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MODEL OF ENERGY EXCHANGE THROUGH ELECTRON-PHONON COUPLING DURING TRANSIENT PHENOMENA IN MATERIALS FOR DETECTORS

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Abstract. The direct detection of dark matter candidates, for which semiconductor materials are used, is based on the detection of low energy selfrecoils. We show that the corrections to the energy partition curves due to the energy exchange during the transient processes modify the predictions of the standard Lindhard theory. These effects, calculated in the frame of a new model developed by the authors, depend on the initial temperature at which the detector operates, and on the energy of the recoil. Most of the available experimental data accumulated during more than fifty years support these results.

Key words: direct dark matter detection, nuclear recoil, low energy, ionisation, transient thermal effects.

1. INTRODUCTION

Currently, our understanding of the observable universe is based on the standard model of cosmology. Cosmological observations in the frame of different experiments including the measure of abundance of primordial elements, precise mapping of anisotropies in the cosmic microwave background, distribution of matter on different scales, are made in order to validate or invalidate it. At present we know that the universe is spatially flat, and is composed of 5% atoms, 27% dark matter and 68% dark energy [1]. An important challenge for astroparticle and particle physics is the understanding of the nature of dark matter: new particles with masses and cross sections characteristic to the electroweak scale are proposed as a possible solution. A generic class of dark matter candidates is represented by the weakly interacting massive particles (WIMPs); it is supposed that they would have been in thermal equilibrium with quarks and leptons in the hot early universe, and decoupled when they were non-relativistic [2]. WIMPs with masses around the

TeV scale are within reach of high-energy colliders and of direct and indirect dark matter searches [3].

Direct detection of WIMPs is based on their elastic collisions with atomic nuclei in low-background detectors [4]. So, the detection of WIMPs comes to the detection of low energy recoils, and consequently detectors with low threshold are of interest. On the other hand, detectors with low radioactivity and active background rejection must be used, as the estimated event rates are low.

Presently, for detecting WIMPs one must detect phonons (heat) or charge (ionization) or light (scintillation), or must detect simultaneously two quantities: heat and ionization, heat and scintillation or scintillation and ionization.

The materials used for direct dark matter detection cover standard scintillators (NaI, CsI), oxides (Al_2O_3, $CaWO_4$), semiconductors (Ge and Si), noble gases in liquid or gas state (Xe and Ar), as well as compounds containing C, Cl, F, I, Br.

The main difficulties in the reconstruction of the low energy recoils in Ge and Si from measured ionization and heat signals are related to background rejection, to cryogenic temperatures and also to the knowledge of energy partition between ionization and atomic motion fist discussed by Lindhard *et al.* [5]. An important aspect is related to defect formation in these detectors [6]. The knowledge of energy loss sharing of low energy recoils in Ge and Si between ionization and atomic motion is mandatory for a correct understanding of the response of detectors to the WIMP – target atom elastic interaction, and therefore for WIMPs correct characterization. On the one hand, measurements are difficult to be performed in the range around 1 keV selfrecoil kinetic energy, and the sets of data reported disagree to a large amount. On the other hand, the calculation of the Lindhard partition for low energy recoils rises a number of problems [7], related to the accuracy of the electronic and nuclear stopping powers, and also to the problem Lindhard himself mentioned, that the discussion of very low energies must be made separately, being somehow at the limit of applicability of the hypotheses used in the derivation of the integro-differential equations governing energy partition.

In the present paper, we will discuss the energy partition of slow selfrecoils in Si and Ge from a quite different point of view, of the energy exchanged between the electronic and atomic subsystem in the semiconductor during the transient phenomena that follow the primary interaction WIMP – target atom. These phenomena are treated in the frame of the thermal spike model [8]. In the next section, the methodology of calculating the energy exchanged between the two subsystems during the slowing down of the primary recoil produced by the WIMP is given, and the results for the linear energy exchanged both for Si and Ge are presented. These results are used in the section 3 for correcting Lindhard curves, in respect to the original calculations presented in Ref. [5], and are compared with the data reported in the literature for the energy partition.

2. ENERGY EXCHANGE DURING TRANSIENT PROCESSES

The equations governing the development of the thermal spike [8–11]:

$$\begin{aligned} C_e(T_e)\frac{\partial T_e}{\partial t} &= \frac{1}{r}\frac{\partial}{\partial r}\left[rK_e(T_e)\frac{\partial T_e}{\partial r}\right] - g(T_e - T_a) + A(r,t) \\ C_a(T_a)\frac{\partial T_a}{\partial t} &= \frac{1}{r}\frac{\partial}{\partial r}\left[rK_a(T_a)\frac{\partial T_a}{\partial r}\right] - g(T_a - T_e) + B(r,t) \end{aligned} \tag{1}$$

describe the space and time dependence of the electronic and atomic temperatures $T_{e(a)}$, as a function of the temperature dependencies of the parameters of the electronic and atomic systems (specific heats $C_{e(a)}$, and thermal conductivities $K_{e(a)}$), of the electron-phonon coupling coefficient g and also on the electronic and nuclear energy losses, $(\mathrm{d}E/\mathrm{d}x)$ and $(\mathrm{d}E/\mathrm{d}x)_n$, which enter in the expressions of the sources $A(r,t)$ and $B(r,t)$:

$$\begin{aligned} \int_0^\infty \mathrm{d}t \int_0^\infty 2\pi r A(r,t)\,\mathrm{d}r &= \left(\frac{\mathrm{d}E}{\mathrm{d}x}\right)_{el} \\ \int_0^\infty \mathrm{d}t \int_0^\infty 2\pi r B(r,t)\,\mathrm{d}r &= \left(\frac{\mathrm{d}E}{\mathrm{d}x}\right)_{n}. \end{aligned} \tag{2}$$

The term:

$$\frac{\mathrm{d}E_{ex}}{\mathrm{d}x} = \int_0^\infty \mathrm{d}t \int_0^\infty 2\pi r g(T_a - T_e)\,\mathrm{d}r \tag{3}$$

is the linear energy exchanged between the two subsystems, *i.e*. the energy exchanged in a thin layer, perpendicular to the recoil trajectory, in accordance to the hypotheses under which the model of the thermal spike is developed [8]. The integral of this term over the recoil range is the total energy exchanged:

$$E_{ex} = \int_0^R \frac{\mathrm{d}E_{ex}}{\mathrm{d}x}\,\mathrm{d}x. \tag{4}$$

There are two classes of problems related to the evaluation of the energy exchanged, as a function on the starting temperature of the detector and on the kinetic energy of the recoil. The first is related to the knowledge of the parameters of the atomic and electronic subsystems, while the second is a problem of convergence in the computations of T_a and T_e as solutions of the system of partial differential equations (1), and then in the integral (3).

While the specific heats and thermal conductivities of the lattice are well known from experimental measurements in the whole range of temperatures, from

cryogenic temperature up to the melting point (see Ref. [12] and references cited therein), the physical quantities characterising the electronic subsystem are known only at cryogenic temperatures from experiments, while for the rest of temperatures of interest there are theoretical dependencies, obtained from the analogy with the electronic system in metals, and experimental data for $T < 1$K. As there are a lot of possibilities, we investigated the sensitivity of the solution of the system of partial differential equations to $C_e(T_e)$ and $K_e(T_e)$, and we found that there is a high sensitivity in respect to $C_e(T_e)$.

Silicon. The numerical integration of the solutions of eqs. (1) in eq. (3) was made using Mathematica, and the difficulty is the slow convergence, due to the very sharp dependence of $(T_e–T_a)$ both in time and in distance. Thus, the error estimated for the integral is relatively high.

By choosing $C_e(T_e) = 3 \times 10^{-6} T_e$, we have found the dependencies of $dE_{ex}/dx(E)$ at different starting temperatures (working temperatures of the detector) shown in Fig. 1.

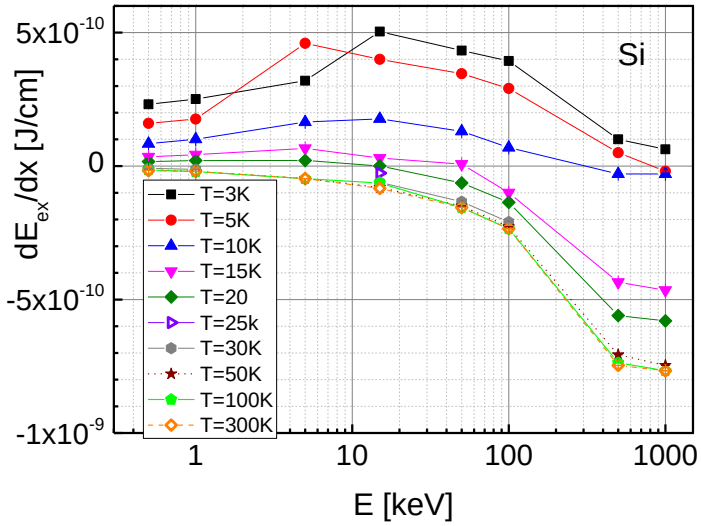

Fig. 1 – Linear energy exchanged by a Si selfrecoil as a function of its kinetic energy.

In this graph, the energy transferred from the atomic toward the electronic subsystems is positive, and the energy transferred from the electronic system to the atomic one is negative. One can see that the increase of the starting temperature favours the transfer from electronic toward atomic system, and the same is true for the increase of the kinetic energy of the recoil. On contrary, at very low temperatures and low kinetic energy of selfrecoils, the energy flows from the atomic toward the electronic system. One can also observe that with the increase of

the temperature, the curves move to lower values of dE_{ex}/dx, but the displacement decreases with increase of temperature, and the curves crowd toward the 300 K curve.

Germanium. In Ge, the numerical integration in (3) converges even slower in respect to the situation for Si, and the accuracy of the computation is relatively bad. The errors estimated for the integral are high. The results for the energy dependence of dE_{ex}/dx at different temperatures are plotted in Fig. 2.

The dependence of $dE_{ex}/dx(E)$ has the same trend for Ge as for Si: the transfer in predominantly from the electronic toward the atomic system at high temperatures or high recoil energies, and has the reverse sign for low temperatures and low kinetic energies of selfrecoils.

The comparison between Ge and Si reveals that in Ge the errors associated with the calculations are much higher, and that the values of energy flow from atomic toward electronic system are lower. In both Si and Ge, at the lowest temperatures ($T < 20$ K) the curve dE_{ex}/dx has a small maximum, while for higher temperatures there is a monotonic decrease. In Si, at energies higher than 500 keV a plateau is reached. The increase of the temperature produces lower and lower shifts of the curves, as in the case of Si.

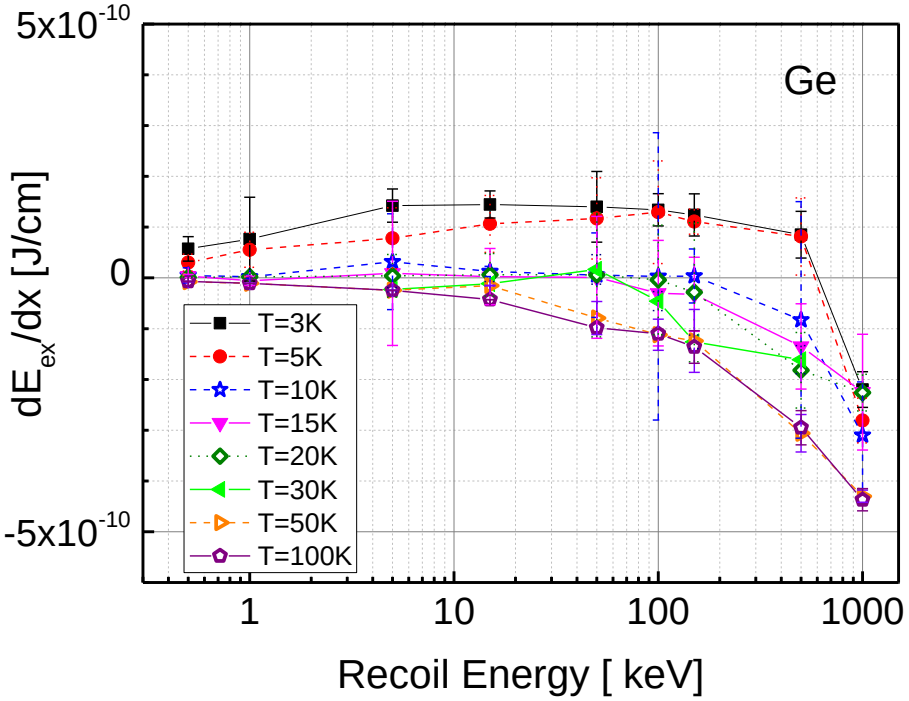

Fig. 2 – Linear energy exchanged by a Ge selfrecoil as a function of its kinetic energy.

3. LINDHARD CURVES AND CORRECTIONS DUE TO THE ENERGY EXCHANGED IN TRANSIENT PROCESSES

The curves representing the fraction of the energy of the selfrecoil ultimately transferred to electrons are given in Figs. 3 and 4 as dashed lines, for Si and Ge respectively, and were calculated under the following hypotheses [5]:

– the nuclear stopping cross section is based on the Thomas-Fermi potential;

– the electronic stopping cross section is proportional to the velocity for velocities of the selfrecoil lower than the corresponding Bohr velocity;

– electrons do not produce recoil atoms;

– the atomic binding energy is neglected (*);

– the energy transferred to electrons is neglected (*);

– nuclear and electronic collisions are separated;

– the energy transferred to nuclei is smaller than the energy of the selfrecoil for which we calculate the partition.

The hypotheses with (*) correspond to not too low energies of selfrecoils.

Different authors reported measurements for the energy partition in both Si and Ge. The data were measured on a time span of fifty years. The measurements were performed at different temperatures from room temperature up to cryogenic temperatures, and using different methods. Compilations of published data are presented in Figs. 3 and 4 for Si and Ge respectively, superposed on the calculated curves. In the last years, related to the searches for WIMPs, the region corresponding to low energy recoils (less than 1 keV) and cryogenic temperatures became of much interest.

In the case of Si, the data reported in Refs. [13–16] were used. The major problem in the interpretation of the data is the lack of complete information on the properties of the material (as doping concentration and, correlated, concentration of free charge carriers) and also measurement temperature. When available, measurement temperatures were indicated in the legends of the graphs. In respect to the calculated Lindhard curve, corresponding to the numerical result of the integro-differential equation, most of the data are situated below.

By integrating the linear energy exchange along the selfrecoil path up to its stop, one calculates the total energy exchanged between the two subsystems. From the data presented in Fig. 3, it is evident the highest transfer from atomic to electronic system corresponds to 3K, and that the maximum transfer in reverse direction is for 300 K. With these maximum values, we calculated the maximum corrections to the Lindhard curves, which are also represented in Fig. 3 as shadowed areas. As can be seen, most of the data reported for low energy Si selfrecoils enter in the shadowed area. As remarked before, a general trend of the data is that they are generally situated under the curve, fact that can be attributed to the energy transferred by the electronic system to the atomic one, at temperatures above LN_2 one.

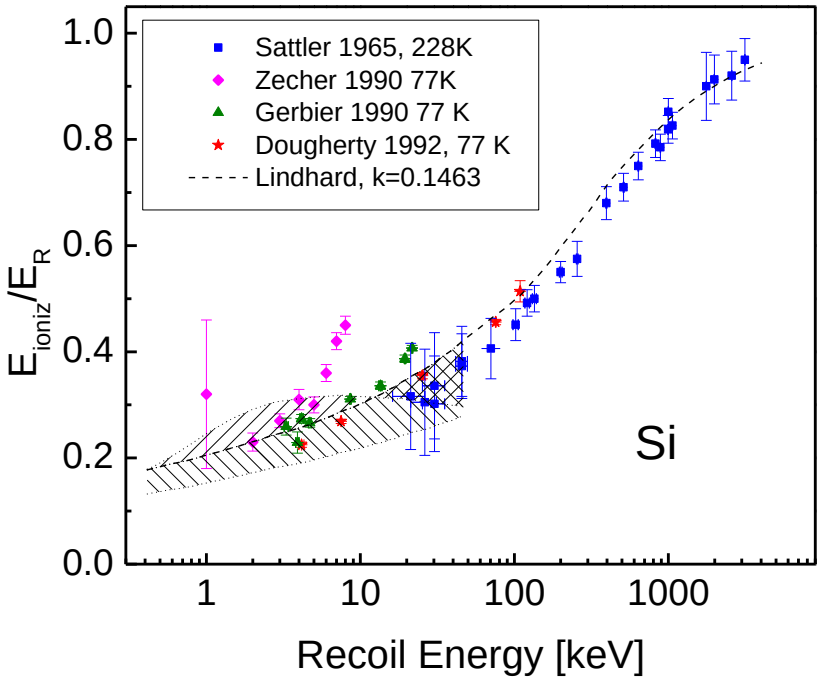

Fig. 3 – Dependence of energy partition on recoil energy for Si.

A similar situation exists for Ge. The data from Refs. [17–27] were used and are represented in Fig. 4. The filled symbols are associated with temperatures higher than LN_2, while the empty ones are associated with low temperatures. As one can see, for energies of the selfrecoil less than 2 keV experimental data 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.

We evaluated the energy transfer between the two subsystems. Similarly to Si, the direction of energy flow is reversed by increasing the temperature. The corrected Lindhard curves are also represented in Fig. 4.

We would like to emphasise that the upper borders of the shadowed regions depend on the parameters of the electronic system, both in Si and Ge. In the case of Si, using the mentioned dependences $C_e(T_e)$ and $K_e(T_e)$, the correction to the Lindhard curve corresponding to the energy exchanged at 3 K has a maximum at about 3 keV kinetic energy of the selfrecoil, decreases and passes through zero, changing then sign. The change of sign means that, even at 3 K, with the mentioned parameters of the electronic system, there is no transfer from the atomic to the electronic system in Si.

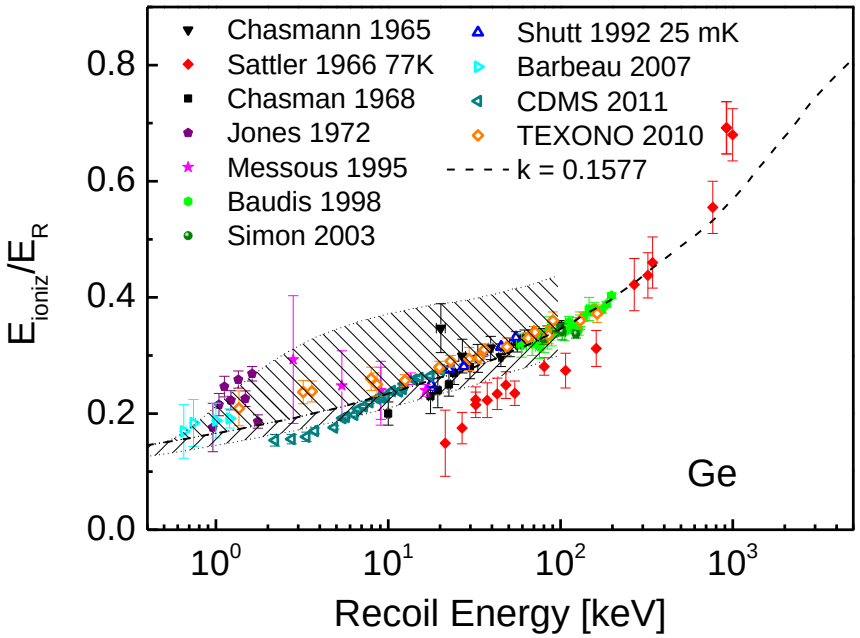

Fig. 4 – Dependence of energy partition on recoil energy for Ge.

4. SUMMARY AND CONCLUSIONS

The energy exchange between electronic and nuclear subsystems in Si and Ge, associated to the transient phenomena related to the slowing down of selfrecoils following the primary interaction, are analysed in the frame of a model previously developed by the authors. The kinetic energy of the selfrecoil is partitioned between ionization and atomic motion, and the subsystems exchange energy due to electron-phonon coupling. We showed that for low energy of selfrecoils, both directions of the energy flow between electronic and atomic subsystems are possible, and this depends mainly on the initial temperature of the target (detector).

These new results present a particular interest for astroparticle experiments searching for WIMPs, where low energy selfrecoils are at the base of the detection processes.

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REFERENCES

1. P.A.R. Ade *et al.*, Planck 2015 Results, XIII, Cosmological parameters. arXiv:1502.01589.
2. B.W. Lee, S. Weinberg, Phys. Rev. Lett. **39**, 165–168 (1977).
3. G. Bertone, D. Hooper, J. Silk, Phys. Rept. **405**, 279 – 390 (2005).
4. M.W. Goodman, E. Witten, Phys. Rev. D **31**, 3059 – 3063 (1985).
5. J. Lindhard, V. Nielsen, M. Scharff, P. Thomsen, Mat. Fys. Medd. Dan. Vid. Selsk., **33**, 10 (1963).
6. I. Lazanu, M.L. Ciurea, I. Lazanu, Astroparticle Phys. **44**, 9 – 14 (2013).
7. S. Lazanu, I. Lazanu, *Modifications on Lindhard energy partition for low energy recoils in Ge and Si for detectors due to electron-phonon coupling*, Rom. Rep. Phys. **68**, 594–603 (2016).
8. I. Lazanu, S. Lazanu, Nucl. Instrum. Meth. B **268,** 2241 – 2245 (2010).
9. I. Lazanu, S. Lazanu, Rom. Rep. Phys. **63**, 707 – 716 (2011).
10. I. Lazanu, S. Lazanu, Rom. Rep. Phys. **66**, 963 – 972 (2014).
11. I. Lazanu, S. Lazanu, JCAP **07**, 013 (2011).
12. I. Lazanu, S. Lazanu, *Contribution of the electron–phonon coupling to Lindhard partition at low energy in Ge and Si detectors for astroparticle physics*; arXiv:1505.06340.
13. A. R. Sattler, Phys. Rev. **138,** A1815 – A1821 (1995).
14. G. Gerbier *et al*., Phys. Rev. D **42,** 3211 – 3215 (1990).
15. P. Zecher, D. Wang, J. Rapaport, C. J. Martoff, B.A. Young, Phys. Rev. A **41**, 4058 – 4061 (1990).
16. B.L. Dougherty, Phys. Rev. A **45**, 2104 – 2107 (1992).
17. C. Chasman, K. W. Jones, and R. A. Ristinen, Phys. Rev. Lett. **15**, 245 – 248 (1965).
18. A. R. Sattler, F. L. Vook, and J. L. Palms, Phys. Rev. **143**, 588 – 594 (1966).
19. C. Chasman, K. W. Jones, H. W. Kraner, and W. Brandt, Phys. Rev. Lett. **21**, 1430 – 1433 (1968).
20. K. W. Jones and H. W. Kraner, Phys. Rev. C **4**, 125 – 129 (1971).
21. T. Shutt *et al.*, Phys. Rev. Lett. **69**, 3425 – 3427 (1992).
22. Y. Messous *et al*., Astroparticle Phys. **3**, 361 – 366 (1995).
23. L. Baudis, J. Hellmig, H.V. Klapdor-Kleingrothaus, Y. Ramachers, J.W. Hammer, A. Mayer, Nucl. Instr. Meth. Phys. Res. A **418**, 348 – 354(1998).
24. E. Simon *et al*., Nucl. Instr. Meth. Phys. Res. A **507**, 643 – 656 (2003).
25. P.S. Barbeau, J.I. Collar and O Tench, JCAP **09**, 009 (2007).
26. Z. Ahmed *et al*. (CDMS Coll.), Phys. Rev. Lett. **106**, 131302 (2011).
27. X. Ruan for CDEX-TEXONO collaboration, *Nuclear recoil quenching factor measurement for HPGe detector*, presented at *Application of Germanium Detector in Fundamental Research*, Tsinghua University, March 24–26, 2011; https://wwwgerda.mpp.mpg.de/symp/20_Ruan.pdf.