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Point and extended defects in irradiated silicon and consequences for detectors

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The interactions by which ions lose their energy in silicon are investigated at the microscopic level. This theoretical study put in evidence that the ionization could also represent a source of structural defects, and, contrary to the processes initiated by elementary particles, could generate extended primary defects, as, e.g. four-fold coordinated defects, due to the simultaneous breaking of bonds for more neighbouring atoms in the lattice in a single interaction, in the ionisation core. The average energy transferred per atom is calculated, and also the energy spent by ionisation. The time dependence of the temperature in the ionisation core is derived in some simplifying assumptions. These contributions were not considered yet in the studies of degradation of silicon detectors in radiation fields and could account for the discrepancies observed between models and measurements at microscopic versus device level for hadrons and ions.

1 Introduction The development of new electronic devices able to work in hostile conditions represents an important goal of the physics of semiconductors. In particular, silicon detectors will represent a major option for the next generation of experiments (in elementary particles or astroparticle physics, for example), where these devices must be able to work long time in very high radiation fields. Actual materials are not adequate to satisfy these conditions. Other applications require a very good control of ion penetration and related phenomena: material physics, reactor waste technologies, medical applications, dosimetry, etc. So, the understanding of elementary physical processes in the material, due to radiation penetration, will be a useful tool in obtaining new materials, radiation harder, new technologies, new principles and techniques of detection. An incompletely clarified aspect in the modelling of detector degradation due to radiation fields is the correlation between the microscopic rate of production of defects and the changes in the electrical device parameters: a relatively good agreement between experiment and models was obtained after photon and electron irradiation and discrepancies up to two orders of magnitude after heavy projectiles [1].

Particles penetrating into solids lose energy by ionisation, displacements, and radiation (not considered in the present paper). Usually, the nuclear interactions are supposed to be the source of permanent degradation.

In this contribution, considering the microscopic scale of the processes by which the projectile loses energy in the material, we put in evidence the mixing of nuclear and electronic stopping powers in the degradation processes. In the primary ionisation core, an increase of temperature must be considered due to energy loss, and thus, because annealing processes are temperature dependent, an increase of the rate of formation of defects, and also the production of defects which are not specific to room temperature is to be waited.

2 Silicon and its primary defects Silicon has the diamond crystal structure, with a lattice constant equal to 5.43095 Å at 300 K and ionisation potentials equal to 8.151, 16.345, 33.493, 45.142, 166.767 eV respectively,

corresponding to the first, second, third, fourth and fifth level.

The structural characteristics of the "classical" *vacancy* are: bond length in the bulk is 2.35 Å and bond angle – 109°. The formation energy is 3.01 eV (p-type silicon), 3.17 eV (intrinsic), 3.14 eV (n-type).

For *interstitials*, different structural configurations are possible: a) the hexagonal configuration, a sixfold coordinated defect with bonds of length 2.36 Å, joining it to six neighbours which are fivefold coordinated; b) the tetrahedral interstitial is fourfold coordinated; has bonds of length 2.44 Å joining it to its four neighbours, which are therefore fivefold coordinated; c) the split - <110> configuration: two atoms forming the defect are fourfold coordinated, and two of the surrounding atoms are fivefold coordinated; d) the 'caged' interstitial contains two normal bonds, of length of 2.32 Å, five longer bonds in the range 2.55 ÷ 2.82 Å and three unbounded neighbours at 3.10 ÷ 3.35 Å. From calculations, it was found that the tetrahedral interstitial and caged interstitial are metastable. For interstitials, the lowest formation energies in eV are 2.80 (for p-type material), 2.98 (for n-type) and 3.31 in the intrinsic case respectively.

In the last years, the existence of a new type of primary defect, *the four fold coordinated defect* (FFCD), obtained by moving atoms from the initial positions [2], has been predicted. This displacement of atoms produces new bonds with the neighbours. The bond lengths are between 2.25 ÷ 2.47 Å and angles vary in the 97 ÷ 116° range. So, the bond length and angle do not deviate significantly from their bulk values. The formation energy is 2.45 eV (for p-type silicon), 2.42 eV (intrinsic), and 2.39 eV (n-type), lower than the energy of formation of both vacancies and interstitials.

3 General aspects of the interactions of heavy charged particles with silicon The starting point in these investigations is represented by the quantitative physics on the penetration of particles and ions through matter.

If the mechanisms for ionisation are relatively clear for particles, the situation is more complicated in the case of ions. A distinctive feature of heavy ions is that they are composite projectiles, having an internal structure and carrying electrons, and their interaction with bounded and free electrons in the stopping medium is a complex problem involving a number of processes that are absent in the case of particles.

For the ionisation energy loss three distinct regions are found in the dependence on the energy of the incoming particle, corresponding to low, intermediate and high energies, and which were modelled by Lindhard–Scharff [3], Andersen–Ziegler [4] and Bohr/Bethe-Bloch respectively. The charge of the projectile is screened due to electrons and the result is a reduced Coulomb interaction between projectile and target electrons, but at the same time excitations must be considered. The screening effect consists in the reduction of electric field strength, depending on the distance from the projectile and on velocity. So, in ionisation processes both projectile and target charges contribute to the phenomenon.

Nuclear interactions were first phenomenologically explained by Kinchin and Pease [5] and in quantum theory by Lindhard et al. [6]. Some extensions were done by Lazanu and Lazanu in Ref. [7] and also by others in Refs. [8–10] for different particles and energies. Nuclear interactions include elastic and inelastic collisions. In the first case, target nuclei are only moved from their lattice positions, while in the second case the identity of the projectile and/or target could be changed.

While electronic processes depend on the velocity of the projectile, nuclear phenomena depend on the energy of the projectile.

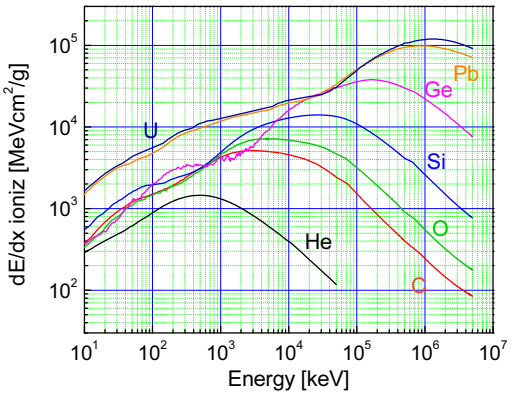

Figure 1 Linear ionisation energy loss dependencies on ions kinetic energy for different ions in Si.

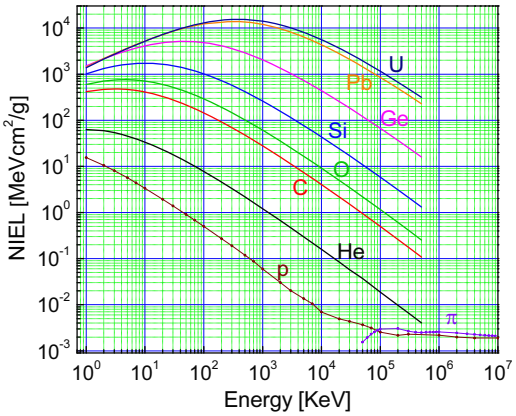

Figure 2 NIEL dependencies on kinetic energy for pions, protons and C, O, Si, Ge, Pb and U ions in silicon.

In Figs. 1 and 2, the ionising and the nonionising energy loss (NIEL) dependencies on ion energy in silicon are represented respectively.

The curves are calculated based on SRIM 2008 [11] simulations, see, e.g. Ref. [12]. The ions considered are He, C, O, Si, Ge, Pb and U, and cover an important part of the periodic table. For NIEL, the same dependencies were represented also on the same graph for protons [13, 14] and pions [15].

4 Microscopic aspects of the energy loss in ionisation processes and defect production The charge state of an ion in interaction is described using the concept of effective charge. For heavy ions, different alternatives for the effective charge were used. The simple empirical formula of Northcliffe [4] was modified by Ziegler [16] for current use. Betz's formula [17] gives an alternative, and another one is given by Sigmund [18].

In Figures 3a and b, the effective charge of He and U ions in silicon, calculated in the frame of different models as dependencies on the ion kinetic energy in silicon are represented.

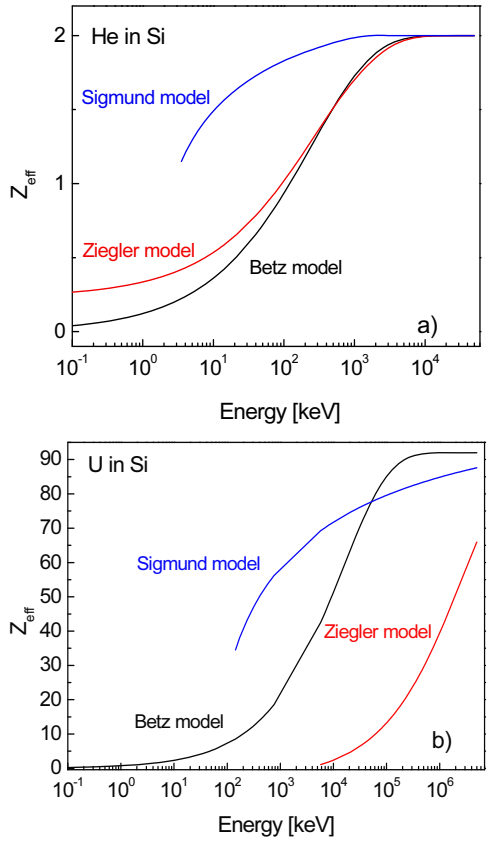

Figure 3 Effective charges of a) He ions and b) U ions incident on silicon versus kinetic energy.

Using the idea of range of interaction, a primary ionisation core could be defined. It has the shape of a cylinder around ion's trajectory, and the critical distance is the radius of this region, the size of which is given by the radial distance from the energetic ion at which the electric field of the projectile is high enough to produce ionisation of the outer electrons of a target atom:

$$r = \left(Z_{eff}\right)^{1/2} r_{Bohr} \tag{1}$$

In Figs. 4a and b, the dependence of the cylinder radius produced by He and U ions respectively in Si is represented as a function of the kinetic energy of the projectile, where the effective charge has been calculated using Ziegler, Betz and Sigmund models respectively.

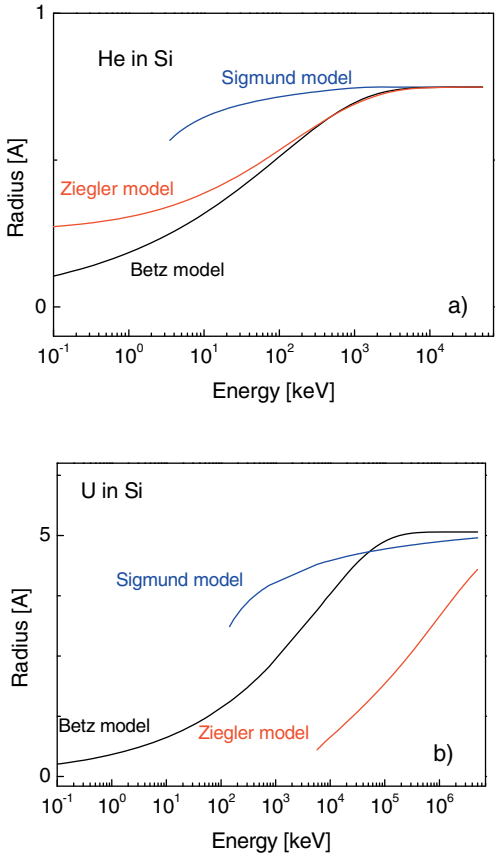

Figure 4 Ionisation radii produced by: a) He ions and b) U ions incident on silicon versus kinetic energy.

A monotonic increase of the radius with the energy of the ion could be observed in the region of low and intermediate energies, which is followed by a plateau, at high energies. While the values of the radius at the highest energies are model independent, and are given by the product of the Bohr radius by the square root of the charge number of the ion, at all other energies it has different values in different models.

For He ions, even at the highest energies, the corresponding radius is lower than the length of the Si–Si bond, while for high energy U ions more Si atoms are comprised in the ionisation core, i.e. more Si–Si bonds could be simultaneously broken by the energy stored in this region.

This could represent a source of FFCD and of other extended defect production directly by swift heavy ions.

In Fig. 5, the dependence of the ionisation radii produced by He, C, O, Si, Ge, Pb and U ions in silicon is represented as a function of kinetic energy. Betz's formula for Z_{eff} has been used. At the same energy, the radius increases with the charge number of the ion. Thus, depending on the ion and energy, more Si atoms could be simultaneously situated inside the ionisation core and in principle extended defects could be produced.

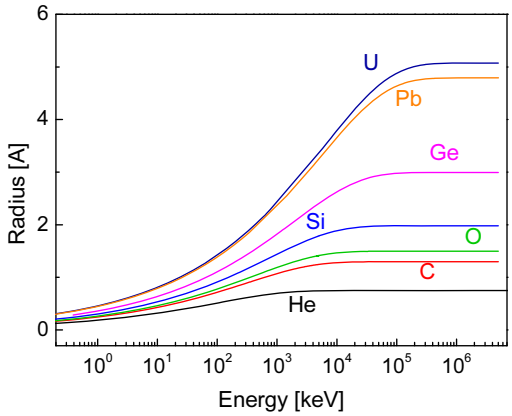

Figure 5 Dependence of the ionisation radii produced by He, C, O, Si, Ge, Pb and U ions in silicon as a function of their kinetic energy.

The very low values of the radius in Bohr's adiabatic approximation suggest that energy is rapidly transported from the initial region where it was deposited [19].
Starting from the interaction radius, the energy transferred by the projectile, by ionisation, to each atom in the ionisation core has been calculated. Its dependence on the kinetic energy of the projectile is represented in Figure 6 for He and U ions respectively, as continuous curves, that were calculated in the frame of Betz's model.

The total energy per atom represents a physical quantity that folds two distinct aspects: energy dependence of the energy loss in ionisation processes and the variation of the dimension of the core of the interaction region respectively.

The energy transferred by the ion in the primary core is used to eject electrons from the atoms, and to give kinetic energy to these electrons. So, radial energy transfer is by energetic electrons, and there exists a transport process mediated by recombination and energy transfer to ions. We suppose here that the "damaged" zone is the primary ionisation core defined above. In this zone, a rise of temperature takes place. The heat wave can be considered to have a step-like front structure, and the temperature at any spatial point an instantaneous maximum at the time the heat wave arrives. The temperature at that spatial point then falls rapidly with time as the heat wave propagates [20].

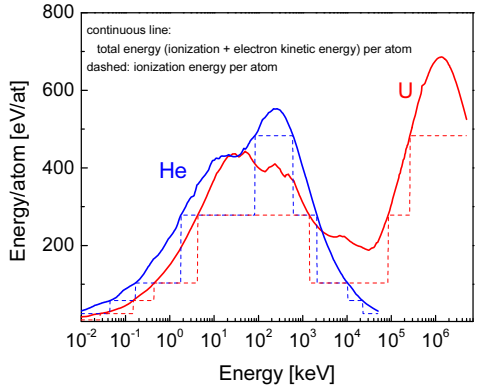

Figure 6 Energy dependence of the average energy/atom in the ionisation core (continuous curve) and energy spent by ionisation (dashed curve) for He and U ions incident on Si.

Using the thermal spike model of Szenes [21] and the simplified procedure from Ref. [20], the space–temperature profile may be described as Gaussian-like, with an exponentially long leading edge, with the maximum in temperature produced at $t = 0$. The time variation of the temperature is dependent on the projectile and material characteristics: So, for He ions in silicon, a time dependence of the temperature, expressed in K (with the time expressed in sec.), of the order of $T = 10^{-11}/t$ has been found, while for U ions it is given by $T = 5 \times 10^{-7}/t$.

Defect annealing is a temperature activated process. If, in the region of interaction, the increase of temperature has a time scale comparable with the time necessary to produce complex defects, this aspect must be considered in the kinetics of defects, with implications at the device level. The degradation is more important for heavy ions in respect to light ions. This work is in progress.

5 Summary and conclusions We have shown that mixing of nuclear and electronic stopping powers must be considered in the degradation processes.

For heavy projectiles, depending on energy, in the primary region affected by the energy deposited in ionisation processes, the simultaneous breaking of bonds for more atoms is possible, and also the production of extended primary defects (as FFCD for example) starts to be possible.

The local increase of temperature in ionisation processes and its time dependence in the primary degradation region imposes the consideration of supplementary defects in respect with those present at room temperature, if their temperature and time scales of activation fit the conditions.

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