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Study of the Irradiation Damage in Simple Crystals by Channeling

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Abstract

Several experiments have been carried out in the past in order to examine the impact of medium and heavy ions in crystals in the MeV range, which is of particular interest in high energy implantations. In the present work, the gradual amorphisation of simple crystals such as Si (100), Ge (100) and W (100) when irradiated with 18 MeV ¹⁶O in a random direction is being studied using the progressive change of channeling parameters, up to a maximum dose of approximately $1 \cdot 10^{16}$ particles/cm². The results are compared to the ones present in literature and an attempt is made in order to explain the peculiarities of the experimental spectra.

1 Introduction

The effects of irradiation on the properties of solids are of significant interest in scientific and technological context. Several papers have been presented recently concerning irradiations with ions having an energy of the order of 1 MeV/nucleon [1, 2]. These ions find an ever increasing application in the modification of the properties of metals and semiconductors. There exists a growing interest in the physical nature of the effect of this high-energy ion implantation as it is considered to be a promising way of increasing the micro-electronic chip integration by the formation of multilayer three-dimensional structures [4]. Moreover, there are strong indications that the increase of ion

energy does not lead exclusively to quantitative changes of the ion implanted layer parameters but also to qualitative changes of the defect-impurity structure of the whole irradiated area [5].

This type of implantation is mainly characterized by the high linear density of the energy contribution by ions into the electronic subsystem of the target, resulting to electronic energy losses of the order of tens of keV/nm and also by the fact that this type of losses strongly prevail over the direct transmission of the ion energy to the nuclear subsystem of the target, which is predominant at the end of the mean ion projected range but almost negligible otherwise (less than 3% in our case as shown with the use of the TRIM code).

It should be noted here however, that the data on defect production and annealing at depths of the order of 1 μ m inside a target are sparse, often contradictory and by no means conclusive as to the very nature of the mechanism of the phenomenon. Recently, an anomalous behavior of silicon when bombarded with 16 MeV ^{14}N ions has been observed and analyzed [3].

This work is an attempt to present and analyze the damage induced by high dose irradiation of 18 MeV $^{16}\text{O}^{5+}$ ions, in the case of two classic semiconductors (Si, Ge) and a metal (W), all showing excellent crystalline behavior, by means of the progressive change of channeling parameters.

2 Experimental setup

The experiments were carried out using the 5.5 MV Tandem Accelerator at N.C.S.R. Demokritos which produces a very stable beam over a large period of time, a factor which is of great importance as far as irradiation measurements are concerned. The final ion energy was determined via NMR with an estimated error of 8 keV.

The experimental setup includes a goniometer system (RBS-400 by Charles Evans and Associates) which permits experiments for backscattering spectroscopy of oriented or non-oriented crystalline targets. It consists of a vacuum chamber, a silicon surface-barrier detector (situated at $\theta = 160^\circ$ relative to the beam propagation axis), a four-axis goniometer with the appropriate motor drivers and controller, a fixed laser pointer for the determination of the precise beam-target orientation and the corresponding standard electronics. Data acquisition and control hardware are driven by a personal computer with the use of the appropriate software.

The goniometer is also accompanied by a set of differential collimators which allows us - through micrometric movements - to fix the beam spot size. The

accuracy of the measurements (including several systematic errors like finite solid angle corrections, imperfect charge collection, changes in the detector resolution etc.) is estimated to be in the order of 7-10 %. The targets used were high purity Si, Ge and W crystals cut in the [100] direction.

3 Experimental procedure

The experiment proceeds by the following steps:

- a) The crystals are aligned with the use of a light ion beam, namely protons at 1.2 MeV, and after the polar scan and the fine angle scan, the position for the axial channeling is precisely determined.
- b) The experiment is carried out through irradiations with the 18 MeV $^{16}\text{O}^{5+}$ ions in the random direction (which is achieved via a random rotation of the sample during the spectrum acquisition), so that the dose per step varies between 0.3 and $1 \cdot 10^{15}$ particles/cm². This allows us to examine any possible short range effect showing a non monotonic behavior of the target relative to the accumulated dose. The dose for each step is also determined by the corresponding statistics.
- c) After each step follows a short irradiation ($\sim 5 \cdot 10^{14}$ particles/cm²) in the channeling direction using the same beam, in order to check the progressive change in the χ values (with χ denoting the dechanneled fraction of the beam) at different depths inside the crystal. This check is performed for a much lower total accumulated charge at the expense of statistics, because although initially the irradiation in the channeling direction does not affect the crystal significantly, as the target is progressively damaged, this extra irradiation becomes an additional source of error, introducing an unknown uncertainty in the determination of the total accumulated dose. This may cause an error in the determination of the especially at large depths. The same logic applies to the number of irradiation steps, setting an upper, though not definite limit.
- d) The results are analyzed with the RUMP code, the spectra are compared and the corresponding values are extracted. Subsequently, the curves $\chi = f(\text{dose})$ are studied at various depths x for the crystals into consideration.

During the course of data acquisition, several sources of error affect the precision of our measurements. The exact dimensions of the beam spot have an utmost importance in the accumulated dose per step and any small deviations can lead to uncertainties which are inevitable after a continuous 17 to 24 hours irradiation. During this period one cannot exclude a slight change in the position of the beam spot as well, resulting in small oscillations of the

calculated values. The beam spot was relatively small ($\sim 1.5 \times 1.5 \text{ mm}^2$) in order to avoid any solid angle corrections. The divergence of the beam was small enough to exclude any significant initial dechanneling of the incoming beam. Nevertheless, the resolution of the silicon surface barrier detector in heavy ions, such as O, was mediocre. It should also be noted that the random rotation of a high purity crystalline sample simulates the behavior of an amorphous material only to a 95-98% depending on the quality of the crystal.

4 Results and discussion

The results from the irradiated Ge and W are presented in Figs. 1 and 2 respectively where the progressive changes of the χ_r values at different depths inside each target, relative to the accumulated dose are recorded; χ_r is defined as follows:

$$\chi_r = 1 - \frac{\chi(Dose) - \chi(0)}{1 - \chi(0)} \quad (1)$$

where $\chi(0)$ corresponds to the virgin crystal [8].

The fitted curves presented are empirical, since there is no generally accepted multiparameter formalism concerning the phenomenon. The total estimated errors for each sample are also indicated in the figures.

It should be noted here that there exist two major drawbacks in the trend of analyzing the experimental data. The first drawback is connected to the assumption of the same dE/dx in both the random and the channeling direction, which introduces an uncertainty in the depth determination of the order of 5-10%. Data in the bibliography concerning channeled oxygen atoms in semiconductors and metals are sparse and the experiments have been carried out in the transmission geometry. Therefore, their results refer to the best channeled particles which are only of relative value in the case of the backscattering geometry and a practically infinitely thick target. If one uses a light ion beam (e.g. protons) in order to examine the progressive change of the χ_r values this uncertainty in the depth determination is enhanced. On the other hand, the use of the oxygen beam has the disadvantage of poorer statistics and the danger to cause a small but not negligible extra damage of the crystal.

The second drawback is related to the secondary electron suppression, which was achieved with the application of a positive voltage directly on the target. This suppression is far from being perfect. Ions of medium mass, such as oxygen, hitting on a target can cause the escape of a large number of secondary electrons in the backscattering direction, thus requiring a large correction fac-

tor for the normalization of the charge. There is substantial evidence [6, 7] suggesting that the secondary electron emission in the channeling direction is strongly related to the dE/dx of the incoming ion.

FIGURE 1. Plot of χ_r versus the accumulated dose, at different depths (0.2, 1.1, 1.5 and 2.0 μm) inside the target, in the case of germanium [100]. The total dose for this experiment was $1.25 \cdot 10^{16}$ particles/cm².

FIGURE 2. Plot of χ_r versus the accumulated dose, at different depths (0.2, 0.5, 0.8 and 1 μm) inside the target, in the case of tungsten [100]. The total dose for this experiment was approximately $1.05 \cdot 10^{16}$ particles/cm².

These two effects, meaning the precise depth determination and the accurate normalization of the charge for both the random and channeled spectra, in the case of the absence of a faraday cup, somehow counteract each other in the case of the values calculation. The former error can cause a slight overestimation of χ_r , depending on the depth, while the latter, a small underestimation due to the different correction factor (since the secondary electron emission is reduced when irradiating in the channeling direction). As a whole, using the same beam for irradiation and diagnostics seems to be more preferable, but the combined statistical and systematic error cannot be less than 10-15% in

the most favorable case, therefore only effects significantly exceeding the above mentioned value can be reliably observed. Such effects have not been observed in any of the three cases.

In the case of germanium, the response is roughly exponential (Fig. 1), reaching a plateau, after which no significant damage with the dose has been observed. The fitting curves show an excellent monotonic behavior.

In the case of W the monotonic behavior is once more confirmed. It is quite surprising though, that the damage induced in W is less evident than the corresponding one in Ge. The χ_r fitting curves (Fig. 2) have a very small inclination with the dose, instead of being more acute than the ones in the case of Ge.

Apart from the irradiations of Ge and W, shown in Figs. 1 and 2, a Si crystal has also been irradiated to a comparable dose. The data are not presented due to the large random and systematic errors ($> 20\%$) caused mainly by the poor statistics. Nevertheless, the trend of these data, as far as χ_r versus dose is concerned, is similar to the one observed in the case of W, though towards lower values, up to a depth of $1\ \mu\text{m}$. The non monotonic dependence of χ with respect to the accumulated dose, which has been reported for Si irradiated with $16\ \text{MeV}\ ^{14}\text{N}$ at comparable doses [3], has not been observed in the present work within experimental errors.

In an attempt to comprehend the behavior of the irradiated crystals, simulations were performed using the TRIM code, which calculates the induced damage according to the Kinchin-Pease model. The results for all targets are summarized in table 1 for the maximum range of the incoming O ions. The nuclear energy loss, especially for the depths into consideration, is just a small percentage of the electronic one, however, due to the high accumulated doses, a lot of displacements per target atom (dpa) are produced. Depending on the initial settings of the simulation (displacement and binding energies), it is evident that, for roughly the same accumulated dose, the damage induced in Ge is much more profound than the one induced in Si, in accordance to experimental data. As far as W and Ge are concerned, it can be seen in table 1 that for the former, the nuclear energy loss is much higher than the corresponding one for the latter, while the induced damage versus the accumulated dose seems to be less severe (as shown in Figs. 1 and 2). This is also evident in Fig. 3 where χ_r is plotted versus dpa for both crystals at a depth of $0.2\ \mu\text{m}$. These figures clearly show that the permanent damage caused in the W crystal is significantly reduced compared to the one caused in the Ge crystal, although the energy distributed to recoils is greater in the case of tungsten.

The saturation of defect creation, as seen in Fig. 3, can be explained by the subsequent passage of an ion along the path of another, which can lead to the

breaking of stable defects, and therefore to their annealing. One cannot also exclude a possible influence of the electronic energy loss in this overlapping region, causing an enhancement of the observed phenomenon.

As a possible explanation for the lower damage observed in W, we propose the following arguments: At room temperature Frenkel defects are mobile in all three materials. Nevertheless, defect clusters like di-vacancies and di-interstitials are stable in Ge and Si. This, however, does not apply in the case of W, where these clusters can diffuse and recombine, thus explaining the radiation hardness of this metal. This phenomenon has been observed in the past as well [9].

TABLE 1. Results with the use of TRIM for 18 MeV ^{16}O ions

Quantity/Crystal	Si	Ge	W
Range (in μm)	11.5	8.87	4.19
Electronic energy loss (%)	99.35	99.22	98.98
Nuclear energy loss (%)	0.65	0.78	1.02

FIGURE 3. Plot of χ_r versus dpa (displacements per atom), at a depth of 0.2 μm inside the target, for both crystalline targets (W and Ge).

5 Conclusions

The damage induced in Si, Ge, and W crystalline targets by 18 MeV $^{16}\text{O}^{5+}$ ions has been studied and analyzed using the progressive change of the χ channeling parameter. The possible random and systematic errors have been reported and their impact on the quality of the measurements has been discussed. A mechanism was suggested in order to explain the differences between

the behavior of metals and semiconductors. A more comprehensive work, including experiments that have been carried out both at Demokritos and at Garching Beschleunigerlaboratorium with medium mass and heavy ions will be presented soon.

Nevertheless, a lot of problems seem to be open for discussion and further analysis, namely the difference in the behavior between metals and semiconductors and the existence of a possible multiparameter general formalism describing the phenomena.

As far as the experimental errors are concerned, it should be noted that special efforts should be undertaken for their control and reduction, since these sensitive measurements are quite time consuming, so during acquisition small changes are most likely to occur, affecting the accuracy of the data. Moreover, the problems of the different dE/dx of the incoming ions and the correction factors for the charge normalization due to the difference in the secondary electron emission between the random and channeled spectra will be the subject of a future study.

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