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MD simulation of ion implantation damage in AlGaAs: III. Defect accumulation and amorphization

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ABSTRACT

The defect accumulation and amorphization in (0 0 1)$Al_xGa_{1-x}As$ due to irradiation with 200 keV Ar ions at 20 K is investigated with the help of classical molecular dynamics computer simulation using a modified Tersoff potential. The amount of disorder as a function of the number of displacements per atom has been calculated for $x = 0$, 0.2, 0.5, 0.75, 0.9 and 1.0. The results reasonably agree with the corresponding RBS data from the literature for $x \leqslant 0.9$, however, they completely disagree in the case of $x = 1$. An artificial increase of thermally activated processes shows that thermal annealing during the irradiation may be responsible for the outstanding behavior of AlAs. In addition, the structure of the damage is investigated by visualizing the amorphous clusters and their evolution. It is shown that dynamic annealing does exist. It is negligible for $x = 0$ but it becomes more and more important with increasing Al content x. Furthermore, it is shown that the generation of damage is supported by pre-damage. This effect dominates the dynamic annealing for $x \leqslant 0.5$.

1. Introduction

The defect accumulation and amorphization in $Al_xGa_{1-x}As$ due to ion irradiation has been widely investigated experimentally since about 20 years [1–12]. Most of the experiments were performed at low temperature ($\leqslant$80 K) providing information about the initial damage formation which is of interest in this paper. In all cases it has been found that the irradiation resistance increases remarkably with increasing Al content x; e.g. the amorphization dose for AlAs is about two orders of magnitude larger than that of GaAs.

Different mechanisms of the defect accumulation and amorphization have been discussed to understand this behavior. There is general consensus that for x below about 0.8 the direct impact amorphization in combination with point defect buildup processes are the dominating processes [1,3,5,6,9,10,12]. Dynamic annealing is negligible for $x = 0$ and may become more and more important with increasing value of x [3]. For compositions x above about 0.8, different damage formation processes have been suggested which induced two models. The first model is mainly described by Tan et al. [3]. For a very high Al content a strong dynamic annealing during the irradiation is assumed, which is caused by very mobile defects and by local bonding rearrangements. The imperfect dynamical annealing leads to extended defects (e.g. stacking faults). If a critical damage density is reached the corresponding free energy may become larger than that of the amorphous phase, which causes a sudden 'collapse' into an amorphous state. The second model is suggested by Lagow et al. [6,10]. They argue that the need of formation of structural transitions (extended defects) prior to amorphization is questionable because it requires dynamic annealing and dynamic annealing is in contradiction to the experimental fact that the damage accumulation at such low temperatures is approximately independent of the dose rate. Therefore, Lagow et al. suggest a model, which avoids the necessity of structural transitions prior to amorphization. They assume the direct impact amorphization and point defect buildup processes to be responsible also for the damage formation in the case of $x > 0.8$, that means the amorphization mechanism does not change in the whole range of x. From the dependencies of the density, the heat capacity and the melting temperature on the composition x, Lagow et al. concluded that the probability for creating an amorphous pocket should decrease rapidly with increasing x, which may explain the strong dependence of the damage formation on the composition x.

Using classical molecular dynamics (MD) computer simulation, Sayed et al. [13] showed qualitatively that the damage caused by recoils in AlAs is less than that in GaAs. In the case of GaAs quantitative theoretical investigations of the damage formation have been performed by Nordlund et al. [14–16]. Besides the formation

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of amorphous material, they also found dynamic annealing during the irradiation of GaAs caused by low energy recoils. To the knowledge of the authors, corresponding simulations for $Al_xGa_{1-x}As$ do not yet exist.

In parts I [17] and II [18] of this series the sub-collision cascades in crystalline $Al_xGa_{1-x}As$ generated by single recoils with energies up to 400 eV and the different kinds of point defects generated by the recoils have been investigated by MD computer simulations. The aim of this paper is to find an appropriate simulation of the damage production in $Al_xGa_{1-x}As$ due to ion irradiation, which provides results immediately comparable with Rutherford backscattering data and to get information about the processes of the defect accumulation and amorphization. The computer simulations are performed for the situation of the irradiation of (0 0 1)$Al_xGa_{1-x}As$ with 200 keV Ar at 20 K, where experimental Rutherford backscattering (RBS) data for a wide range of the composition x (0, 0.2, 0.5, 0.75, 0.9, 1.0) are available [9,12]. The irradiations and the RBS measurements were performed at 20 K without warming the sample in between. Therefore, these results really refer to the initial damage at 20 K.

2. Simulation of the ion irradiation

In the case of 200 keV Ar irradiation considered here, the extension of the collision cascades involves up to 10^9 atoms, which is too large to be fully treated by molecular dynamics simulation. Therefore, similar to the treatment by Björkas et al. [16] the simulation is performed in two steps. First, the generation of primary recoils is treated using the binary collision code TRIM and second, the evolution of the sub-cascades caused by the primary recoils is described by molecular dynamics (MD) simulations.

2.1. TRIM calculations

The MD simulation of the evolution of the sub-cascades caused by the primary recoils requires the average number of primary recoils per ion and per depth and the distribution of the primary recoils with respect to the energy E_r and the polar angle ϑ_r between the velocity of the recoil and the initial velocity of the ion (defines the z-direction). The corresponding azimuth angle φ_r is equally distributed. In order to obtain these data, the corresponding output has been added to the original TRIM code [19]. Because the experimental data to be compared with refer to the depth of the maximum of the defect distribution, the data for the primary recoils are calculated for a depth region at the maximum of the vacancy distribution. The TRIM calculations for the irradiation of $Al_xGa_{1-x}As$ with 200 keV Ar have been performed for different values of the composition x. The results show that in good approximation the distribution of the primary recoils with respect to the energy E_r and the polar angle ϑ_r is given by a product of the energy distribution $p_E(E_r)$ and the angular distribution $p_\vartheta(\vartheta_r)$ with

$$\begin{aligned} &p_E(E_r) \sim E_r^{-n} && n = 1.4, \\ &p_\vartheta(\vartheta_r) \sim \exp[-(\vartheta_r - \vartheta_0)^2/(2\Delta\vartheta_r^2)] && \vartheta_0 = 87^\circ, \quad \Delta\vartheta_r = 28^\circ, \\ &p_\varphi(\varphi_r) \text{ equally distributed.} \end{aligned} \tag{1}$$

The values given for the three parameters n, ϑ_0 and $\Delta\vartheta_r$ can be used for all compositions x because the very small variations with x show no visible influence on the results obtained here. The average number of primary recoils per ion and per depth varies slightly with the composition x between 0.043/(Å ion) and 0.053/(Å ion). The number of primary recoils and their distributions $p_E(E_r)$ and $p_\vartheta(\vartheta_r)$ are the input data for the MD simulations.

2.2. Molecular dynamics simulation

The molecular dynamics simulations were done with a standard MD code, where the integration of the equations of motion is performed using the velocity form of the Verlet algorithm. The time step is given by the velocity of the fastest atom, however, the maximum value is 0.25 fs. In all cases the simulations are performed using periodic boundary conditions for all three directions. The potential for $Al_xGa_{1-x}As$ used is a modified Tersoff potential [20]. It is based on the GaAs and AlAs potential given by Smith [21] and Sayed [13] and splined to a more realistic repulsive interatomic interaction potential [22] for smaller distances. This potential is briefly described in part II [18] of this series and a more detailed description is given in the first part of this series [17].

In order to study the influence of the size of the MD cell on the results, two different MD cells consisting of $10 \times 10 \times 10$ unit lattice cells (8000 atoms) and $15 \times 15 \times 15$ unit lattice cells (27,000 atoms) are used. The $Al_xGa_{1-x}As$ lattice of the composition x is obtained from a GaAs zincblende lattice, where the Ga lattice sites are statistically occupied by Al or Ga according to the probabilities x or $1 - x$, respectively. For the lattice parameter $a_0(x)$ as a function of the composition x the results obtained from the zero pressure simulations in part I [17] ($a_0(x) \cong (5.6536 + 0.0075\ x)$ Å) are used.

The passage of *one ion* through the MD cell (in z-direction) generates n_r *primary recoils* given by the number of primary recoils per ion and per depth z obtained from TRIM and by the z-extension of the MD cell. For the smaller MD cell (mainly used, z-extension 10 a_0), the rounded value is $n_r = 3$. For 200 keV Ar ions the time for crossing the MD cell is about 5 fs, which is very small compared with the vibration period of the atoms (∼ps). This means that the n_r primary recoils generated by one ion can be considered to start at the same time. The starting positions are equally distributed within the MD cell and the energies E_r and directions of motion of the recoils are given by random numbers according to the distributions given in Eq. (1).

The irradiation with a *sequence of ions* (ion beam) is simulated by a *sequence of sets of n_r primary recoils* starting in time intervals of Δt_{rec}. For typical experimental conditions (dose rate $\sim 10^{12}$ $cm^{-2}\ s^{-1}$) the time interval Δt_{rec} is in the order of seconds, which is impossible to simulate. That means that long time annealing, as possible in the experiment, cannot be simulated. As has been shown in parts I and II of this series [17,18], the short time annealing is finished in a time of about 2.5 ps in all cases considered, that means the average numbers of point defects are constant after this time. In order to be sure that the short time annealing is finished before the next set of primary recoils starts, the time interval Δt_{rec} should be larger than 2.5 ps.

In order to maintain the temperature T (here 20 K), the heat introduced by the recoils has to be extracted. In parts I and II of this series [17,18], the energy was deposited mainly in the center of the MD cell and the heat was extracted by velocity scaling of the atoms in a surrounding frame (the usual procedure). However, this can not be applied here because the recoils start from all positions in the MD cell. Therefore, a special procedure for the velocity scaling is used, which is described in the following. There are three time intervals considered: 0–0.2 ps, 0.2–4.5 ps and 4.5–5.0 ps. In the first time interval, up to 0.2 ps after the start of a set of n_r recoils, the system is allowed to relax without velocity scaling. During this time, the temperature decreases because a part of the kinetic energy of the recoils is converted to potential energy, which should not be disturbed by velocity scaling. It has been shown that for