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KINETICS OF DEFECTS IN LOW TEMPERATURE SEMICONDUCTOR DETECTORS AND DIRECT DARK MATTER SEARCH*

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Abstract. The calorimetric technique is a method used at the present time in several experiments in the search for different forms of dark matter, especially the existence of hypothetical Weakly Interacting Massive Particles or other candidates as neutrino, particles that satisfy the criteria to be non-baryonic, non-luminous and possibly non-relativistic. Usually, in several experiments, the simultaneous measurements of the ionization and phonon or light from scintillation signals are used in the identification of particles. Silicon and germanium crystals are used in some experiments, but the energy used in the production of defects in these materials is usually not considered in the energy balance of the processes and could represent a source of errors in particle identification. In this paper we investigate the kinetics of defects in cascade interaction processes at cryogenic temperatures, estimate the energetic cost of defect formation in the energy loss and predict the maximal errors in mass and energy identification for WIMPS and neutrinos respectively.

Key words: dark matter, WIMP, neutrino, low temperature, semiconductors, phonons, ionization, defects.

1. INTRODUCTION

Recent astrophysical and astronomical evidence indicates that only a small fraction of the matter in the Universe is composed of "ordinary" baryonic matter, while the dominant fraction has an unknown nature. This is the so-called "Dark Matter".

During last years, proofs of the possible presence of Dark Matter have been found coming from several and independent investigations in different fields of research. Theoretical independent predictions suggest that this unknown matter

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could be made of a generic class of particles called Weakly Interacting Massive Particles (WIMPs), relics of the Big Bang that still exist today, that should be stable, massive enough and weakly interacting. Alternatively, in a completely independent way, the supersymmetric extension of the Standard Model provides WIMPs as candidates in this sector of the model. Other candidates could be neutrinos, baryonic matter or other new hypothetical particles. The search for dark matter has become a very active research area in the last decades and new detectors or detection methods have been proposed.

The paper has three distinct sections. First, we analyse some general aspects of new calorimetry used in the search and the direct detection of some candidates for dark matter (WIMPS and neutrinos) and we discuss processes by which incident particles lose their energy in the calorimeter. Then, we review the types and characteristics of primary defects produced in silicon and germanium semiconductors, two current options for detectors. Because they operate in the temperature range of mK, we investigate the peculiarities of the processes, with emphasis to the production of defects and their time evolution. In the last part, we estimate the consequences for calorimetric detection in conditions where only ionization and phonons are simultaneously measured, the energetic cost of defect formation in the energy loss and we predict the maximal errors in mass and energy identification, for WIMPs and neutrinos, respectively.

2. PHYSICAL PROCESSES IN DETECTORS

2.1. CASCADE OF INTERACTIONS AND CALORIMETRY IN THE DETECTION OF DARK MATTER

After the interaction of a (dark or "ordinary" matter) particle with a nucleus the following processes occur: the recoiling nucleus loses its energy via collisions with neighbouring atoms in the crystal and with electrons. The recoil loses all energy which was transferred in the primary interaction and is finally stopped. In essence three classes of processes are produced: ionisation, displacements and phonons (heat). The amount of energy transferred to lattice nuclei in the creation of displacements and to the electronic system depends on the magnitude of the recoil energy, on the interatomic forces and crystal structure, and thus on the direction of the recoil. In the WIMP – nucleus interactions, with WIMPs from galaxies, their velocities are in the range of hundreds of km/s and thus recoil nuclei are nonrelativistic, with energies in the range of tens of keV. The neutrinos have energies of the order of MeV.

Both the energy deposited into defect creation and that transmitted as ionization could partially be transferred to the phonon system by defect annihilation and by recombination of electron-hole pairs. In fact, in calorimetric conditions the energy balance is:

$$E_{\text{recoil}} = E_{\text{ionization}} + E_{\text{phonon}} + E_{\text{stable defects}}. \quad (1)$$

The evaluation of the quantity of energy stored in "stable" defects, after the transitory regime, is a difficult task.

Phonons can be detected with methods of classical calorimetry. Calorimeters for low energy particles up to 1keV are used for the search and detection of cosmic neutrinos, WIMPs or other candidates of dark and non-luminous matter. In the last two decades this field of experimental physics has developed intensively and numerous projects are in progress. An important parameter in these experiments is the low detection threshold and one objective for all experiments is to decrease this threshold, because the successful detector of this type must, of course, have an energy threshold that is sufficiently low so that the small amount of energy deposited into the target by the dark matter particle could be detected.

In this type of detector the target crystal is a semiconductor, insulator, or possibly a superconductor at a temperature substantially below its transition temperature so that the number of free electrons is very small. We discuss the phonon physics associated with elementary particle interactions within silicon and germanium crystals at temperatures below 1 K.

This measurement technique provides discrimination between the expected signal of WIMPs and an electromagnetic background. Ionization and phonon signals measured simultaneously allow distinguishing both between electron and nucleon recoils and between nucleon (nucleus) recoil from ordinary matter and exotic type respectively. For detecting these rare events, it is important to utilise information from the prompt phonons (ballistics) that helps suppress backgrounds. The outputs of these sensors are recorded as a function of time. For ballistic phonons the times are in the order of ~ 2 ps/cm for Si. The spectrum and spatial distribution of these prompt phonons could be used to determine the event position, can provide discrimination between electron recoils versus nuclear recoils, and can provide information about the direction of the primary recoil in isotropic pure crystals. If these calorimetric measurements are performed at very low temperatures as in mK range and the specific heat capacity of the device is very small (the lattice contribution to the specific heat is proportional to T^3 at low temperatures), then this method could be used to detect individual particles [1].

2.2. PRIMARY DEFECTS IN SEMICONDUCTOR DETECTORS AT CRYOGENIC TEMPERATURES AND THEIR TIME EVOLUTION

The creation of displacements in silicon and germanium can be described in terms of primary interaction of the incoming particle with a nucleus placed in a site of the lattice, with the creation of the primary knock-on atom, to which an amount of energy has been transferred. If this energy surpasses a specific displacement threshold, E_d, the recoil is the source of a cascade of displacements. These displacements are vacancy-interstitial pairs, which could also be in the form of close (bounded) Frenkel pairs (FP). Another type of primary defect is the fourfolded coordination defect (FFCD) [2, 3, 4], which could also be interpreted as a metastable form of close FPs [5].

The main advantage of low temperature irradiation is that all processes are either frozen or slowed down.

In silicon, at sub-Kelvin irradiation, vacancies are frozen in, close FPs are stable and interstitials have athermal migration by the Bourgoin-Corbett mechanism [6], and have never been found experimentally. Single vacancies and impurity interstitials (as, e.g. Al_i, B_i) [7, 8], have been evidenced. The presence of radiation-produced FPs, stable at the irradiation temperature, has been detected by X-ray measurements on Si irradiated with fast electrons at liquid helium temperature [9]. These defects anneal out in the temperature range 10–70K [10].

The situation is different in germanium; the interstitial can be observed; information about the properties of isolated *I* and *V* in *Ge* has been obtained from experiment [11, 12], following low temperature electron irradiation. It seems that the Frenkel pair in *n*-type germanium could be frozen into the lattice at temperatures below 65K, and thus observed [13]. Germanium self-interstitials and probably vacancies disappear at around 200 K. In *p*-type germanium, the main defects observed are the single vacancy and the gallium interstitial.

In both materials, the interstitial could be found in the following configurations: hexagonal, tetrahedral, split, dumbbell and 'caged'. The stability of different configurations is discussed in relation with different charge states – see Ref. [14]. There is an agreement in the literature regarding the existence of the neutral, positive and double positive ones for both semiconductors. The enthalpies of formation of interstitials are also charge state dependent, and are around 3–4 eV in silicon [15], and in the range 3–6 eV in germanium [16], with a relatively good agreement between calculations and experiment.

The migration energies of interstitials are in silicon in the range 0.18–0.45 eV, depending again on the charge state [17], and 0.3 [5] – 0.7 [16] in germanium.

It has been established that in silicon the vacancy takes on five different charge states in the band gap: V^{2+}, V^{+}, V^{0}, V^{-}, and V^{2-}. Theoretical and experimental values for the formation enthalpy are both in the range $3 \div 4$ eV for silicon and germanium.

The Frenkel pairs are defects that conserve the number of particles, and the formation energy is less than the sum of an isolated vacancy and interstitial. In contrast to all these point defects, in the FFCD only two bonds are broken, the formation energy is lower in respect to previously mentioned defects, and the bond length and angles do not significantly deviate from their bulk values.

In order for a permanent defect to be produced from an initially perfect crystal lattice, the kinetic energy that it receives must obviously be larger than the formation energy of a Frenkel pair. However, while the Frenkel pair formation energies in crystals are typically around 5–10 eV, the average threshold displacement energies are much higher, in the order of 20 eV or higher. The reason for this apparent discrepancy is that the defect formation is a complex multi-body collision process (a small collision cascade) where the atom that receives recoil energy can also bounce back, or kick another atom back to its lattice site. Hence, even the minimum threshold displacement energy is clearly higher than the Frenkel pair formation energy. In fact, the displacement energy is the sum between the energy of formation of vacancy (ΔH_f^V) and interstitial (ΔH_f^I), and a quantity which goes to the lattice (E_L), consisting mostly in a bond-bending component [15]:

$$E_d = \Delta H_f^V + \Delta H_f^I + E_L \tag{2}$$

3. MODELLING DEFECT PRODUCTION IN CRYOGENIC DETECTORS AND RESULTS

Both particles of interest interact elastically with the nuclei of the target, and transmit an amount of energy to the primary knock-on atom.

The quantity of energy transferred in a single interaction is represented as a function of WIMP's mass for both Si and Ge targets in Fig. 1: continuous lines correspond to maximum energy transfer, while dashed ones to the energy transfer averaged over the possible directions of the recoil. The velocity of the WIMP was taken as 230 km/s.

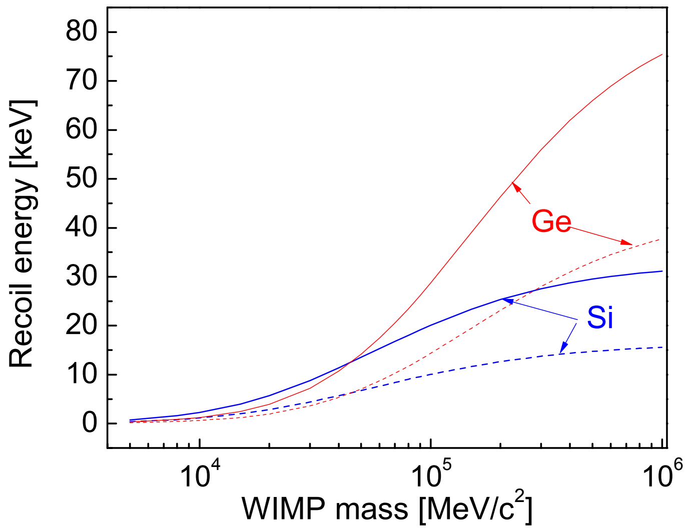

Fig. 1 – Maximum (continuous lines) and average (dashed lines) recoil energies in Si and Ge due to a WIMP interaction, as a function of WIMP's mass.

The average and maximum recoil energies were calculated also for the interaction of the neutrino in the same materials, and are represented in Fig. 2, as a function of the energy of the neutrino. One can see that at all energies less energy is transferred to Ge PKA than to the Si one.

The average number of displaced atoms in the cascade produced by a PKA of energy E has been estimated using the modified Kinchin-Pease displacement damage function [18, 19, 20].

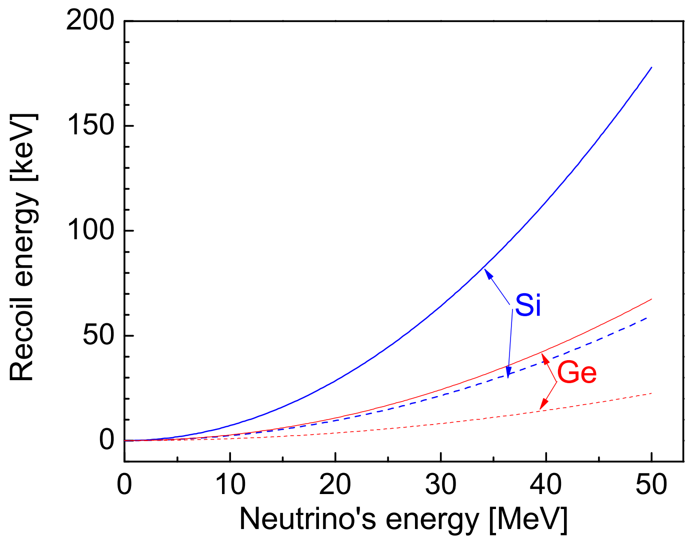

Fig. 2 – Recoil energy in Si and Ge due to a neutrino interaction, as a function of the neutrino's energy.

The basic assumptions used in its derivation are that the collisions in the cascade are binary, elastic and made between similar atoms (implying that if the energy is less than E_d, than there is no displaced atom, while atoms receiving energy between E_d and $2E_d$ are displaced from their lattice position, but do not contribute to any additional displacements due to subsequent collisions); a correction factor ξ is applied for PKA energies greater than $2E_d$, to account for the electronic stopping power of the material. Therefore, the displacement damage function is:

$$< N_d >= \begin{cases} 0 & E < E_d \\ 1 & E_d \le E < 2E_d \\ \dfrac{\xi E}{2E_d} & 2E_d \le E < E_c \;, \\ \dfrac{\xi E_c}{2E_d} & E \ge E_c \end{cases} \qquad (3)$$

where E_c is a cut-off energy, of the order of 28 keV for Si targets and 73 keV for Ge ones [21].

The numbers of vacancy-interstitial pairs created by a single WIMP elastic interaction in silicon and germanium lattices have been calculated, supposing threshold displacement energies of 21 [22] and 25 eV [23] respectively.

The number of displacements produced by a WIMP of 230 km/s, as a function of the mass of the WIMP, is represented in Fig. 3, for Si and Ge targets: continuous lines correspond to maximum energy transfer, while dashed ones to the energy transfer averaged over the possible directions of the recoil. The WIMP is supposed to undergo a single elastic interaction in the detector. The dotted lines in the right of the figure represent the maximum number of displacements, and correspond to an energy transfer equal to the cut-off energy E_C. It could be seen that for high masses of the WIMPs, the number of vacancy-interstitial pairs is higher in Ge; this is mainly due to the higher energy transferred to the lattice recoil in the elastic interaction. Equal energies transferred to silicon and germanium nuclei correspond to a WIMP mass of around 50 GeV/c^2. The process of creation of vacancy – interstitial pairs is the most energy consuming from the possible processes of production of primary defects mentioned above, and this is the reason it was considered here.

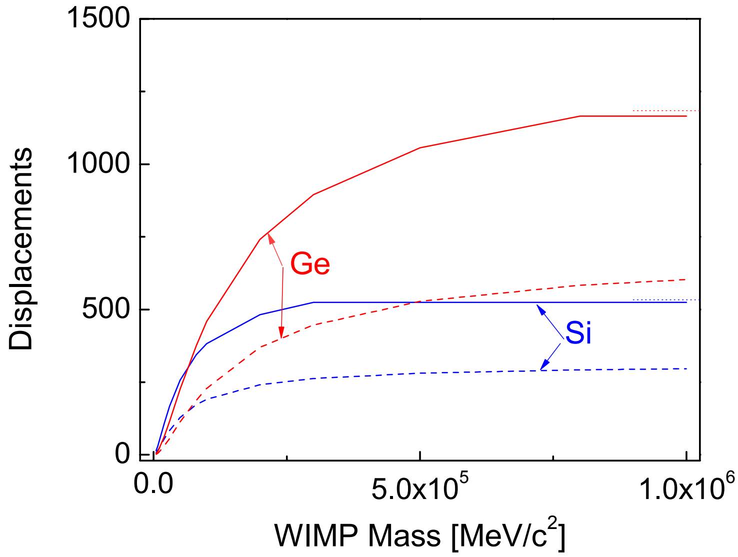

Fig. 3 – Displacement damage function in Si and Ge versus the mass of the WIMP. Continuous lines correspond to an energy transfer maximized over recoil's direction, and dashed ones to averages over the orientation of the recoil.

The displacement function related to the neutrino's interaction in the same targets: silicon and germanium, is represented in Fig. 4 as a function of the particle's energy. Again, it is supposed that the neutrino has a single interaction.

Neutrinos of the same energy produce more displacements in silicon than in Ge. Due to the higher energy transfer in Si, the cut-off energy E_c is attained in this energy range of the neutrino.

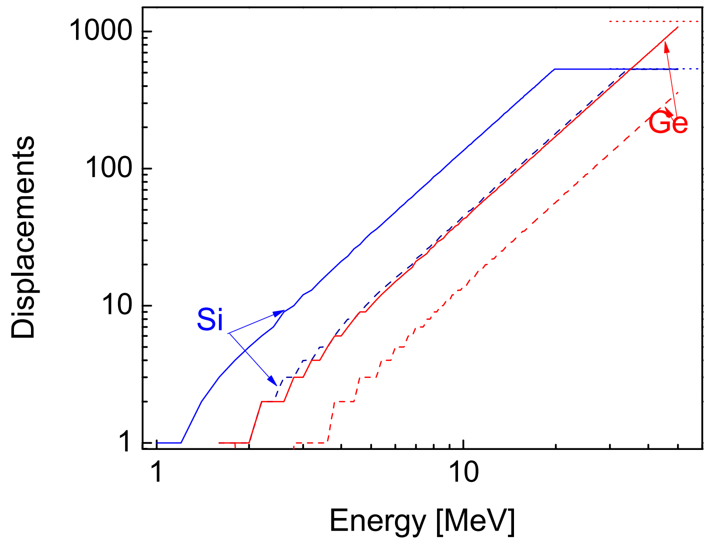

Fig. 4 – Displacement damage function in Si and Ge versus the neutrino's energy. Continuous lines correspond to maximum energy transferred and dashed ones to average energies.

In order to estimate the weight of the energy stored in these defects from the energy transferred to the recoil in the primary interaction, it is necessary first to estimate the survival rate of vacancy interstitial pairs, and then to calculate the energy in the defects as the sum of their formation energy over all defects. As underlined previously, the most energy consuming is the creation of vacancies and interstitials. Using the data from the literature on defect introduction rates after electron irradiation of silicon under 4K – see Ref [24] and references cited therein, one can estimate that around 80% of them do not recombine at sub-Kelvin temperatures.

Supposing that the modified Kinchin-Pease model reproduces correctly the production of defects, considering the same survival rate of defects in both silicon and germanium, and taking into consideration the energy balance (1), we estimate a maximal limit of around 12% of the recoil energy deposited into defects in silicon and 14% for Ge, independent of the incoming particle. This introduces an error in the mass identification of WIMPs considering the kinematics of the interaction up to 25% in silicon and up to 40% in germanium respectively. The corresponding error in the energy of the neutrino is 6% for Si and 7% for Ge.

4. SUMMARY AND POSSIBLE CONCLUSIONS

Silicon and germanium cryogenic detectors represent a current option in actual experiments which are searching for weakly interacting particles, possible component of the dark matter. In this paper we reviewed the mechanism of formation of defects at low temperature in these semiconductors, and also the primary defects produced by the displacement damage. We showed that a fraction of the energy of the PKA is stored in these defects, the other two components being the ionization and the phonons. This maximum weight is 12% and 14% from the energy of the PKA in silicon and germanium respectively. The corresponding maximum error for the mass of the WIMP is 25% in silicon and 40% in germanium, while the maximum error for the energy of the neutrino is 6% and 7% respectively in the two semiconductors.

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