)$$

where $u_1 = c_I / c_0$, $u_2 = c_V / c_0$, $u_3 = c_{bI} / c_0$, $u_4 = c_{bV} / c_0$, $u_5 = r_I / b$, $u_6 = r_b / b$. The dot and the prime denote partial derivatives with respect to the variables t and z, respectively.

The solution to the resulting system of equations (the numerical values of the parameters are given in [2]) gives the dependence $u_1, \ldots, u_6$ on z and the irradiation time at 300 K (Fig. 1-3).

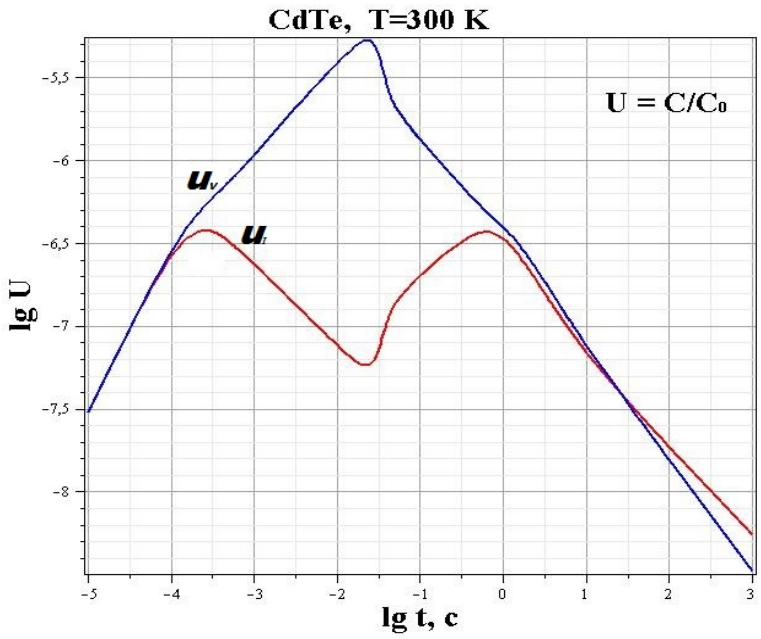

Figure 1. Dependence of u_I and u_V on the irradiation time at 300 K

The results presented in fig. 1 show that in the center of the sample (z = 100 nm) interstitial atoms have greater mobility than vacancies. When moving, the atoms quickly shift to the periphery and their concentration (c_I) decreases more intensively than the concentration of vacancies (c_V). In the time interval 0.1-0.01 seconds the concentration of vacancies reaches its maximum which practically coincides with the minimum of the concentration of interstitial atoms; it is explained by the dynamics of the processes of generation and recombination of Frenkel pairs, as well as agglomeration of Frenkel pairs in the di-interstitials and divacancies, which are assumed to be the nuclei for the formation of the dislocation loops and vacancy voids.

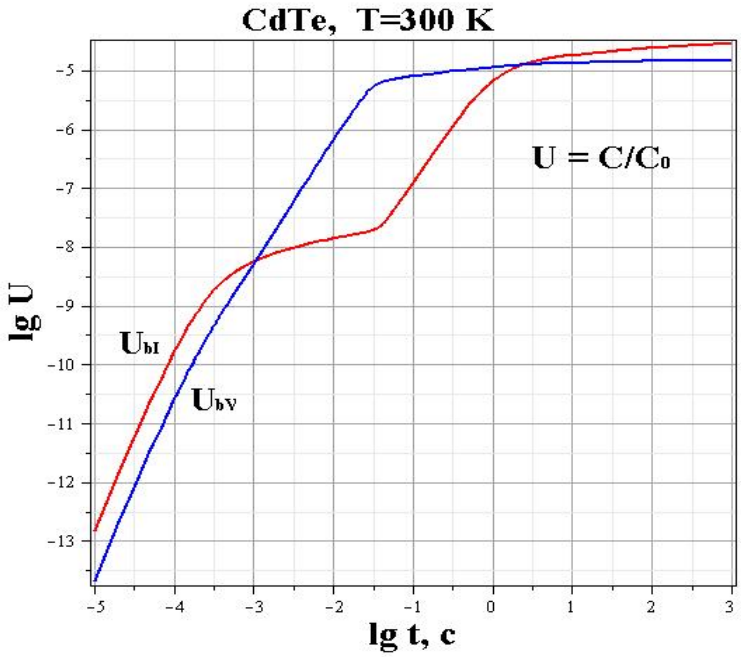

Figure 2. Change in the concentration of di-interstitials (u_3) and divacancies (u_4) within the irradiation time at 300 K

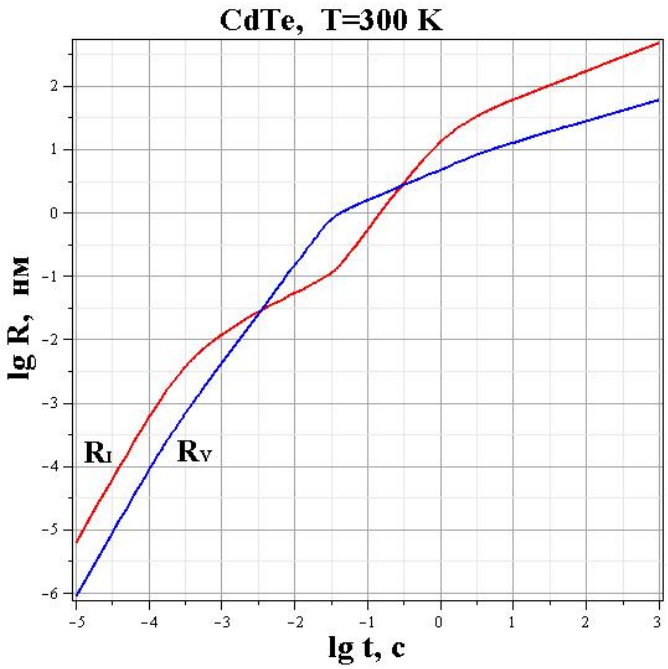

Figure 3. Dependence of the radii of the loops (u_5) and pores (u_6) on the irradiation time at 300 K

We note that the radii of dislocation loops and vacancy voids begin to exceed parameter b only a few seconds after the start of irradiation, and the final values of these radii practically do not depend on the initial conditions.

From Fig. 2 and 3, it can be seen that the growth of the radii of dislocation loops and the density of di-interstitials slow down. In the process of the sample irradiation the concentration of c_V begins to decrease, and c_I

increases, which causes the increase in the growth of the di-interstitials (u_3) and the loop radii (u_5) and slowing the growth of the divacancies (u_4) and the radii of voids (u_6).

3. Conclusion

Comparing the results of numerical modeling of cluster formation (point defects of interstitial and vacancy types) in cadmium telluride with the experimental data of a number of works [7,9], we come to the conclusion that the experiment and theory agree. However, in order to achieve maximum consistency, it is necessary to improve the existing model and introduce two parameters into it: firstly, taking into account the number of semiconductor nodes, since their number decreases upon irradiation; secondly, it is necessary to take into account the initial distribution of point defects, which is spatially inhomogeneous. The values of the initial concentrations depend on the energy of thermal activation of Frenkel pairs and the physical conditions under which the sample of the CdTe crystal is processed. This will allow to confirm the initial conditions of the experiment and theoretical modeling more accurately.

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