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A phenomenological model for the behaviour of irradiated silicon

S.Lazanu
Institute of Physics and Technology of Materials, Bucharest, Romania

U.Biggeri, E.Borchi, M.Bruzzi
University of Florence, Florence, Italy

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Abstract

Starting from the fundamental equations governing the transport of charge carriers in the presence of the deep energy levels corresponding to lattice defects, as well as from the empirical laws describing donor removal and acceptor-like centre creation during irradiation, the dependencies of the Fermi level position, carrier concentrations, resistivity and Hall coefficient on the neutron irradiation fluence of high resistivity silicon have been modelled. The free parameters of the model are the initial doping of the semiconductor, the energies levels in the band gap associated to the defects and their introduction rates.

Based on this model, from the analysis of experimental data for the dependencies of resistivity and Hall coefficient of n-type irradiated silicon versus the neutron fluence, the main responsible for the radiation effects has been identified to be an acceptor-like centre, situated at 0.4 eV below the conduction band edge. The same value of the position of the energetic level in the silicon band gap has been found for different sets of samples characterised by different initial doping concentrations.

It has also been shown that during the short time annealing after irradiation, the donor and acceptor-like centres have different kinetic characteristics.

* The original talk - in romanian

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Introduction

By the most discussed effects observed in high resistivity silicon are the inversion of the conductivity type after heavy particle irradiation, and, connected to this, the phenomena that determine the behaviour of the semiconductor immediately after irradiation.

It was previously shown that resistivity and Hall coefficient measurements as a function on the particle fluence and on the selfannealing time are a good tool to have an insight on the phenomena produced in the silicon bulk at low electric field [1].

Of particular interest is to correlate the information obtained by different physical methods, e.g. from the microscopical characterisation of the lattice defects produced in the semiconductor lattice by irradiation. So, it was stressed that, with the increase of the irradiation fluence, a great number of permitted energy levels in the silicon gap could by detected, these corresponding to lattice defects [2].

The present paper proposes a simple model for the calculation of the resistivity and of the Hall coefficient of high resistivity irradiated silicon, starting from some simple hypothesis reguarding defect creation. It is than shown that although a lot of deep centres are induced by irradiation, the behaviour of the semiconductor, long time after irradiation, can be modelled with only one centre, acceptor-like, responsible for the inversion of the conductivity type. The modelling of the behaviour of the material short time after irradiation necessitates the introduction of either some hypothesis on concentration of the deep acceptor-like centre, or the introduction of a donor-like centre.

Model

As was previously mentioned, as a result of the interaction of the primary radiation defects (vacancies and silicon interstitials) with the impurities and defects already present in the lattice, a lot of defect centres are formed, all characterised by deep energy levels in the gap (e.g.[3] for reactions and [2] for e review of the levels). Both donor and acceptor centres are produced. In parallel to this effect, a removal of doping donors is to be noted, due to the formation of the V-P centre [4]. The combined effect of these two processes is the modification of free carrier concentrations, and correlated of all macroscopic properties of the semiconductor. There is experimental evidence that irradiation could induce the inversion of the conductivity type of n-type high resistivity silicon [5]. So, acceptor centres production seems to be preponderant on the donor ones.

The forthcoming quantitative analysis is valid in the following simplifying assumptions:

(i) only room temperature situation is analysed, where all shallow donors are ionised; their concentration is N_d.

(ii) we refer to a stable situation in the lattice, long time after irradiation, when the selfannealing is completed.

(iii) donor removal could be characterised by an exponential decrease of the donor concentration with the neutron fluence described by the equation:

$$N_d = N_{d0} \exp(-d\Phi) \qquad (1)$$

where N_{d0} is the initial doping of the material, Φ is the

(iv) during irradiation, one simple acceptor-like centre forms; it is characterised by the energy level E_t in the forbidden gap, and by the concentration N_A. Its concentration depends linearly on the irradiation fluence:

$$N_A = b\cdot\Phi \qquad (2)$$

The fundamental equations governing this process are: the dependencies of the carrier concentrations of the Fermi level position, the occupation function on the deep acceptor centre [6], and the neutrality equation. This way, in the hypothesis (1) -(2), the Fermi level position as a function of the irradiation fluence could be determined. It has been shown in [7] that the shape of this curve is very sensitive to the acceptor level position, to the initial doping of the semiconductor and to the introduction rate of the deep acceptors. Before irradiation, the Fermi level is situated in the upper half of the forbidden band, corresponding to n-type material. With the increase of the fluence, it goes down, and at a certain fluence it crosses the intrinsic level, after that the material being p-type.

In Fig. 1, the influence of the different parameters on the dependence of the Fermi level position of the irradiation fluence is illustrated. The origin of the energy axis is considered at the edge of the valence band. Higher inversion fluences correspond to acceptor-like levels nearer to the conduction band. The increase of the introduction rate of the deep centre decreases the value of the fluence where the Fermi level crosses the intrinsic one, as more acceptors are produced, and correspondingly more electrons occupy them.

It is of high interest to illustrate the inversion process from the dependence of the carrier concentrations (electrons and holes) versus the irradiation fluence, this being shown in Fig. 2.

As the Fermi level position is not a direct measurable physical quantity, it is of high interest to characterise the influence of the irradiation fluence on, e.g. the resistivity and Hall coefficient. If the conduction mobilities of both electrons and holes, and the Hall factor are considered independent on the particle fluence, the dependencies of the resistivity and Hall coefficient on the neutron

fluence are illustrated in Figs 3 and 4 respectively, for the same parameters for which the position of the Fermi level on neutron fluence was represented in Fig. 1. The energetic position of the deep level influences very much the width of the resistivity and Hall coefficient vs fluence dependencies (in a semilog representation). Two orders of magnitude variation of the introduction factor of the deep level changes the point corresponding to the maximum of the resistivity in a fluence range from 2 10^{12} n/cm^2 to 10^{13} n/cm^2, for the same N_{do} and E_t. The maximum of the resistivity corresponds to the intrinsic material. At fluences lower that the value corresponding to the maximum of the resistivity, the material is n-type, and at fluences higher that this value the material is p-type.

Experimental results

The present model is to be utilised in the interpretation of the experimental data obtained for the dependence of the resistivity and of the Hall coefficient of n-type, irradiated silicon samples on the neutron fluence. As was previously reported [1], the resistivity increases up to a maximum, and than decreases, while the Hall coefficient starts from low negative values, decreases up to a minimum, and than increases and changes sign in a very small fluence interval.

The measurements of resistivity and Hall coefficient were performed at room temperature using the four points probe method [8], at the Dipartimento di Energetica di Universita di Firenze, using the experimental set-up described in [9]. Four sets of square shaped samples, 10x10 mm^2 area and 1mm and respectively 400 μm thickness, made on n-type, phosphorous doped, Wacker silicon, with low compensation, of initially 2-6 KΩcm resistivity, were used. The samples were produced at the Brookhaven National Laboratory, USA. Each set was irradiated with fast neutrons of average energy 1MeV, in a separate run, at the University of Lowell [10]. The fluences ranged in the interval 5 10^{11} - 2 10^{14} n/cm^2.

The experimentally measured resistivity and Hall coefficient versus fluence dependencies, reported in [1] are all of the shape of the curves calculated and represented in Fig 3 and 4 respectively, indicating an inversion of the conductivity type from n to p at fluences around 10^{13} n/cm^2.

The measurements performed short time after irradiation evidence a different resistivity, and respectively Hall coefficient, vs the irradiation fluence, as shown in Fig.5.

Discussion

A superposition of the measured data (resistivity and Hall coefficient) for the samples of set 3a, irradiated with fluences ranging in the interval 2 10^{12} - 2 10^{14} n /cm^2, and of the calculated dependencies on fluence of the resistivity and Hall coefficient are represented in Fig. 6, a and b respectively. The parameters used in the calculations are: the initial doping of the material N_{do} = 3.5 10^{11} cm^{-3}, the donor removal cross section d = 9 10^{-14} cm^2, the energy of the deep level E_t=0.72 eV measured from the edge of the valence band, and its introduction rate b = 9 cm^{-1}.

So, from the multitude of the centres with deep energy levels in the gap, induced by irradiation, both the resistivity and the Hall coefficient dependencies on the fluence have been modelled with only one acceptor-like centre.

The behaviour of the resistivity and of the Hall coefficient short time after irradiation, as shown in Fig.5, could be understood with the formation, at irradiation, of a donor-like centre, that anneals-out at high selfannealing times, where a dependence of the type seen in Fig. 6 is recorded each time [1]. More, the production of this deep donor-like centre must be a phenomenon with a fluence threshold of formation, corresponding approximately to the minimum in the ρ(Φ) dependence.

In Fig. 7 the calculated resistivity vs neutron fluence is represented. It has been supposed that the dependence of the deep donor centres on the fluence is of the type:

$$N_{d_{td}} = \frac{bb * \Phi}{1 + \exp[-a(\Phi - \Phi_o)]} \qquad (3)$$

All the previously mentioned hypothesis have been used, both on the shallow donor removal, and on acceptor-like centre creation. The parameters used in the construction of Fig. 7 are: N_{do}=5.10^{11} cm^{-3}, E_{ta}=0.72 eV, b=18 cm^{-1}, bb=1.5 cm^{-1}, E_{td}=0.4 eV, Φ_o=4.10^{13} n/cm^2.

Summary and conclusions

A calculation method for the resistivity and the Hall coefficient in high resistivity silicon was developed, starting from the hypothesis that the main phenomena that take place during irradiation are donor removal and acceptor creation.

The model has been found in reasonable agreement with the experimental measurements, performed on three different sets of samples, irradiated with neutron fluences up to 2 10^{14} n/cm^2. The resistivity and Hall coefficient variation as a function of the neutron irradiation have been modelled with one acceptor centre, of energy E_t= 0.72 eV, measured from the valence band edge.

The behaviour of the resistivity and of the Hall coefficient short time after irradiation could be explained by the introduction of an unstable deep donor-like centre, that forms after a threshold fluence, and that anneals out at long times after irradiation.

Acknowledgements

The authors would like to thank Zheng Li from the Brookhaven National Laboratory for helpful discussions on the parallel between the phenomena occurring in the electrical neutral bulk and space charge region of the p-n junctions after heavy particle irradiation, as well as for the preparation and the irradiation of the samples.

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$$N_d = N_{do} \exp(-d \cdot \Phi)$$

$$N_A = b \cdot \Phi$$

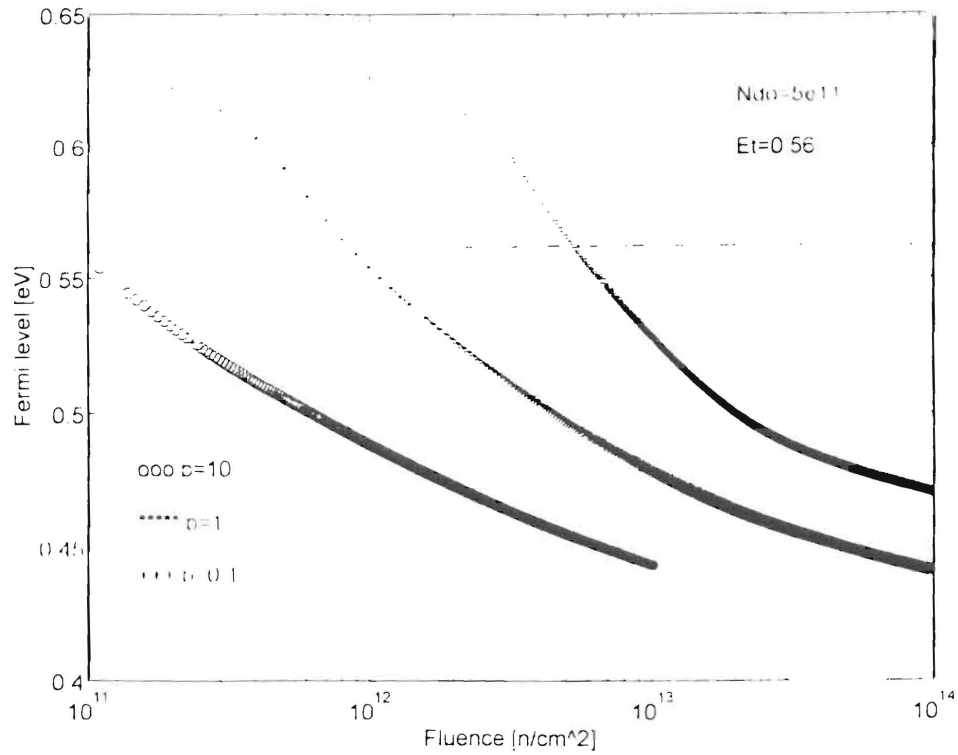
$$n = N_c \exp\left(-\frac{E_c - E_F}{k_B T}\right)$$

$$p = N_v \exp\left(-\frac{E_F - E_V}{k_B T}\right)$$

$$\frac{A}{N_A - A} = \exp\left(\frac{E_F - E_t}{k_B T}\right)$$

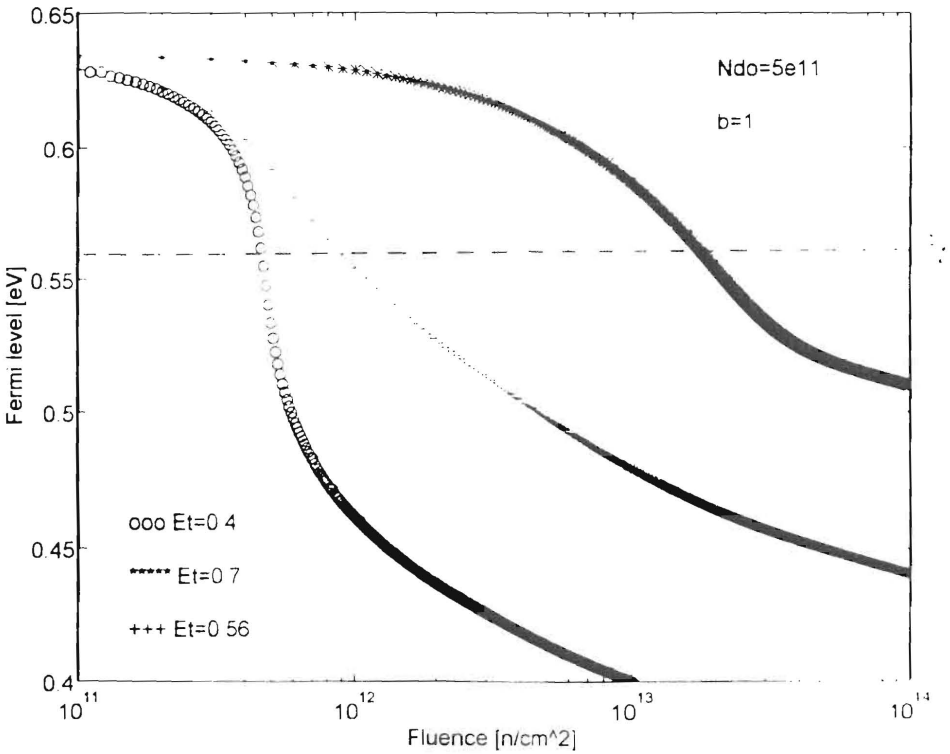
N_A - conc. of deep acc. like centres

A - conc. of occupied acceptors

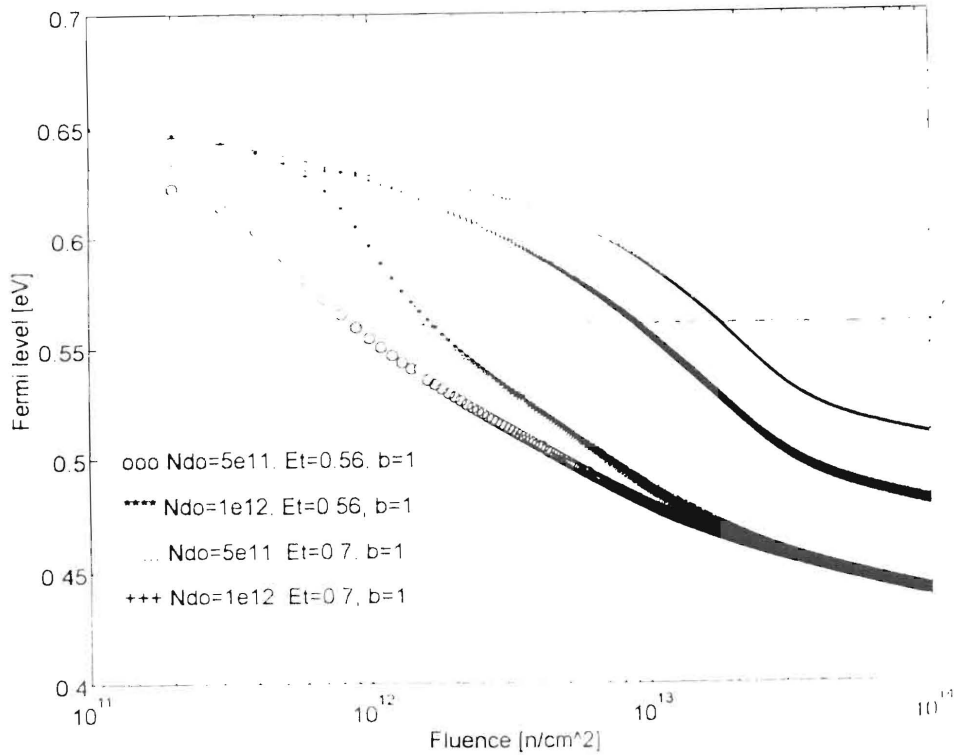


b - introduction rate of the deep acceptor-like centre

$N_A = b \cdot \Phi$

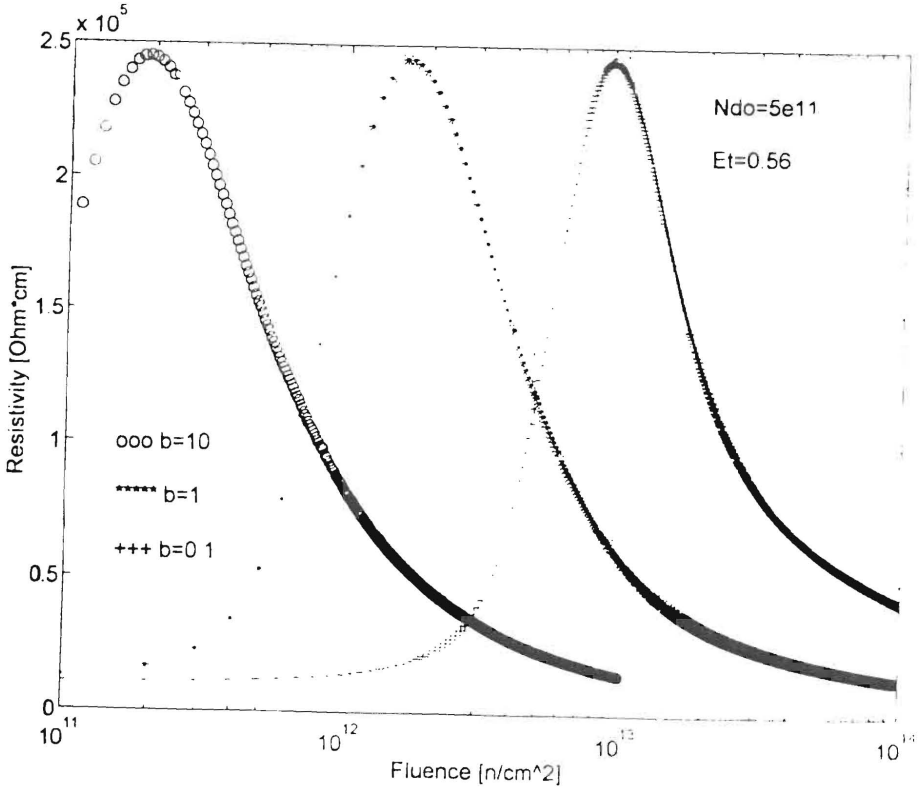


E_t - energy level of the deep acceptor-like centre, measured from the edge of the valence band.

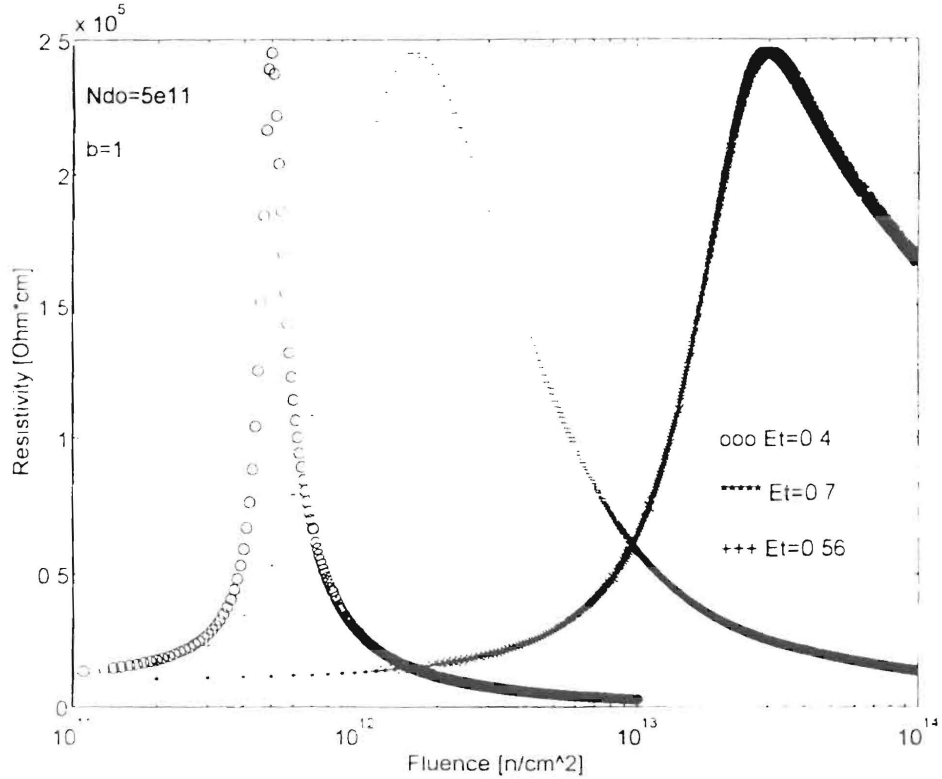


N_{do} - initial doping of the starting material

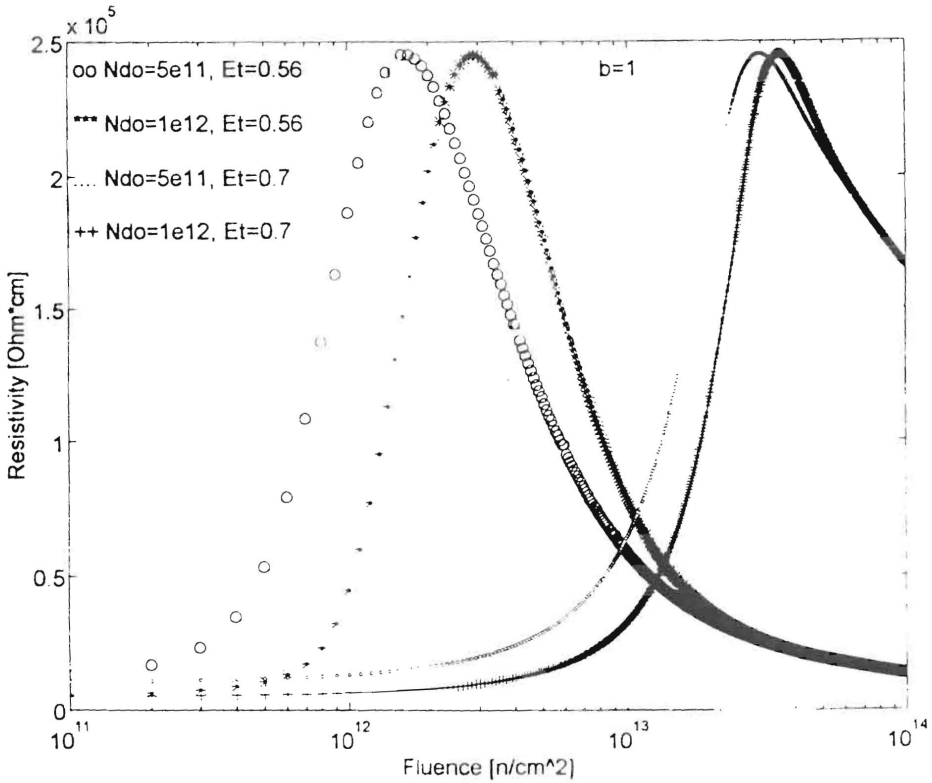
E_t - energy level of the deep acceptor-like centre

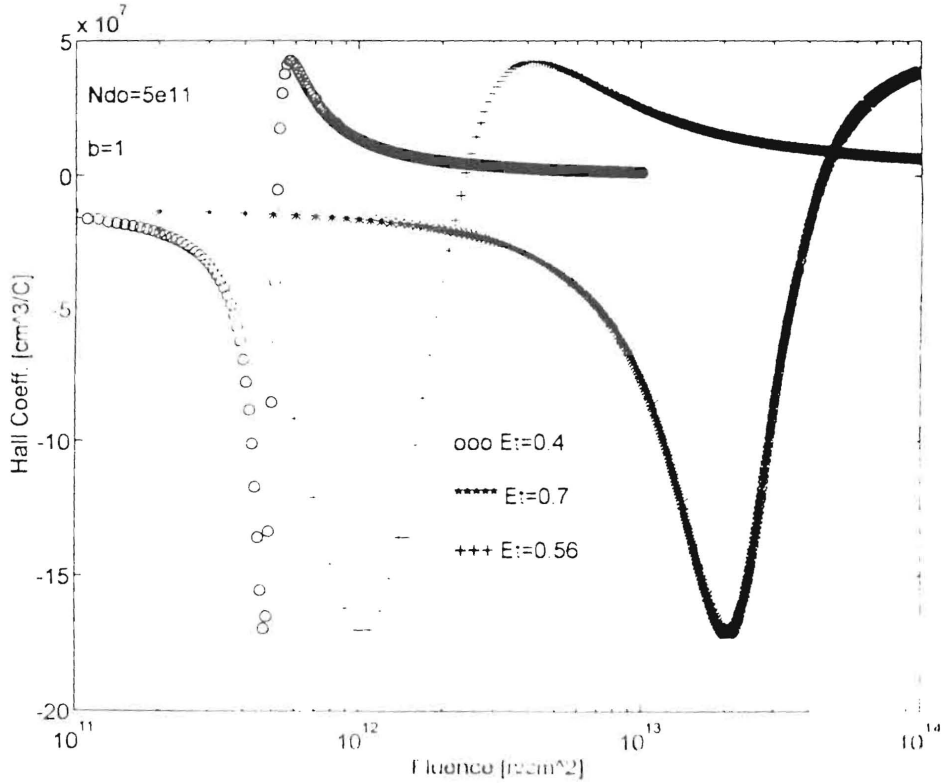


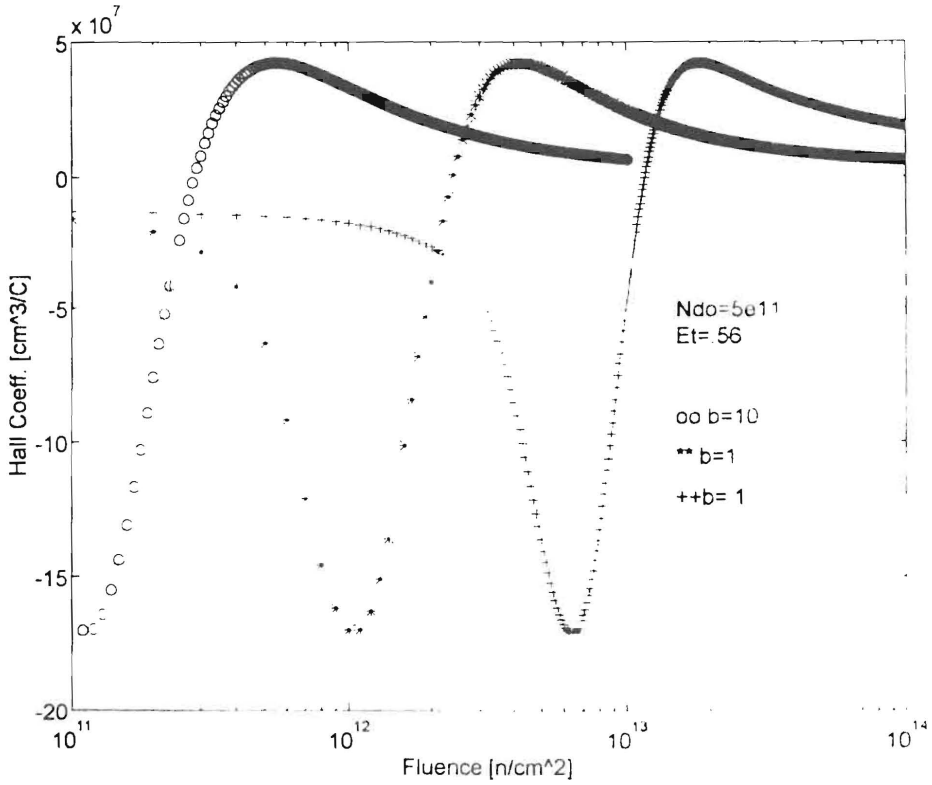
$N_A = b \cdot \phi$

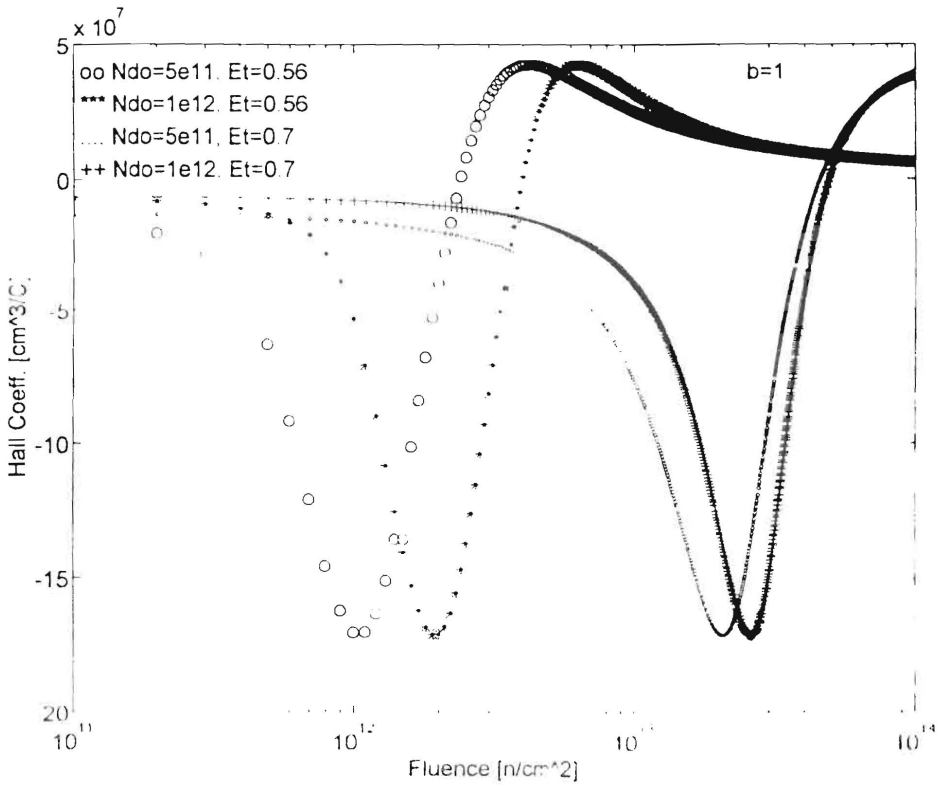


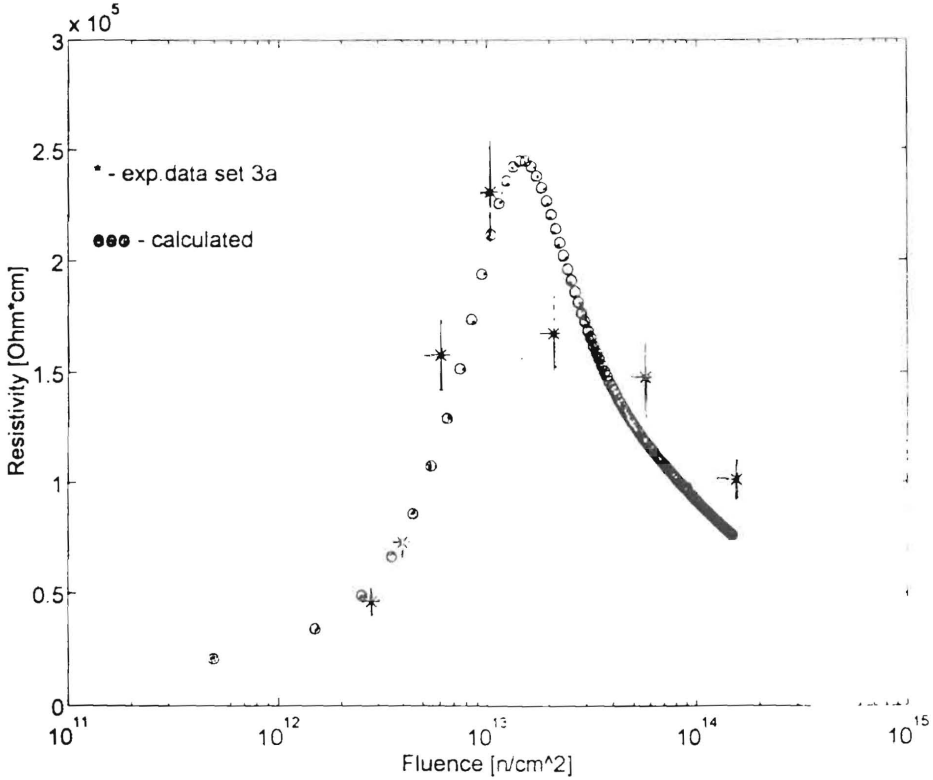
E_t

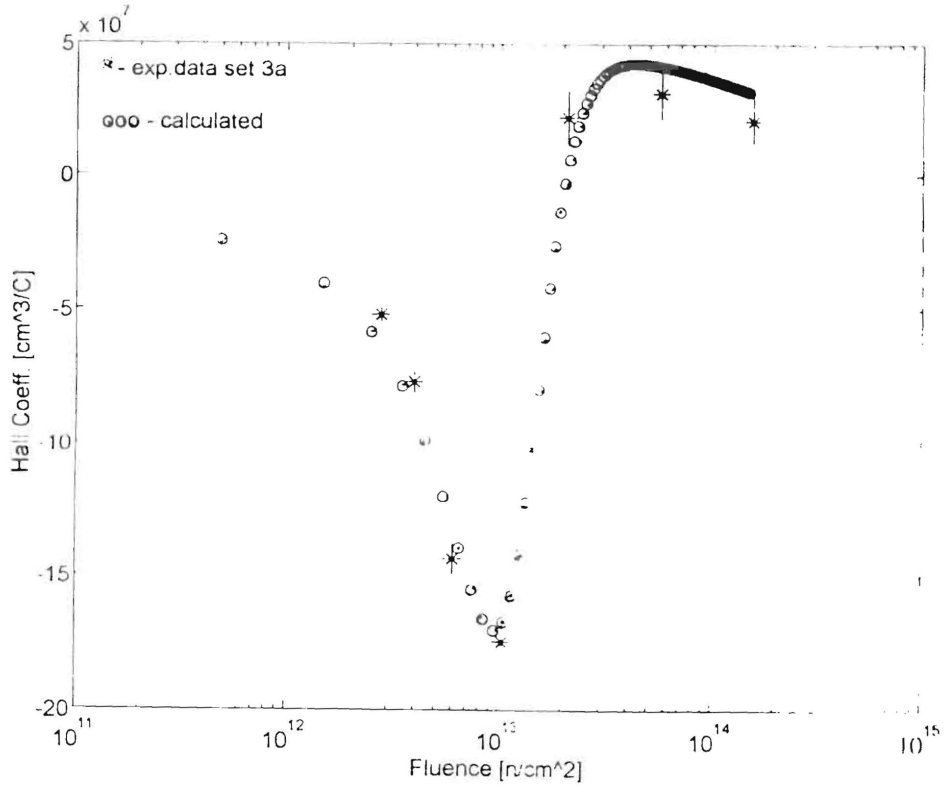

x 10^5
oo Ndo=5e11, Et=0.56
*** Ndo=1e12, Et=0.56
.... Ndo=5e11, Et=0.7
++ Ndo=1e12, Et=0.7
b=1
Resistivity [Ohm*cm]
Fluence [n/cm^2]

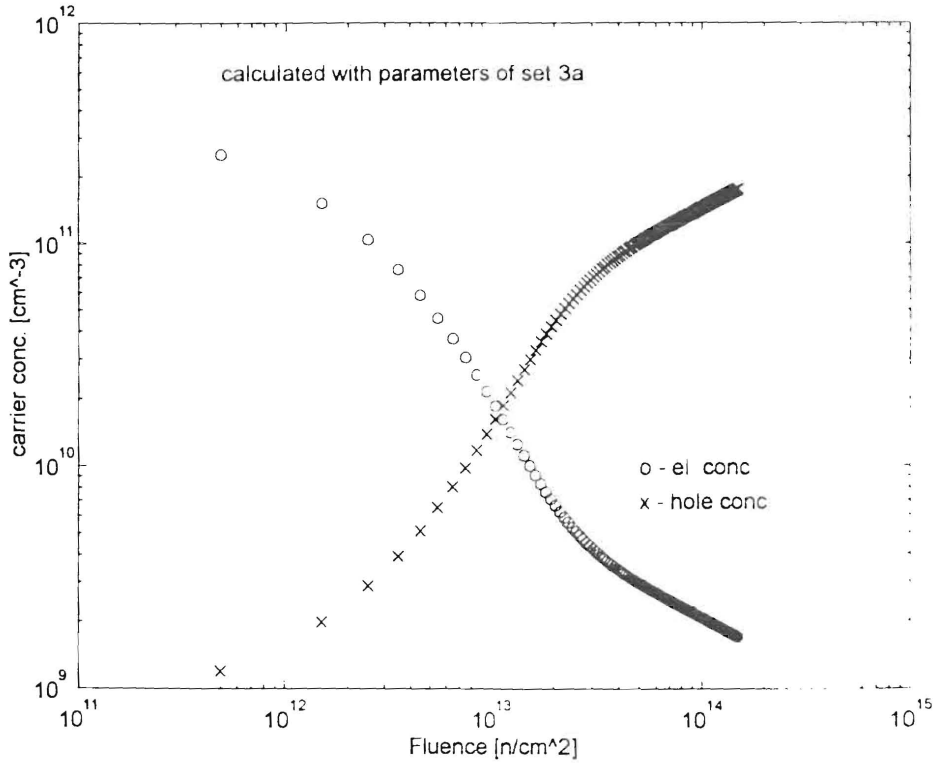

x 10^7
Ndo=5e11
b=1
ooo Et=0.4
***** Et=0.7
+++ Et=0.56
Hall Coeff. [cm^3/C]


x 10^7
5
0
-5
-10
-15
-20
Hall Coeff. [cm^3/C]
10^11
10^12
10^13
10^14
Fluence [n/cm^2]
Ndo=5e11
Et=.56
oo b=10
** b=1
++b= 1


x 10^7
5
0
-5
-10
-15
20
Hall Coeff. [cm^3/C]
10^11
10^14
Fluence [n/cm^2]
oo Ndo=5e11, Et=0.56
*** Ndo=1e12, Et=0.56
.... Ndo=5e11, Et=0.7
++ Ndo=1e12, Et=0.7
b=1


x 10^5
3
2.5
2
1.5
1
0.5
0
Resistivity [Ohm*cm]
* - exp.data set 3a
ooo - calculated
10^11
10^12
10^13
10^14
10^15
Fluence [n/cm^2]


x 10^7
5
0
-5
-10
-15
-20
Hall Coeff. [cm^3/C]
* - exp.data set 3a
ooo - calculated
10^11
10^12
10^13
10^14
10^15
Fluence [n/cm^2]



$N_{do} = 3.5 \cdot 10^{11} cm^{-3}$
$d = 9 \cdot 10^{-14} cm^{2}$
$E_t = 0.72$ eV
$b = 9\ cm^{-1}$

$t = 15$ [illegible]

$N_d = N_{do} \exp(-d \cdot \phi)$

$N_a = b \cdot \phi$

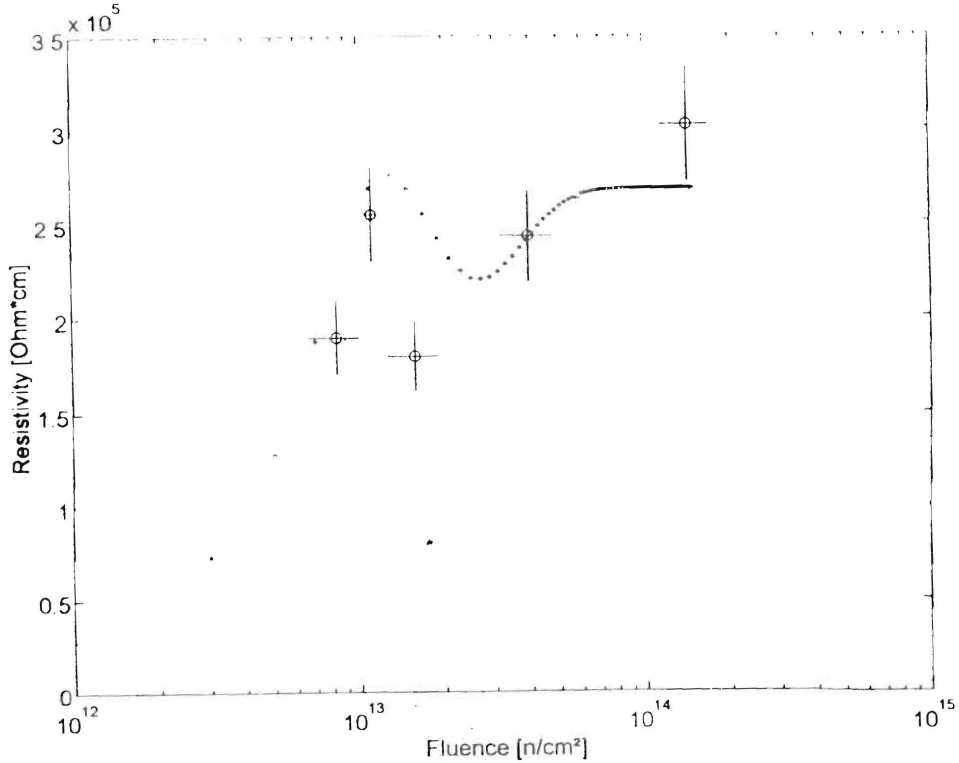
$N_{dom} = \dfrac{b \cdot \phi}{1 + \exp[-a(\phi - \phi_0)]}$

E_{ta}

E_{td}

$N_{do} = [illegible] cm^{-3}$
$E_{ta} = [illegible]$
$b = [illegible]$

$b = 1.5\ cm^{-1}$
$E_{td} = 0.4$ eV
$\phi_0 = 4 \cdot 10^{[illegible]}$ [illegible]



Summary and conclusions

- in a model with one deep acceptor-like centre:
  - the position of the deep acceptor trap influences the inversion fluence and the width of the $\rho(\Phi)$ and $R_H(\Phi)$ curves
  - its introduction rate changes the inversion fluence

- the experimental dependencies of the resistivity and Hall coefficient on the neutron fluence have been modelled, supposing that the irradiation introduces one deep acceptor-like centre in the semiconductor band-gap, at $\approx$0.4 eV below the conduction band edge.

- the short-time annealing can be modelled with another deep centre, donor-like, situated at $\approx$0.4 eV above the valence band edge.