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ENERGY DEPOSITED BY RADIATION IN SOLIDS: REGISTRATION PHYSICS[*,**]

I. LAZANU[1], S. LAZANU[2]

[1] *University of Bucharest, Faculty of Physics, POBox MG-11, Bucharest-Măgurele, Romania*
[2] *National Institute for Materials Physics, POBox MG-7, Bucharest-Măgurele, Romania*

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Abstract. General aspects of the interactions of ions in silicon are investigated: energy lost in electronic and nuclear processes, as well as their consequences, creation of point and extended defects in the crystal structure. The correlations between irradiation ions, their energy, ionization and nuclear energy loss per atom, radius of interaction and spatial extension of the primary damaged region are also investigated.

Key words: radiation effects, electronic and nuclear stopping, heavy ions, silicon, damage.

1. INTRODUCTION

Quantitative physics on the penetration of ions through matter represents a fundamental aspect for a wide diversity of applications: the development of new materials for devices able to work in hostile conditions (high fields of radiation, extreme temperature or pressure), new principles and techniques of detection, reactor waste technologies, medical applications, dosimetry, etc.

In this contribution, energy loss processes of charged particles and heavy ions in silicon are investigated, as well as their consequences, creation of point and extended defects in the crystal structure. The correlations between irradiation particles, their energy, ionization, energy loss per atom, radius of interaction and spatial extension of the primary damaged region are also investigated.

2. GENERAL ASPECTS OF THE INTERACTIONS OF SWIFT IONS IN SILICON

Energy loss processes for charged particles in matter may be classified considering excitations, ionisation or capture of electrons from target or projectile

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atoms, nuclear stopping in which the energy of projectiles is lost by nuclear recoils in elastic and inelastic collisions, or radiative interactions. Radiative processes become dominating at extremely high velocities. In crystalline materials, phonons – vibrations of the lattice – are generated, and this process remains the dominant mechanism of interaction below the thresholds for other processes. All these competitive processes are dependent on energy, type of incident projectile and target material.

In principle, the energy lost by an incoming particle in materials can be separated into individual components:

$$\left(-\frac{\mathrm{d}E}{\mathrm{d}x}\right)_{total} = \left(-\frac{\mathrm{d}E}{\mathrm{d}x}\right)_{electronic} + \left(-\frac{\mathrm{d}E}{\mathrm{d}x}\right)_{nuclear} + \left(-\frac{\mathrm{d}E}{\mathrm{d}x}\right)_{radiation}. \quad (1)$$

In this work we concentrate on the ionization energy loss. Usually, for these processes, 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 [1], Andersen – Ziegler [2] and Bethe-Bloch respectively. These regions could be immediately identified in Fig. 1, where the ionization energy loss of Si ions in silicon is obtained from simulation, using the SRIM program [3].

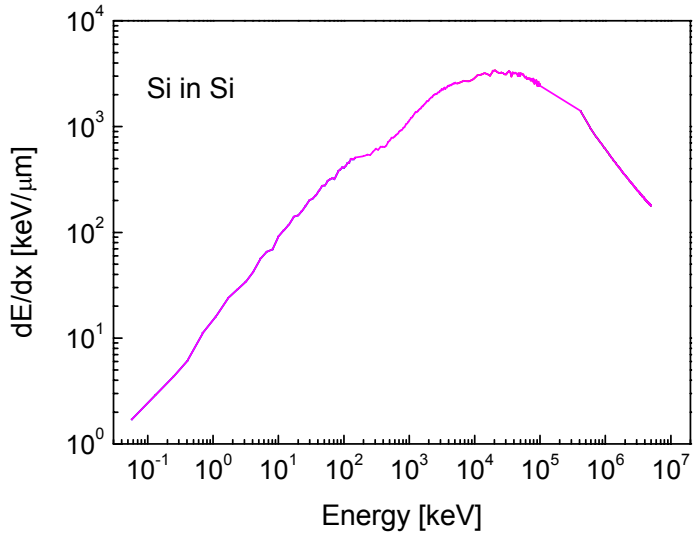


Fig. 1 – Electronic energy loss of Si ions in a silicon target, simulated using SRIM.

In this particular case, the first region, corresponding to low energies, extends up to around 10^3 keV, the intermediate region covers the next energy range up to 10^5 keV, and for higher values of energy the mechanisms are well explained by Bethe's theory.

The nuclear interactions were first explained by Lindhard et. al. [4], and also some extensions were done by Lazanu and Lazanu [5], and others [6], for different particles and energies. In Fig. 2, the nuclear energy loss for the same incident projectile in the same material as in figure 1 is presented; the calculations of the present work are done in the frame of the Lindhard theory.

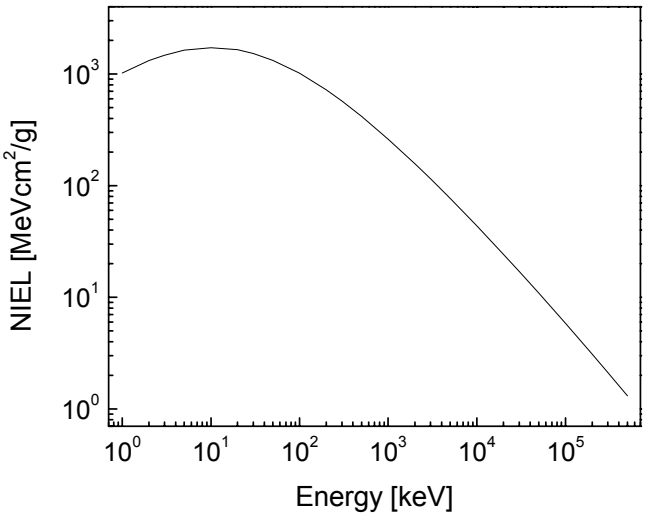


Fig. 2 – Nuclear energy loss of Si ions in a silicon target.

If the mechanisms of interaction 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 bound and free electrons in the stopping medium is a complex problem involving a number of processes that are absent in the case of particles, as for example the number of electrons that remain bound to ions in interaction processes and their interactions with the medium, or the Barkas-Andersen effect, representing a correction on the energy loss, with a Z_{pr}^3 dependence [7].

The charge of the projectile is screened due to electrons and reduces Coulomb interactions 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 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.

In the present work we concentrate only on phenomena in silicon. The choice of silicon is due to the fact that silicon is a major option for detectors in space experiments, at Tevatron, LEP-like and LHC facilities – see Table 1, adapted from [8]. For each experiment, the aria of silicon detectors in squared meters is specified.

Table 1

Experiments using silicon detectors

Experiment / Aria of silicon detectors [m^2]							
Space		Tevatron		LHC		LEP – like	
NINA	0.12	DO	3.00	LHCB	0.77	HERMES	0.02
AGILE	2.02	CDF	11.10	ALICE	5.58	TOSCA	0.14
AMS	2.10			ATLAS	61.00	FINUDA	0.19
PAMELA	2.40			CMS	214.00	BELLE	0.20
GLAST 1	2.70					H1	0.39
AMS-02	5.53					L3	0.62
GLAST	74.00					OPAL	0.63
						CLEO3	0.64
						BABAR	0.86
						ALEPH	0.96
						NOMAD	1.20
						DELPHI	1.63
						ZEUS	2.46

3. PRIMARY DEFECTS IN SILICON

Silicon has the crystal structure of diamond, with a lattice constant of 5.43095 Å at 300K.

The primary mechanism of defect formation during irradiation in semiconductors in general and in silicon in particular is the collision of the incoming particle with the atoms of the crystal, which leads to the departure of an atom to a rather large distance from its original site, i.e., to the formation of separated Frenkel pairs (vacancies and interstitials), as well as to the Si_{FFCD} defect formation, which is an extended defect - because more nuclei change simultaneously their bound state, fact which introduces a new type of symmetry in the lattice [9], [10]:

$$\text{Transfered energy} \rightarrow \text{Si} \rightarrow \text{Si}_{\text{FFCD}} . \quad (2)$$

The following four regimes and their timescale have been identified [11]:

(1) carrier excitation (10^{-14} – 5×10^{-12}s),

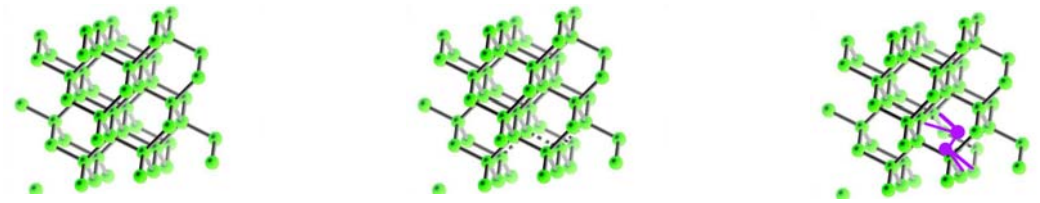
(2) thermalization between 10^{-14} and 5×10^{-12}s,

(3) carrier removal (from to 5×10^{-12} up to 10^{-5} s and

(4) thermal and structural effects between 5×10^{-10} up to 5×10^{-6} s.

In silicon, the primary defects (*V* and *I*) are mobile over a broad temperature range, including room temperature, and diffusing they are trapped by other primary defects or by impurity atoms forming secondary defects, or migrate to sinks. The main characteristics of the kinetics of defects are summarised in reference [12]. The Si_{FFCD} defect represents an elementary centre of amorphization, changing the symmetry of the crystal, and could form new extended defects.

Fig. 3 presents the successive modifications in the silicon bonds in an elementary cell, whit the production of the FFCD defect, and implicitly elementary amorphization.



a) b) c)

Fig. 3 – a) Normal structure of silicon; b) the bounds of the silicon affected by the transferred energy that contribute to create Si_{FFCD} defect; c) the new bonds of the Si_{FFCD} defect.

Due to the mobility of primary vacancy-interstitial pairs and to the existence of different impurities, processes of migration, formation of new types of defects as well as annihilation are all annealing processes.

4. THE MODEL

4.1. HYPOTHESES

In the modelling of ion-atom collisions, a full quantum mechanical treatment is used. Ion-atom interactions are screened Coulomb collision, including exchange and correlation interactions between the overlapping electron shells. The ion has long range interactions creating electron excitations and plasmons within the target. These are described including target's collective electronic structure and interatomic bond structure. The charge state of the ion in the target is described using the concept of effective charge, which includes a velocity dependent charge state and long range screening due to the collective electron sea of the target.

The basic assumption in the calculation of electronic stopping of ions is that electron density in the target varies slowly with position and is described by a free electron gas. There are no significant band-gap effects on electronic stopping.

The charge of the ion can be reduced to a scalar quantity called ion's effective charge.

For heavy ions, different alternatives for the effective charge were used. The simple empirical formula of Northcliffe [2] was modified by Ziegler [13] for current use as:

$$Z_{ion}^{eff}/Z = 1-\left[\exp(-a)\right]\left[1.034-0.1777\cdot\exp\left(-.08114\times Z_1\right)\right], \tag{3}$$

with practical values for a and b:

$$a = b + .0378\times\sin\left(\pi\cdot b/2\right),$$

and

$$b = 0.886\cdot\left(\frac{E\left[\text{keV}\right]}{25\cdot M_1\left[\text{amu}\right]}\right)^{\frac{1}{2}}\cdot\frac{1}{Z_1^{2/3}}.$$

Betz's formula [14] for Z_{eff}: is given by the alternative expression:

$$Z_{eff} = Z\cdot\left[1-\exp\left(-\frac{v}{v_0 Z^{2/3}}\right)\right] \tag{4}$$

where v and v_0 are projectile and Bohr's velocities respectively, while Sigmund [15] roughly approximated the effective charge, disregarding screening, shell and higher order Z (charge number of the projectile) corrections as

$$\frac{Z_{eff}}{Z} = \begin{cases} 1 & \text{for} \quad v > 2Z\cdot v_0 \\ 1-\dfrac{\log(2Zv_0/C\text{v})}{\log(2m\text{v}^2/I)} & \text{for} \quad v < 2Z\cdot v_0. \end{cases} \tag{5}$$

Using the ideas of range of interaction, we could define a primary ionization core, 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 ionization of the outer electrons of a target atom. The radius of this cylinder is approximated as:

$$r = Z_{eff}^{1/2}\cdot r_{Bohr}, \tag{6}$$

where r_{Bohr} is Bohr's radius and Z_{eff} is the effective charge of the ion.

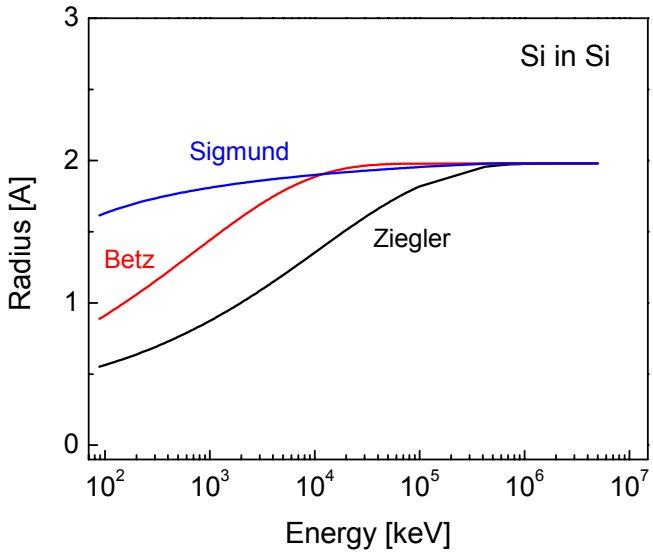


Fig. 4 – Energy dependence of ionization radii induced by silicon ions in silicon in different models.

In Fig. 4, the dependence of these radii on the kinetic energy of Si ions in silicon is presented. It could be seen that Betz, Sigmund and Ziegler expressions for Z_{eff} agree at high enough energies of the ions, where the effective charge equals the charge number of the ions, and this limits the radius of ionization given by formula (6).

4.2. PROCESSES OF INTERACTION AND DAMAGE INDUCED IN SILICON

When an ion penetrates into the target, it loses its energy through collisions with nuclei and electrons. Target amorphization could be the result of damage accumulation due to nuclear and electronic processes.

Generally, energy transferred to the electronic system is considered as inelastic loss, while energy deposited in the form of nuclear collisions is considered as an elastic one. When swift ions move through matter, their energy dissipation is almost exclusively due to interactions with and energy transfer to electrons. Low energy ions lose energy especially by nuclear interactions. When energetic ions slow down in solids, the energy is locally deposited to the electrons and finally can be transferred to the atoms by electron-electron and electron-atom interactions.

Numerous experiments on defect formation in insulators, metals, alloys, and amorphous semiconductors have shown that these materials are sensitive to track formation when they are bombarded by high-energy heavy ions. Nevertheless, the conditions of track formation and the inner structure of tracks (phase composition)

in metals, insulators and semiconductors, crystalline and amorphous solids, films, and massive specimens differ substantially.

The irradiation of crystalline silicon, germanium, and gallium arsenide at room temperature by swift ions, conducted at numerous accelerators all over the world, did not lead to any specific effects caused by the high intensity of electronic excitations [16, 17, 18, 19, 20, 21, 22, 23, 24]. The effectiveness of defect formation or defect annealing stimulated by the high level of electronic excitations depends on $(dE/dx)_e$ and ion velocity. The specific ionization energy loss for monoatomic ions in silicon does not exceed 28 keV/nm. However, recent experiments [25] on irradiation of crystal silicon by fullerene ions C_{60}^{2+} with $E \sim 30$ MeV and $(dE/dx)_e \sim 48$ keV/nm, as well as with $E \sim 40$ MeV and $(dE/dx)_e \sim 57$ keV/nm revealed the formation of tracks with entrance diameters amounting to 8.4 and 10.5 nm, respectively. The track diameters remain constant down to a depth of roughly 80–100 nm [25], and at larger depths gradually decrease. Very often the tracks end in a series of droplets of disturbed material along the ion paths (the discontinuous section of the tracks).

The radius of interaction for helium, silicon and uranium projectiles are considered, for a large range of energies, in the hypothesis of the Betz approximation. The results are presented in Fig. 5.

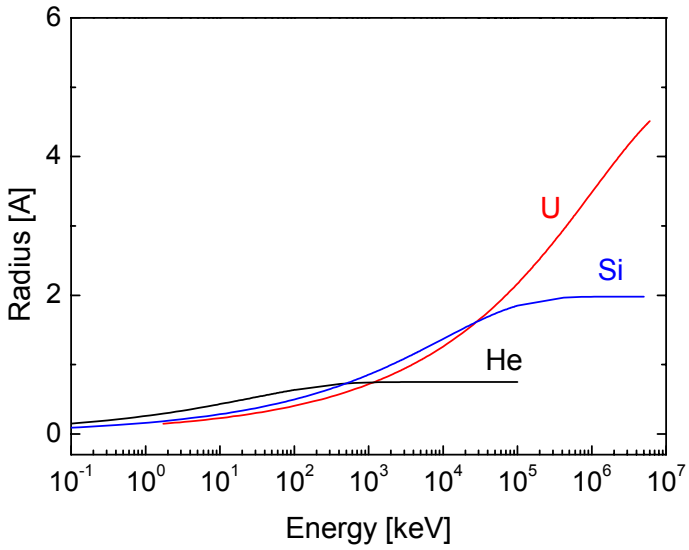


Fig. 5 – Ionization radii (calculated with Betz's formula for Z_{eff}) induced by He, Si and U ions in Si, as a function of their kinetic energy.

It could be observed that the radius of the corresponding cylinder is very small in respect to the separation of Si atoms in the lattice. Only at high energies

and for heavy ions, one interaction affects more that 1 atom. These preliminary results could explain why the Si_{FFCD} has not been put yet in evidence experimentally.

Supposing that in the first stage all electronic energy loss is transmitted to atoms in the ionization core, the dependence of the atomic density of energy on ion kinetic energy has been extracted, and is represented in Fig. 6 for the same ions. These estimations are done using Betz's model.

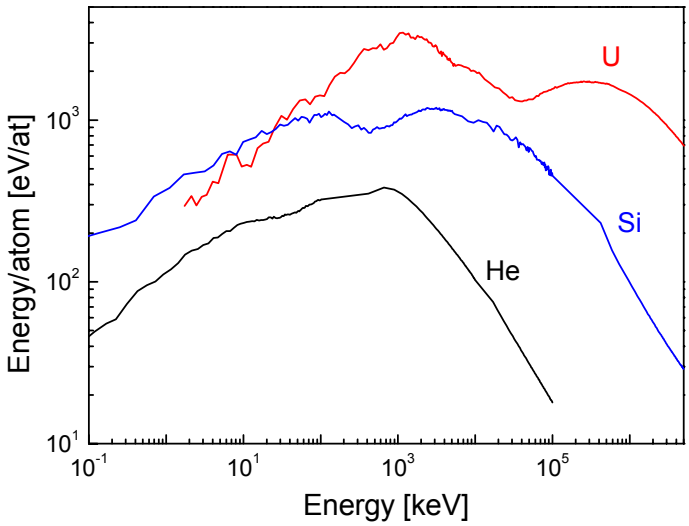


Fig. 6 – Energy/atom transferred in the ionization core due to $(dE/dx)_e$ by He, Si and U ions in silicon as a function of kinetic energy.

On the other side, the energy lost in nuclear interactions with the nuclei of the target has as a consequence cascades of displacements produced by the primary knock-on atom. Vacancies and interstitials interact with other impurities and defects in the lattice, or between themselves, producing "stable" defects. Studies involving deep level transient spectroscopy (DLTS), Hall measurements, transmission spectroscopy, optical absorption measurements, electron paramagnetic resonance (EPR), and measurements of electrical resistance did not reveal other types of structural defects, as a consequence of ion irradiation in respect to particle irradiation in silicon. But, while in electron-damaged samples defects are distributed randomly, neutron and ion irradiation produce defect distributions which are not spatially homogeneous.

In the process of energy loss of the incident particle an electron gas is created around its trajectory. We suppose that in the initial stages this gas is in equilibrium and a temperature could be defined. In the vicinity of the projectile the increase of the temperature is significant in respect to environment temperature, where

processes are currently studied, and thus supplementary mechanisms for the formation of extended/complex defects must be considered: multiple self-interstitials [26] and vacancy clusters [27] as well as oxygen dimers and complexes with other impurities.

Neutrons or ions eject energetic Si knock-on atoms that subsequently produce locally dense cascades of Si vacancies and interstitials. The concentration of defects in these cascades has been estimated [28] to be as high as 10^{20} cm^{-3}, exceeding the spatially averaged defect density by 4–7 orders of magnitude. This locally dense defect production impacts not only the types and efficiency of defect creation, but also affects the electronic properties of the irradiated material. With locally dense defect clusters one must consider defect correlations that impact, for example, local changes in the defect capture rate, emission rate, and energy levels due to nearby defects [29]. These complications make the extension of classic studies of isolated defects to a clustered environment a significant challenge.

5. SUMMARY

In the present work the peculiarities of ionisation energy loss in silicon due to heavy ions were investigated on a large range of energies, below Bethe-Bloch formalism.

The concepts of effective charge for the projectile in different approximations used in the literature, the radius of interaction, energy loss per atom were discussed

Analytical calculations and / or numerical simulations of these quantities permitted to estimate the spatial extension of the primary damaged region and to suggest an explanation for the formation of Si_{FFCD} as primary defect.

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