Predictions about the behaviour of diamond, silicon, SiC and some $A^{III}B^{V}$ semiconductor materials in hadron fields

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Abstract

The utilisation of crystalline semiconductor materials as detectors and devices operating in high radiation environments, at the future particle colliders, in space applications, in medicine and industry, makes necessary to obtain radiation harder materials. Diamond, SiC and different $A^{III}B^{V}$ compounds (GaAs, GaP, InP, InAs, InSb) are possible competitors for silicon to different electronic devices for the up-mentioned applications. The main goal of this paper is to give theoretical predictions about the behaviour of these semiconductors in hadron fields (pions, protons). The effects of the interaction between the incident particle and the semiconductor are characterised in the present paper both from the point of view of the projectile, the relevant quantity being the energy loss by nuclear interactions, and of the target, using the concentration of primary radiation induced defects on unit particle fluence. Some predictions about the damage induced by hadrons in these materials in possible applications in particle physics and space experiments are done.

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1 Introduction

The crystalline materials for semiconductor devices used in high fluences of particles are strongly affected by the effects of radiation. After the interaction
between the incoming particle and the target, mainly two classes of degrada-
tion effects are observed: surface and bulk material damage, the last due to the
displacement of atoms from their sites in the lattice. After lepton irradiation,
the effects are dominantly at the surface, while heavy particles (hadrons and
ions) produce both types of damages.

Up to now, in spite of the experimental and theoretical efforts, the under-
standing of the behaviour of semiconductor materials in radiation fields, the
identification of the induced defects and their characterisation, as well as the
explanation of the degradation mechanisms are still open problems.

The utilisation of semiconductor materials as detectors and devices operating
in high radiation environments, at the future particle colliders, in space appli-
cations, in medicine and industry, makes necessary to obtain radiation harder
materials.

Diamond, SiC and different $A^{III}B^{V}$ compounds (GaAs, GaP, InP, InAs, InSb)
are in principle, possible competitors for silicon in the realisation of different
electronic devices.

All analysed materials have a zinc-blend crystalline structure, with the excep-
tion of SiC, that presents the property of polytypism [1]. The polytypism refers
to one-dimensional polymorphism, i.e. the existence of different stackings of
the basic structural elements along one direction. More than 200 polytypes
have been reported in literature [2], but only few of them have practical im-
portance. These include the cubic form $3C(\beta)$, and the $4H$ and $6H$ hexagonal
forms. For the cubic polytype, the symmetry group is $T_d^2$, while for the hexag-
onal ones this is $C_{6v}^4$. Silicon is at the base of electronic industry, diamond
and the $A^{III}B^{V}$ compounds present attractive electrical and/or luminescence
properties, of interest for different applications, while the utilisation of SiC
as a radiation detector, both in high energy physics and in the field of X-ray
astronomy is now under extensive investigation more conferences in the field
having sections dedicated to SiC.

The diamond has the reputation of being a radiation hard material and it
is considered as a good competitor to silicon, but non all its properties as a
radiation hard material have been proved experimentally.

The main goal of this paper is to give some theoretical predictions about the
behaviour of different semiconductors in hadron fields (pions, protons), these
materials representing potential candidates for detectors and electronic devices
working in hostile environments.

The treatment of the interaction between the incident particle and the solid
can be performed from the point of view of the projectile or of the target.
In the first case, the relevant quantity is the energy loss (or equivalently the
stopping power) and in the second situation the effects of the interactions are described by different physical quantities characterising material degradation. There is no a physical quantity dedicated to the global characterisation of the effects of radiation in the semiconductor material. A possible choice is the concentration of primary radiation induced defects on the unit particle fluence (CPD), introduced by [3]. It permits the correlation of damages produced in different materials at the same kinetic energy of the incident hadron. For the comparison of the effects of different particles in the same semiconductor material, the non ionising energy loss (NIEL) is useful.

As a measure of the degradation to radiation, in the present paper the energy lost by the incident particle in the nuclear interaction and the concentration of primary defects induced in semiconductor bulk are calculated. If the energy loss of the incident projectile is, in principle, a measurable physical quantity, the concentration of primary defects is not directly observable and measurable and can be put in evidence only indirectly, e.g. from the variation of macroscopic parameters of the material or/and of electronic devices. It is to be noted that there exists also a kinetics of the defects induced by irradiation giving rise to the annealing process. A general treatment of the evolution processes is not possible, so, only some particular models exist in literature, see for example [4] and the references cited therein in the case of silicon. In these circumstances, in the present paper only the primary process of defect generation is modelled. This way, the energy range of incident hadrons for which the concentration of primary defects do not affect irreversibly the device properties could be established (theoretically predicted).

2 Model of the degradation

2.1 Energy loss

At the passage of the incident charged particle in the semiconductor material same of its energy is deposited into the target. The charged particles interact with both atomic and electronic systems in a solid. The total rate of energy loss, could, in general, be divided artificially into two components, the nuclear and the electronic part.

The energy lost due to interactions with the electrons of the target gives rise to material ionisation, while the energy lost in interactions with nuclei is at the origin of defect creation.

A comprehensive theoretical treatment of electronic stopping, which covers all energies of interest, cannot be formulated simply because of different approxi-
mations concerning both the scattering and contribution of different electrons in the solid. For fast particles with velocities higher than the orbital velocities of electrons, the Bethe-Bloch formula is to be used [5]. At lower velocities, inner electrons have velocities greater than particle velocity, and therefore do not contribute to the energy loss. This regime has been modelled for the general case by Lindhard and Scharff [6] and particular cases have been treated, e.g. in reference [7]. If the particle has a positive charge, and a velocity close to the orbital velocity of its outer electrons, it has a high probability of capturing an electron from one of the atoms of the medium through which it passes. This process contributes to the total inelastic energy loss since the moving ion has to expend energy in the removal of the electrons which it captures.

The nuclear stopping depends on the detailed nature of the atomic scattering, and this in turn depends intimately on the form of the interaction potential. At low energies, a realistic potential based on the Thomas-Fermi approximation has been used in the literature [6] and at higher energies, where scattering results from the interaction of unscreened nuclei, a Rutherford collision model is to be used.

2.2 Bulk defect production

The mechanism considered in the study of the interaction between the incoming particle and the solid, by which bulk defects are produced, is the following: the particle, heavier than the electron, with electrical charge or not, interacts with the electrons and with the nuclei of the crystalline lattice. The nuclear interaction produces bulk defects. As a result of the interaction, depending on the energy and on the nature of the incident particle, one or more light particles are produced, and usually one or more heavy recoil nuclei. These nuclei have charge and mass numbers lower or at least equal to those of the medium. After the interaction process, the recoil nucleus or nuclei, if they have sufficient energy, are displaced from the lattice positions into interstitials. Then, the primary knock-on nucleus, if its energy is large enough, can produce the displacement of a new nucleus, and the process could continue as a cascade, until the energy of the nucleus becomes lower than the threshold for atomic displacements.

The concentration of the primary radiation induced defects on unit fluence has been calculated starting from the following equation:

\[ CPD(E) = \frac{1}{2E_d} \int \sum \frac{d\sigma}{d\Omega} L(E_{Ri}) \ d\Omega \]  

(1)

where \( E \) is the kinetic energy of the incident particle, \( E_d \) the threshold energy.
for displacements in the lattice, $E_{Ri}$ the recoil energy of the residual nucleus, $L(E_{Ri})$ the Lindhard factor describing the partition between ionisation and displacements and $d\sigma_i/d\Omega$ the differential cross section for the process responsible in defect production. In the concrete calculations, all nuclear processes, and all mechanisms inside each process are included in the summation over index $i$. Because of the regular nature of the crystalline lattice, the displacement energy is anisotropic.

In the concrete evaluation of defect production, the nuclear interactions must be modelled, see for example references [3,8–10]. The primary interaction between the hadron and the nucleus of the lattice presents characteristics reflecting the peculiarities of the hadron, especially at relatively low energies. If the inelastic process is initiated by nucleons, the identity of the incoming projectile is lost, and the creation of secondary particles is associated with energy exchanges which are of the order of MeV or larger. For pion nucleus processes, the absorption, the process by which the pion disappears as a real particle, is also possible.

The energy dependence of cross sections, for proton and pion interaction with the nucleus, presents very different behaviours: the proton-nucleus cross sections decrease with the increase of the projectile energy, then have a minimum at relatively low energies, followed by a smooth increase, while the pion nucleus cross sections present for all processes a large maximum, at about 160 MeV, reflecting the resonant structure of interaction (the $\Delta_{33}$ resonance production), followed by other resonances, at higher energies, but with much less importance. Due to the multitude of open channels in these processes, some simplifying hypothesis have been done [10].

The process of partitioning the energy of the recoil nuclei (produced due the interaction of the incident particle with the nucleus, placed in its lattice site) by new interaction processes, between electrons (ionisation) and atomic motion (displacements) is considered in the frame of the Lindhard theory [11].

The factor characterising recoil energy partition between ionisation and displacements has been calculated analytically, solving the general equations of the Lindhard theory in some physical approximations. Details about the hypothesis used could be found in reference [12]. All curves start, at low energies, from the same curve; they have at low energies identical values of the energy spent into displacements, independent on the charge and mass number of the recoil. At higher energies, the curves start to detach from this main branch. This happens at lower energies if their charge and mass numbers are smaller. The maximum energy transferred into displacements corresponds to recoils of maximum possible charge and mass numbers. The curves present then a smooth increase with the energy. For the energy range considered here, the asymptotic limit of the displacement energy is not reached.
For binary compounds, the Lindhard curves have been calculated separately for each component of the material, and the average weight Bragg additivity has been used. In this case, a threshold for atomic displacements must be considered for each atomic species and for each direction in the crystal. In the concrete calculations, a weighted value, independent on the crystalline direction has been used.

3 Results, discussions and some possible applications

The nuclear stopping power presents an energy dependence with a pronounced maximum. It is greater for heavier incident particles: protons compared to pions. In a given medium, the position of the maximum is the same for all particles with the same charge. In figure 1, the nuclear energy loss in diamond, silicon, silicon carbide, GaP, GaAs, InP, InAs and InSb is represented for protons and pions respectively, as a function of their kinetic energy. In the same medium, the position of the maximum is the same for pions and protons.

The behaviour of these materials in proton and pion fields is characterised by the CPD. In Figure 2, the dependence of the CPD as a function of the protons kinetic energy and medium mass number is presented for diamond, silicon, SiC GaAs and InP - see reference [13] and references cited therein. The values for diamond degradation are from reference [9], the corresponding ones for silicon are averaged values from references [14] and [15], SiC - from reference [16] and those for GaAs and InP are from reference [15]. Low kinetic energy protons produce higher degradation in all materials. The discontinuity in the surface is related to differences in the behaviour of the CPD for monoatomic materials (or binary ones with close elements), and binary ones with remote elements in the periodic table.

For pion induced degradation, the energy dependence of CPD (as well as of the NIEL) presents two maxima, the relative importance of which depends on the target mass number: one in the region of the $\Delta_{33}$ resonance, more pronounced for light elements and compounds containing light elements, and another one around 1 GeV kinetic energy, more pronounced for heavy elements. At higher energies, an weak energy dependence is observed, and a general $A_{\text{average}}^{3/2}$ dependence of the NIEL can be approximated [10,12]. In Figure 3, the CPD for all analysed materials (diamond, Si, SiC, GaP, GaAs, InP, InAs, InSb) is represented as a function of the pion kinetic energy and of material average mass number. The differences in the behaviour of these materials are clearly suggested by the discontinuity in the mesh surfaces.

In the energy range considered in the paper, it could be observed that the CPD produced by pions and protons, and characterising the bulk degrada-
tion, are very different and reflect the peculiarities of the interactions of the two particles with the semiconductors. For pions, there are two maxima, one in the region of the $\Delta_{33}$ resonance, corresponding to about 140 - 160 MeV kinetic energy, and the other at higher energies, around 1 GeV. The relative importance of these maxima depends on the mass number of the material. In comparison with this behaviour, the CPD produced by protons decreases abruptly with the increase of energy at low energies, followed by a smooth and slow increase at higher energies.

In relation to their behaviour in pion fields, these materials could be separated into two classes, the first with monoatomic materials or materials with relatively close mass numbers (diamond, silicon, GaAs and InSb), and the second comprising binary materials with remote mass numbers of the elements (SiC, GaP, InP, InAs) with similar behaviours inside each group. The diamond is the hardest material from all considered here. A slow variation of the primary defect concentration has been found for pion irradiation of diamond, silicon, SiC, GaP and GaAs, in the whole energy range of interest, with less than 2 displacements/cm/unit of fluence. In contrast to these materials, there are others, characterised by a low CPD in the energy range up to 200 MeV, (which represents this way the upper limit of the energy range where their utilisation in pion field is recommended), followed by a pronounced increase of displacement concentration with energy to more than 8 displacements/cm/unit fluence for InSb.

It is to be mentioned that, in the present model hypothesis, for SiC, negligible differences have been found between different polytypes in what regards the effects of pion and proton degradation [16], conclusions in accord with the experimental results [17]. The behaviour of SiC in radiation fields is between the corresponding one of diamond and silicon.

As it is well known, the analysed semiconductors are possible materials for detectors and electronic devices which have to work long time in particle physics experiments, space applications, etc., in intense fields of hadrons, and in experimental configurations which impose high reliability of devices, and must present a controlled degradation of their parameters. As possible applications we will analyse two hypothetical cases: the utilisation of diamond, silicon, SiC or GaAs as detectors at the Large Hadron Collider (LHC) at CERN, and the long time exposure of the electronic devices in the field produced by cosmic rays.

For the LHC, the standard physics programme is based on the study of proton - proton interactions, at about 7 TeV beam energy, on an integrated luminosity of $5 \times 10^5$ pb$^{-1}$ which corresponds to 9 year of operation, for an annual operation time of $1.9 \times 10^7$ s. The irradiation background is continuous. The charged hadrons are produced in the primary interactions, while the neutrons
are albedo particles. The charged pions are the dominant particles, followed by protons, antiprotons and kaons. As an illustration of the above calculations for the degradation of different semiconductors in proton and pion fields, the results of the simulation of Gorfine and Taylor [18] have been chosen, for pion and proton fluxes in the inner detector assembly region, parallel to the beam axis. Both protons and pions are transported down to thermal energies in the detector, by nuclear interactions. The particle flux energy spectra have been simulated for a first layer of Si detectors (situated at 11.5 cm), and with complete moderator. The obtained spectra have been found to be slowly dependent on the material of the inner detector and so, in the present paper the same hadron spectra for diamond, silicon carbide, silicon and gallium arsenide have been utilised.

The convolution of the pion and proton spectra with the energy dependence of the CPD has been done in the energy range 50 MeV - 10 GeV, and 10 MeV - 10 GeV for pions and protons respectively. Below 50 MeV, a realistic estimation of materials degradation to pions is very difficult due to the lack of experimental data on pion-nucleus interaction and also to the increase of the weight of Coulomb interaction.

The results of these calculations are summarised in Fig. 4, for the diamond, silicon carbide, silicon and GaAs options, both for pion and proton degradation. In the analysed case, diamond and SiC are the hardest materials in both pion and proton fields; the diamond is harder to pions than to protons. The behaviour of silicon is similar in both particle fields. The GaAs option is not recommended because of an order of magnitude higher degradation in comparison with all other considered materials.

Another possible utilisation of semiconductor devices in radiation fields is related to space applications. In the primary cosmic radiation, the most abundant particles are the protons [5]. Other charged particles (for example $\pi^{+/-}$, $e^{+/-}$, $\mu^{+/-}$, $\nu_{\mu}$, etc.) are produced in the interaction of the primary cosmic rays in air. The damage induced in diamond, Si, SiC, GaAs and InP by the primary cosmic field has been estimated for protons in the energy range 10 MeV - 10 GeV, and the results are presented in Figure 5. The devices have been supposed to be exposed directly to the cosmic field. In this case too, diamond has been found to be the hardest material. GaAs and InP suffer a degradation of a factor of about 50 times higher in comparison with diamond and this behaviour can affect irreversibly the properties of these materials for long time operation.

The degradation produced by the particle field at LHC (pions and protons) and by the free protons from the primary cosmic rays respectively are of the same order of magnitude for each of the materials investigated.
4 Summary

A systematic theoretical study has been performed, investigating the interaction of charged hadrons with semiconductor materials and the mechanisms of defect creation by irradiation.

The nuclear stopping power has been found to be greater for heavier incident particles (protons compared to pions), and for lighter media. The position of its maximum is the same for protons and pions in the same medium.

The mechanisms of the primary interaction of the hadron with the nucleus (nuclei) of the semiconductor lattice have been explicitly modelled and the Lindhard theory of the partition between ionisation and displacements has been applied.

For protons, the low kinetic energy particles produce higher degradation in all materials.

For pions, the energy dependence of CPD presents two maxima, the relative importance of which depends on the target mass number: one in the region of the $\Delta_{33}$ resonance, more pronounced for light elements and compounds containing light elements, and another one around 1 GeV kinetic energy, more pronounced for heavy elements. At higher energies, an weak energy dependence is observed. A slow variation of the primary defect concentration has been found for pion irradiation of diamond, silicon, GaP and GaAs, in the whole energy range of interest, with less than 2 displacements/cm/unit of fluence. In contrast to this situation, for the other semiconductor materials analysed, a low CPD is estimated in the energy range up to 200 MeV (which represent the energy range up to their utilisation in pion field is recommended), followed by a pronounced increase of displacement concentration to more than 8 displacements/cm/unit of fluence at high energies.

The behaviour of this semiconductor materials has been analysed comparatively both in relation to particle physics experiments (inner part of the detection system at LHC) and to space applications (the devices being considered to be exposed directly to the cosmic ray field.

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Figure captions

Figure 1: The nuclear energy loss in diamond, silicon, silicon carbide, GaP, GaAs, InP, InAs and InSb as a function of the kinetic energy of the incident particle: protons (up) and pions (down) respectively.

Figure 2a: The concentration of primary defects on unit fluence (CPD) in diamond, silicon, SiC, GaAs and InP induced by protons, as a function of the kinetic energy and average mass number of the semiconductor material. The mesh surfaces are drawn only to guide the eye.

Figure 2b: The dependence of CPD as a function of proton kinetic energy, for the same semiconductors.

Figure 3a: The energy and material dependence of the CPD on unit pion fluence for diamond, Si, SiC, GaP, GaAs, InP, InAs and InSb. The mesh surfaces are drawn to guide the eyes.

Figure 3b: The CPD as a function of the kinetic energy of incident pions, for the same semiconductors.

Figure 4: Estimated CPD on unit fluence induced in diamond, silicon, SiC and GaAs, by the simulated flux energy spectra of pions and protons in the inner detector at LHC.

Figure 5: Estimated CPD on unit fluence induced by the primary cosmic ray flux energy spectra in diamond, Si, SiC, GaAs and InP (only the effects produced by protons are considered), in the hypothesis that these semiconductor materials are exposed directly in the radiation field.
The diagram shows the number of charged particles per square centimeter (CPD) for different materials: C, SiC, Si, and GaAs.

- **C** (Carbon) has a CPD of approximately $10^2$ for pions and $10^3$ for protons.
- **SiC** (Silicon Carbide) has a CPD of approximately $10^2$ for pions and $10^3$ for protons.
- **Si** (Silicon) has a CPD of approximately $10^3$ for pions and $10^4$ for protons.
- **GaAs** (Gallium Arsenide) has a CPD of approximately $10^4$ for pions and $10^4$ for protons.

The y-axis represents the CPD in units of [1/cm], ranging from $10^2$ to $10^4$. The x-axis indicates the different materials tested.
