

MODIFICATION OF LINDHARD ENERGY PARTITION FOR LOW ENERGY RECOILS IN GERMANIUM AND SILICON FOR DETECTORS DUE TO ELECTRON – PHONON COUPLING

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Abstract. One of the methods of direct detection of the massive component of dark matter is the registration of self-recoils in semiconductor detectors at cryogenic temperatures after the WIMPs scattering. In this contribution, after a short presentation of Lindhard curves, derived from the integro-differential equations of the general theory, we discuss the discrepancies between experimental data and theoretical predictions, as well as the corrections suggested in the literature. A new correction is proposed, which is due to the energy transfer between the electronic and atomic subsystems in the solid during the transient phenomena following the primary interaction, and some numerical results are presented.

Key words: energy partition, Lindhard theory, detectors, semiconductors, electron phonon coupling, cryogenic temperature, direct detection of dark matter.

1. INTRODUCTION

The interest in the thematic of the electron – phonon coupling in semiconductors in the last years is related to searches for dark matter using bolometric detectors at cryogenic temperatures. Starting from the fact that the most important part of dark matter in the universe is non-baryonic, non-luminous and non-relativistic, direct search for dark matter is a very active research field. The weakly interacting massive particles (WIMPs) predicted by super symmetric theories are characterized only by weak and gravitational interaction. The principle on which their direct detection is based is the scattering of the target atoms following the primary binary interaction of a WIMP with a target atom. Consequently, the detection of low energy recoils is of interest. At the present time, there are more ongoing experiments, which use Ge or Si detectors operating in these conditions [1, 2].

The partition of the energy of recoils in Si and Ge targets into energy ultimately transferred to the electrons and energy transferred to atoms depends on the relative values of the interaction cross sections characterizing these processes.

The most general formalism has been proposed by Lindhard and co-workers in 1963 [3] who have formulated an integro-differential equation. Based on different approximations, average values are calculated.

Experimental measurements of the energy which goes into electronic excitation started to be reported two years later, both for Ge [4] and Si [5]. The results were obtained through the measurement of the ionization produced by prompt Si recoil atoms resulting from monoenergetic neutron bombardment of germanium / silicon solid-state detectors, observed in a pulse height analyzer.

A resurgence of interest for such measurements was brought by direct dark matter searches, and new data were recently reported, especially for Ge [6, 7]. The region of low energy recoils, under 10 keV kinetic energy, is under study, both theoretically and experimentally.

After introducing Lindhard curves, as derived from the integro-differential equations, we shall shortly present the deviations of last experimental findings from these curves. We shall then review models proposed to correct Lindhard theory in the energy region of interest, and eventually propose a new correction, due to the energy transfer between the electronic and atomic subsystems in the solid during the transient phenomena following the primary interaction.

2. LINDHARD THEORY AND ENERGY PARTITION AT LOW ENERGY

The theoretical study of radiation effects can be performed using different types of methods, from transport theories relating the rate of change of the density of particles in an element of space, velocity, and time to integrals over scattering events occurring in other elements [3, 8, 9, 10], to simulations which use atomistic numerical models which start from classical mechanics and follow out the consequences of introducing an energetic atom into an assembly of initially stationary ones [11, 12].

The first step in producing radiation effects is the generation of a primary recoil atom (PKA, primary knock-on atom). This is the self-recoil in which we are interested, and which results, for example, from the binary collision of a WIMP with an atom in the target. It dissipates its initial kinetic energy in two types of processes: excitation of the electrons of the target that may lead to ionization of some of the particles, and elastic collisions with atoms of the target. The individual electron excitation energies are small and electrons carry a small momentum, and consequently they can be ignored in collision dynamics, and the events are said to be quasielastic [13]. Atoms with which the primary recoil collides can receive enough kinetic energy to displace them from their lattice sites to make similar collisions of their own. A collision cascade is so produced.

The treatment of atomic collisions is based in Lindhard theory on the Thomas-Fermi theory of atoms [14, 15]. Under a series of approximations, an

integro-differential equation is derived, for the total energy given to atoms by a self-recoil of kinetic energy E which is stopped into the target. The theory is completely scalable from material to material by using dimensionless (reduced) variables for energy, distance and time. In the case when the particle which stops is a particle of the medium (selfrecoil), the reduced variables are defined as:

$$\begin{aligned}\varepsilon &= E / E_L, \quad \text{with } E_L = \frac{2Z^2 e^2}{a_{12}}, \\ \rho &= x / R_L, \quad \text{with } R_L = \frac{1}{n\pi a_{12}^2}, \\ \tau &= t / T_L, \quad \text{with } T_L = \left(\frac{M}{2E_L} \right)^{1/2} R_L,\end{aligned}\tag{1}$$

where Z and M are atomic number and mass, e is the electron charge ($e^2 = 1.4399 \text{ eV} \times \text{nm}$), n is the atomic density of the target, and a_{12} is a screening length used in the Thomas-Fermi description of the atoms:

$$a_{12} = \left(\frac{9\pi^2}{128} \right) \frac{a_B}{(2Z^{2/3})^{1/2}},\tag{2}$$

with $a_B = 52.92 \text{ pm}$ being the Bohr radius.

In Lindhard theory, the electronic stopping power, in dimensionless variables, for projectiles with the velocity below Bohr velocity in the material ($v < \frac{e^2}{h} Z^{2/3}$) is:

$$\left(\frac{d\varepsilon}{d\rho} \right)_{el} = k_L \varepsilon^{1/2},\tag{3}$$

where:

$$k_L = \frac{32}{3\pi} \left(\frac{m_e}{M} \right)^{1/2} 2^{3/4} Z^{2/3}\tag{4}$$

and with m_e the electron mass. The nuclear stopping power considered is the Thomas Fermi one.

In the approximations considered, the integro-differential equation for the energy transferred to the atomic system, ν , is the following:

$$\left(\frac{d\varepsilon}{d\rho} \right)_{el} \nu'(\varepsilon) = \int_0^{\varepsilon^2} \frac{dt}{2t^{3/2}} f(t^{1/2}) \left[\nu\left(\varepsilon - \frac{t}{\varepsilon}\right) - \nu(\varepsilon) + \nu\left(\frac{t}{\varepsilon}\right) \right],\tag{5}$$

with $f(t^{1/2})$ the Thomas-Fermi function. Numerical solutions for the above integro-differential equations are presented in the original article for $k_L = 0.10, 0.15$ and 0.20 .

From the analysis of these numerical solutions, an analytic approximate dependence for $\nu(\varepsilon)$ has been derived, which transferred into usual variables reads:

$$E_{at} = \frac{E}{1 + k_L g(E/E_L)}, \quad (6)$$

where E_{at} is the energy ultimately transferred to the atomic system, and for the function g one can use the approximation [16]:

$$g(\varepsilon) = \varepsilon + 0.40244\varepsilon^{3/4} + 3.4008\varepsilon^{1/6}. \quad (7)$$

In Ge, for energies of the selfrecoil less than 2 keV, experimental data [6,7] show a deviation from the Lindhard curves so that the energy eventually given to the electronic system is higher than that predicted by Lindhard theory. The same trend appears for Si, for selfrecoil energies lower than 10 keV [17].

In order to assign the discrepancies between the measured values and the calculated ones, one must first revisit the calculations. A major problem is the accuracy of electronic and nuclear stopping powers for low energy recoils.

In this energy range, the nuclear stopping power based on Thomas-Fermi potential is overestimated (see [18] and also sputtering data).

Tilinin [19] argued that for $\varepsilon \ll 1$ the electronic stopping power decreases more rapidly than $\varepsilon^{1/2}$, fact which implies that a factor of up to 3 in respect to the curves calculated in the frame of Lindhard theory could appear. Arista and co-workers underlined the impact parameter dependence of the electronic stopping power [20, 21], *i.e.* of its angular dependence.

3. TRANSIENT PHENOMENA

Lindhard theory describes the partition of the energy imparted by the particle passing through a material, here a selfrecoil, to the electronic and atomic subsystems.

In fact, in spreading the primary recoil energy over a small region of crystal, a local heating effect is produced. Such regions have been considered first by Seitz [22] and Brinkman [23], who named them 'thermal spikes' or 'displacement spikes' according to whether displaced atoms accompanied the heating effect. For a given energy of the selfrecoil, in most cases it transfers energy predominantly by collisions with electrons or atoms as a whole. So, the regime of high electronic

energy loss has been treated in the frame of the thermal spike model in order to explain the track of the ion as due to the modifications of the structural characteristics of the material in metals [24], insulators [25] and semiconductors [26].

The spike model with two heat sources, one from the ionizing energy loss the other from nuclear energy loss, developed by the authors [27, 28, 29], is suitable for energy ranges of selfrecoils where nuclear and electronic energy losses are comparable.

In this model, considering the phenomena of interaction of the primary selfrecoil with the atoms and electrons of the target taking place in a thickness Δx (with the limit dx), perpendicular on the trajectory of the selfrecoil, and considering a cylindrical geometry, the time and space dependencies of the temperatures of the electronic and atomic systems near the track of the selfrecoil are calculated as solutions of the coupled differential equations:

$$\begin{aligned} C_e(T_e) \frac{\partial T_e}{\partial t} &= \frac{1}{r} \frac{\partial}{\partial t} \left[r K_e(T_e) \frac{\partial T_e}{\partial r} \right] - g(T_e^p - T_a^p) + A(r, t), \\ C_a(T_a) \frac{\partial T_a}{\partial t} &= \frac{1}{r} \frac{\partial}{\partial t} \left[r K_a(T_a) \frac{\partial T_a}{\partial r} \right] - g(T_a^p - T_e^p) + B(r, t), \end{aligned} \quad (8)$$

where C_e , C_a are the heat capacities of electronic and atomic systems, K_e , K_a are their corresponding thermal diffusivities, the coupling is given by the term $g(T_e^p - T_a^p)$ with $p = 1$ at RT, and $p = 5$ [30] or 6 [31] at very low temperatures, and the sources satisfy the conservation laws:

$$\begin{aligned} \int_0^\infty dt \int_0^\infty 2\pi r A(r, t) dr &= S_e, \\ \int_0^\infty dt \int_0^\infty 2\pi r B(r, t) dr &= S_n, \end{aligned} \quad (9)$$

with S_e , S_n – electronic and nuclear stopping powers respectively.

During the rise and fall of the thermal spike, the two subsystems (atomic and electronic) exchange energy through the electron-phonon coupling. This energy flows in different points in space, and at different times, either from the atomic toward the electronic subsystems, or reversely, depending on the sign of the difference $(T_a - T_e)$.

The energy eventually exchanged between the two subsystems along the whole range of the selfrecoil is found by integrating the exchange term first on the time and plane in which the thermal spike develops, and then on the whole trajectory of the selfrecoil, up to its stop:

$$E_{ex} = \int_0^R dx \int_0^\infty dt \int_0^\infty 2\pi r g(T_e^p - T_a^p) dr, \quad (10)$$

where E_{ex} represents the energy exchanged between the subsystems, and R the range of the selfrecoil.

The solution of the system of coupled differential equations, and consequently the time and space distribution of the coupling term $g(T_e^p - T_a^p)$ depends strongly on the temperature dependencies of the material parameters, and also on the relative magnitudes of the electronic and nuclear stopping powers.

For Si and Ge, while the temperature dependencies of the atomic heat capacities and thermal conductivities are well known from experimental measurements reported in the literature, for the electronic heat capacities there are only few data for cryogenic temperatures (see Refs. [32, 33] and [34, 35, 36] for Si and Ge respectively), and only theoretical considerations for the rest [37, 38]. It is known that in semiconductors the heat capacities of the electronic and atomic subsystems are of the same order of magnitude only at cryogenic temperatures. In what regards thermal conductivities, always that corresponding to the electronic subsystem is much lower, and it becomes comparable to the atomic heat capacity only at high temperatures, in the order of some hundreds degrees Kelvin. Due to this fact, the temperature rise in the electronic subsystem is much higher, and consequently the energy transfer is predominantly from the electronic toward the atomic one.

In what regards the stopping powers in Si and Ge, the maxima of the nuclear ones correspond to about 15 keV and 95 keV, and the maxima of electronic ones correspond to about 25 MeV and 155 MeV respectively; the equality of nuclear and electronic stopping powers correspond to the energies of the selfrecoils of 75 keV and 1.4 MeV respectively [11, 39]. Consequently, due mainly to the different atomic masses, the regimes of low and high energies have different extensions in the two semiconductors.

To illustrate the exchange of energy between the two subsystems, we present in Figs. 1 and 2 the space and time distribution of the difference $(T_a - T_e)$ produced by selfrecoils of energy 100 eV and 1 MeV in Si with initial temperature 3 K and 300 K respectively. In both cases, the development of the spike produces an important increase of the electronic temperature, which lasts less in time and space than the peak of the atomic temperature, which has a lower increase, due to the fact that both the heat capacity and the thermal conductivity of the atomic subsystem are much higher, but it extends more in space and time. The final heat transfer between these subsystems has opposite directions in the two cases illustrated here. In order to make clear these ideas, in both cases we represented together with the time and space distribution of the difference $(T_a - T_e)$ the contour plots of this temperature difference.

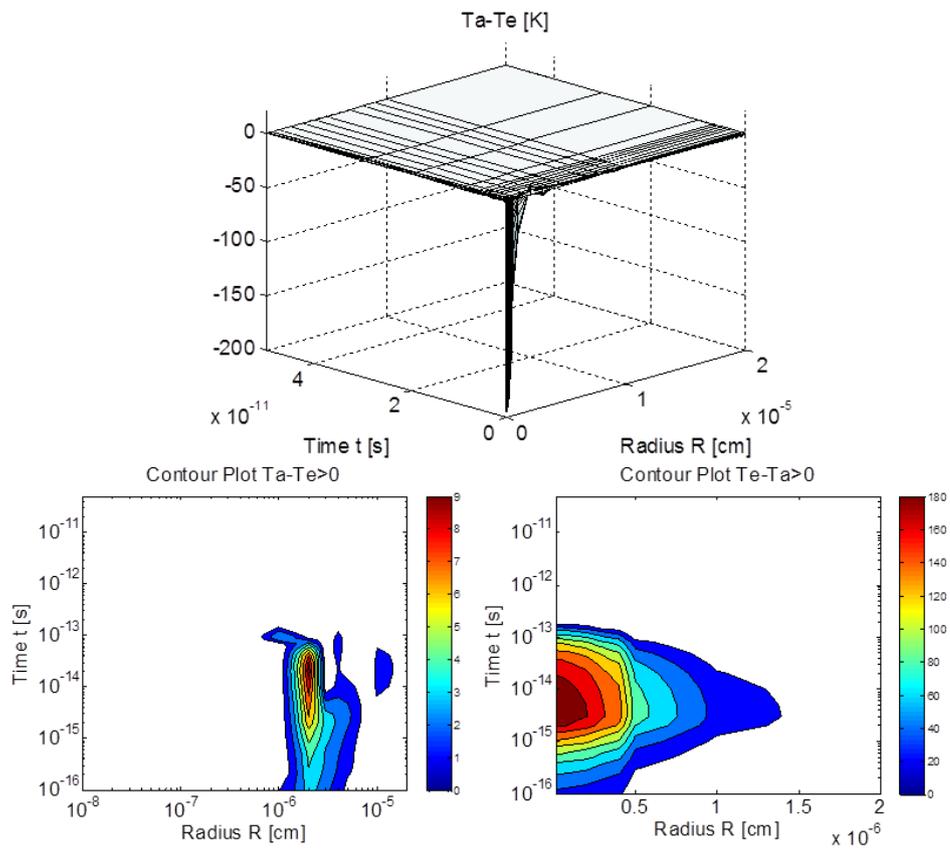


Fig. 1 – Space and time distribution of the difference ($T_a - T_e$) produced by a selfrecoil of energy 100 eV in Si with initial temperature 3 K.

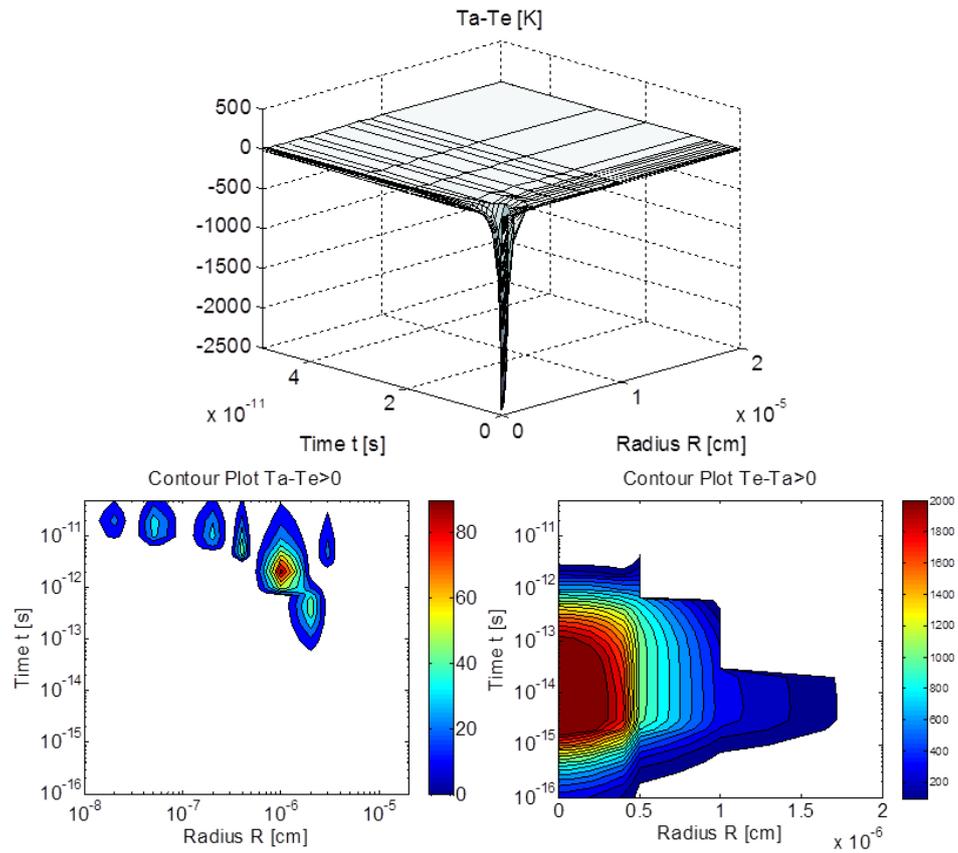


Fig. 2 – Space and time distribution of the difference $(T_a - T_e)$ produced by a selfrecoil of energy 1 MeV in Si with initial temperature 300 K.

A similar situation exists for Ge, where the energy exchanged between the subsystems has different signs depending on the energy of the selfrecoil and on the initial temperature.

4. SUMMARY AND CONCLUSIONS

Starting from the discrepancies in the energy partition of selfrecoils as energy ultimately transferred to atomic and electronic subsystems in Si and Ge between theory predictions and experimental data we propose here the consideration of the transient effects taking place during and after the intimate process of energy transfer.

Thermal effects are treated in the frame of a thermal spike model with two sources, related to atomic and electronic stopping powers.

We put in evidence the fact that the energy transfer can take place in both directions, and this depends on the relative values of the heat capacities and thermal conductivities of the electronic and atomic subsystems at the temperature of interest, as well as on the relative values of the stopping powers. At low energies of recoils and at cryogenic temperatures, the atomic subsystem transfers energy to the electronic one in the transient processes.

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