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Light and heavy ion effects on damage clustering in GaAs quantum wells

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Abstract

Recent experiments have shown that ion irradiation can strongly affect charge carrier dynamics in GaAs quantum wells. The irradiation conditions are such that the ions penetrate deep beyond the active layer, showing that the effect is due to damage in the lattice. Moreover, ions of different mass and energy can lead to clearly different effects even after normalization with the nuclear deposited energy. Using molecular dynamics simulation of the damage production, we show that the experimentally observed effects on charge carrier lifetime correlate well with the production of large (more than 100 disordered atoms) damage clusters. Moreover, we show that 400 keV Ne and 10 MeV Ni produce very similar damage in the near-surface active regions, indicating that 500 kV ion implanters are sufficient to achieve the desired modification effects.

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1. Introduction

Semiconductors based on gallium arsenide are of great interest for a wide range of existing and possible device applications [1]. In particular, semiconductor heterostructures based on GaAs compounds are widely used as the active region in semiconductor saturable absorber mirrors (SESAMs) and quantum well lasers operating at 1.3–1.55 μm wavelength range [2–6]. Recently, it has been established that heavy ion irradiation can be used to strongly modify the charge carrier dynamics in GaAs based semiconductor devices [2,7–11]. Reductions in the charge carrier lifetime of up to 3 orders of magnitude have been reported [10,11], making ion irradiation a promising method for manufacturing very fast SESAMs [7].

Many of the irradiations carried out have used ion energies high enough that the mean range of ions is well beyond the active regions. Hence the effects of ion irradiation on the carrier dynamics have been attributed to crystal defects, but which defect types in particular affect the dynamics is not fully understood. Previous studies of the effect [8–10] have attributed the reduction to large defect clusters, based on the observation that heavy ions are most efficient in facilitating the effect, and on transmission electron microscopy (TEM) experiments where large defect clusters are visible. Until recently, there were no systematic studies of what ion mass and energy ranges, and correspondingly what defect cluster sizes, cause the desired effects. Moreover, the attribution of the carrier lifetimes to defect clusters visible in a TEM is complicated by the experimental observation that such clusters anneal away with time even at room temperature [12]. Recently Dhaka et al. have systematically examined the effects of different ions, fluences, and ion energies on the charge carrier dynamics in

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GaAs-based semiconductor structures [13,11,14]. The results clearly show that different kinds of ion irradiations at energies and fluences that produce the same nuclear energy deposition in the active region, yield very different carrier decay times. This indicates that the decay time not only depends on the total amount of damage, but also on its type, and is thus well in line with the previous interpretation that defect clusters are responsible for the damage.

Our aim is to obtain additional atom-level understanding of what kind of defect clusters are related to the charge carrier lifetimes. To this end, we use atomistic computer simulations of the ion irradiation process to predict the defect cluster sizes obtained for the same 100 keV H, 200 keV He, 400 keV Ne and 10 MeV Ni ion irradiation conditions as those used in related experiments [11].

2. Method

Because of the long (order of microns) penetration depths of the few hundred keV ions in GaAs, it is impossible to simulate the damage production of the 0.1–10 MeV ions in a single molecular dynamics (MD) simulation. Hence we first use MD range calculations [15] to obtain the recoil spectra of the high-energy ions (with initial kinetic energy E_{ion}) in the depth region of interest, and then MD simulations of the full development of collision cascades to obtain the damage production by individual recoils (with initial kinetic energy E_{rec}). By integrating the two, we obtain the damage production of the ions in the active semiconductor layers.

Ion irradiation simulations on GaAs were performed using the MDRANGE code [16]. The universal ZBL repulsive potential and the ZBL96 electronic stopping power [17,18] were included in the MDRANGE calculations. Ions of 100 keV H, 200 keV He, 400 keV Ne and 10 MeV Ni were allowed to irradiate bulk GaAs at an incident direction of 7° off the [1 0 0] crystal direction normal to the sample surface, respectively. Ten thousands recoil events were computed for each ion. The deposited energy and damage production was calculated between the depths of 80 and 200 nm from the sample surface, corresponding to typical depths of the active region [2,7,11].

Statistics on the number of primary recoils of energy E_{rec} produced in the active region per incoming ion of energy E_{ion}, i.e. the integrated primary recoil spectra $n_{\text{t}}(E_{\text{rec}})\text{d}E_{\text{rec}}$ (t represents the atom type, Ga or As), were used to estimate the primary damage. The number of defects, N_{t}^{D}, produced in the collision cascade simulations in bulk GaAs, was also calculated. Then, by integrating $n_{\text{t}}(E_{\text{rec}})\text{d}E_{\text{rec}}$ and N_{t}^{D}, using a procedure described in detail elsewhere [19,20], the total amount of damage, $N_{\text{tot}}^{\text{D}}$, was obtained.

The collision cascade simulations were carried out with the MD code PARCAS [21], at 300 K and 0 pressure using procedures described in e.g. [19,22,23]. The cascades were initiated by As-recoils of kinetic energies ranging from 10 eV to 10 keV. The simulation cells were as large as 33 unit cells in all three dimensions. Periodic boundary conditions [24] were used. The interatomic potential used in these simulations was developed by Albe et al. [25].

Two different types of defect analyses were performed. At first, a Wigner–Seitz (WS) cell [26], centered on each lattice site, was used to find vacancies and interstitial atoms. A single Ga atom on an As site was defined as an antisite defect. Second, a potential energy (E_{pot}) analysis was performed. In this case an atom with E_{pot} more than 0.2 eV above potential energy equilibrium was regarded as a structural defect.

A cluster connectivity analysis was carried out by defining all defects that were within a fixed cut-off radius from each other were a part of the same defect cluster. Point defects, small and large clusters were distinguished from each other such that small clusters contained 2–10 WS defects or 10–70 E_{pot} defects. These limits were found to correspond well to each other based on visual analysis.

3. Results

The results of the cascade simulations are shown in Figs. 1 and 2. The fitted lines are asymptotically linear and the error bars show the standard error of the average. The insets show the damage production at low E_{rec}.

Low-energy simulations ($E_{\text{rec}} < 400$ eV) provided threshold energies for the formation of point defects, small clusters, and large clusters. According to Fig. 1, these energies are about 25, 50, and 650 eV, respectively, for the WS defect analysis. The corresponding thresholds for the E_{pot} analysis are approximately 15, 20 and 120 eV (see Fig. 2).

Antisites are produced in GaAs at energies above a threshold energy of approximately 35 eV. Similarly to the

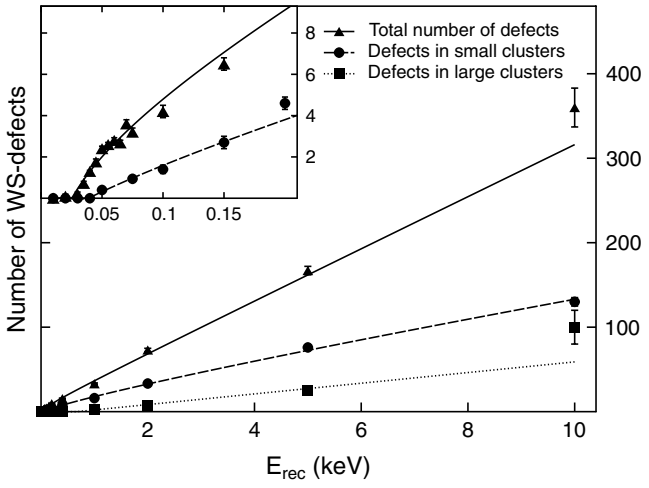

Fig. 1. The number of Wigner–Seitz-defects (WS-defects) (vacancies and interstitials) produced by collision cascades initiated by As-recoils in GaAs. Small clusters contain 2–10 WS-defects. The inset shows the defect production at low recoil energies.

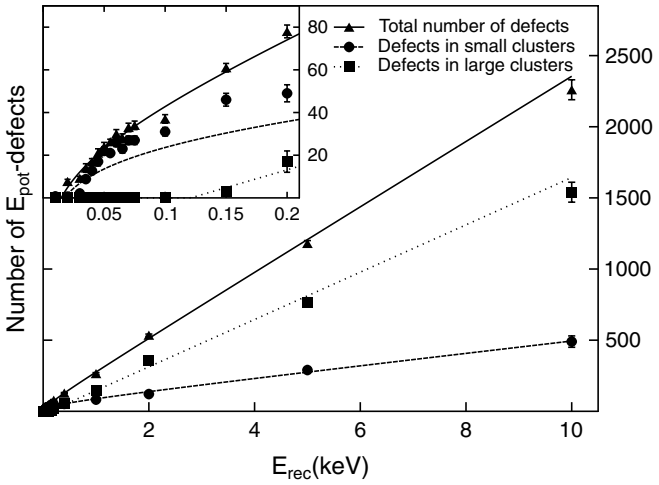

Fig. 2. The number of atoms with a potential energy of more than 0.2 eV above equilibrium value (E_{pot}-defects) after collision cascades in GaAs. Small clusters are clusters containing 10–70 defects. The inset illustrates the amount produced at low recoil energies.

case of other WS defects (vacancies and interstitials), the number of antisites exhibit an asymptotically linear behavior, as E_{rec} is varied. The simulations showed that the ratio between the amount of antisites and the sum of interstitials and vacancies is significant. At low recoil energies, it is as high as 40%, and at higher energies about 20%.

The results of the total damage production are illustrated in Fig. 3. The damage in large clusters is seen to depend on the type of the incoming ion. Seventeen percent of the damage were in clusters with more than 10 WS defects (large clusters), or alternatively 64% in large E_{pot} defect clusters, when the irradiating ion was Ni, whereas when irradiated with H ions, these numbers were 3% and 23%, respectively.

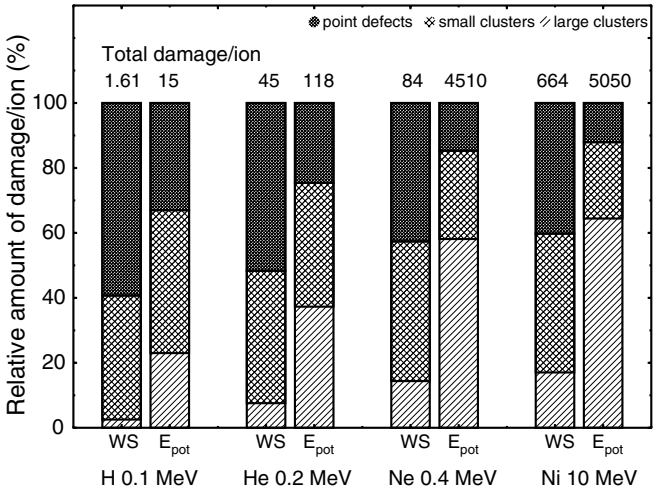

Fig. 3. The final defect distribution of the implantation. The total amount of damage per ion, as well as the fraction of defects in clusters of different sizes, is shown for both the Wigner–Seitz (WS) and the potential energy (E_{pot}) analysis.

4. Discussion

Figs. 1 and 2 show that a major fraction of the primary damage induced by self-recoils in GaAs is in clusters, for all recoil energies above roughly 100 eV. The large clusters are strongly disordered (amorphous). These results are in line with other simulations and experiments on ion-irradiated damages in elemental and binary semiconductors [27,23,20,28,29]. Experiments have also shown that in GaAs amorphous pockets recrystallize at room temperature [12]. While this effect is not included in our simulations, it does not change the observation that the differences in ion damage normalized by deposited energy must be reflected in the primary damage.

A relatively low threshold energy needed to form antisites is consistent with earlier reports [30,31], suggesting that antisites can be formed directly by single atom recoils in GaAs. The high fraction of damage in antisites is important since antisites at least in pure GaAs are quite stable, requiring high temperatures to anneal out [32]. In a previous work, we have shown that antisites persist also after annealing of an amorphous zone [20]. This, in combination with the observation that the amorphous zones are vacancy-rich, indicates that even though the amorphous zones anneal even at room temperature, a sizable fraction of the damage in them will remain in the form of vacancies and/or antisites.

The distribution of the final damage, illustrated in Fig. 3, shows that the fraction of damage in small and large clusters is significant even by H irradiation at $E_{ion} = 100$ keV. The fraction of damage in large clusters (more than 10 WS defects or more than about 70 atoms), does increase strongly with mass, however. Our criteria for defining a "large" cluster are of course somewhat arbitrary, and thus it is not surprising that the Wigner–Seitz and E_{pot} criteria give different fractions of damage large clusters. However, both show a similar strong increase in damage in large clusters going from H and He to Ne and Ni ions, see Fig. 3. It is also interesting to note that the damage produced by 400 keV Ne and 10 MeV Ni is very similar for both defect analysis methods, indicating that desired effects can be obtained efficiently with irradiation energies below 1 MeV. This conclusion is well in line with recent experimental observations [11].

Our results indicate that differences in carrier dynamics, due to ion irradiations by various ion species having the same nuclear deposited energy, are related to the types of defects generated. The defects can be attributed to the existence of large clusters either in the form of amorphous zones or clustered vacancies and antisites, which persist in the samples after the zones have recrystallized. Therefore, we suggest that the carrier decay time decreases with an increasing fraction of damage particularly in large clusters.

A recent report on thermal stability of Ni-induced damage in InGaAs shows that the carrier lifetime depends on an aging process [13]. A twofold increase in lifetime was obtained in all Ni irradiated samples when the measure-

ments were made after 45 days of aging at room temperature. On the other hand, rapid thermal annealing (RTA) at 610 °C for 1 s gave rise to quick lattice recovery and, consequently, much longer lifetimes. This effect can also be interpreted by the present calculations. Ni irradiation produces large amorphous defect clusters, which, however, can be removed by maintaining the sample at room temperature for a long time [12], or even more effectively, by annealing at high temperature where the defects with high formation energies, including most of the point defects, are removed.

5. Conclusions

Using molecular dynamics computer simulations we studied the damage production by high-energy (100 keV–10 MeV) H, He, Ne and Ni ions in GaAs at depths corresponding to quantum well active regions. We find, using two different damage analysis methods, that the heavier Ne and Ni ions produce a larger fraction of damage in large clusters. Our results indicate that experimentally observed differences in charge carrier lifetimes between light and heavy ion irradiation, and before and after annealing, can be understood in terms of the large defect clusters. An increasing amount of damage in large clusters decreases the carrier decay time. Moreover, the damage production by 400 keV Ne and 10 MeV Ni ions is almost identical near the surface, indicating that 500 kV ion implanters may be sufficient to obtain the desired ion beam modification of the material.

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