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Monte Carlo Simulation of Carrier Capture at Deep Centers for Silicon and Gallium Arsenide Devices

A. Palma, J.A. Jiménez-Tejada, A. Godoy and J.E. Carceller

Departamento de Electrónica y Tecnologia de Computadores. Facultad de Ciencias. Universidad de Granada. 18071 Granada, SPAIN

Abstract

This work provides a direct way to include multiphonon capture at deep levels in the simulation of electron transport by the Monte Carlo method. This has been possible by adding the capture probability as one more scattering probability together with lattice mechanisms. To check this probability, numerical capture cross sections for deep centers in Si and GaAs obtained by our method have been fitted with experimental measurements.

1. Introduction

The multiphonon-emission process, responsible for carrier capture in bulk deep centers, has been included in the framework of a standard Monte Carlo simulation [1] of the electron transport in Si and GaAs semiconductors doped with deep neutral impurities. Multiphonon-emission probability has been added to the simulation lattice-scattering mechanisms. This work comprises a first step in the implementation of this process in device simulators.

At the limit of low temperatures and weak coupling, the probability of emission of p phonons with energy $\hbar\omega$, W^{mph}, has been calculated on the basis of the adiabatic formalism developed by Ridley [2, 3]:

$$W^{mph} = \frac{16\pi^2 \omega S^p e^{-S} (\nu_T a^*)^3}{V (2\pi p)^{1/2} (p/e)^p} p[0.4 + 0.18(p-1)](n+1)^p e^{-2nS}, \qquad (1)$$

where S is the Huang-Rhys factor (S<<p), V the crystal volume, and a* the effective Bohr radius in the semiconductor. The delta function model has been used to model the center bound state, $\phi_T(r) \propto r^{-1} e^{-r/\nu_T a^*}$. Dependence with the deep energy level, E_T, is through ν_T as follows:

$$\nu_T^2 = \frac{E_H^*}{E_T}, \qquad (2)$$

where E_H^* is the effective Rydberg energy (32 meV in Si and 5.3 meV in GaAs), and dependence with the temperature T is included in the occupation factor of phonons,

$n = (e^{\hbar\omega/k_B T} - 1)^{-1}$,where k_B is the Boltzmman constant. In this eq., we considered the emitted phonons to be the non-polar LO phonons ($\hbar\omega$=63 meV) in Si and ($\hbar\omega$ =30 meV) in GaAs. Therefore, the Huang-Rhys factor is the only free parameter in Expression 1. In order to verify the capture probability, in the next section we have numerically calculated the thermal dependence of the capture cross sections for several deep centers in Si and in GaAs.

2. Numerical procedure

The task of incorporating this probability in the Monte Carlo simulation was solved by restricting the carrier motion to one impurity space. Therefore, in a sample with an empty impurity concentration of N_T, the real probabilities included were:

$$< W^{mph} >= W^{mph} V N_T, \tag{3}$$

which means that we are simulating the motion of one electron in the average volume corresponding to one trap. The third body [3] and the screening effects were neglected.

In the Monte Carlo simulation, all phonon mechanisms were included and the non-parabolicity effects were accounted for both in Si and in GaAs. The numerical procedure was as follows: One electron is introduced with the thermal energy corresponding to the lattice temperature and is allowed to move without including for the multi-phonon process in order to avoid dependencies with the initial carrier state. After a certain number of scatterings (15000), the multiphonon mechanism is activated. At precisely the moment when this mechanism is stochastically chosen, the electron is considered captured, and the mean velocity and the time spent since the multiphonon probability inclusion, the so-called capture time, are recorded. This one-electron procedure is repeated for a very large number of carriers, and the average values of the mean velocities, $< v >$, and the capture times, $< \tau_c >$, are used to calculate the average thermal capture cross section for electrons, σ_n:

$$\sigma_n = \frac{1}{N_T < v >< \tau_c >}. \tag{4}$$

3. Results

In order to check whether the average capture time is the proper value to use in Eq. 4, the distribution of electrons, N_e, with the capture-time interval is plotted is Fig. 1. This figure shows one example of the exponentiality of this numerical magnitude as the Schokley-Read-Hall statistic predicts. We have fitted our results with experimental data [4, 5] of capture cross sections vs. temperature for the acceptor level of Au in silicon (Fig.2) and the A defect in gallium arsenide (Fig.3). The Huang-Rhys factors obtained in these fittings agree with theoretical and experimental measurements [2, 6].

In summary, the inclusion of the capture mechanism with the rest of the lattice mechanisms allows a better understanding of this phenomena, showing as it does the relationship between the multiphonon process and the scattering mechanisms. The agreement between our results and experimental data has been achieved with physical values of the different parameters of Eq. 1, resulting in an easy way of implementing this capture mechanism in carrier transport simulators.

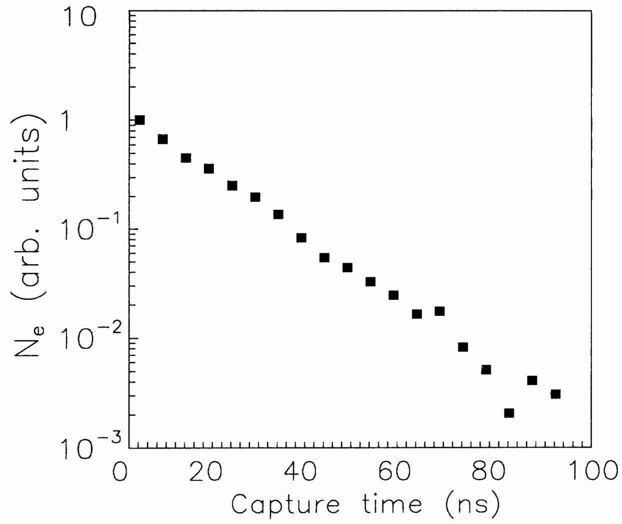

Figure 1: Histogram of N_e vs. capture time. Simulation for Pt acceptor level in Si with $N_T = 5 \cdot 10^{14}$ cm^{-3} at T=80 K

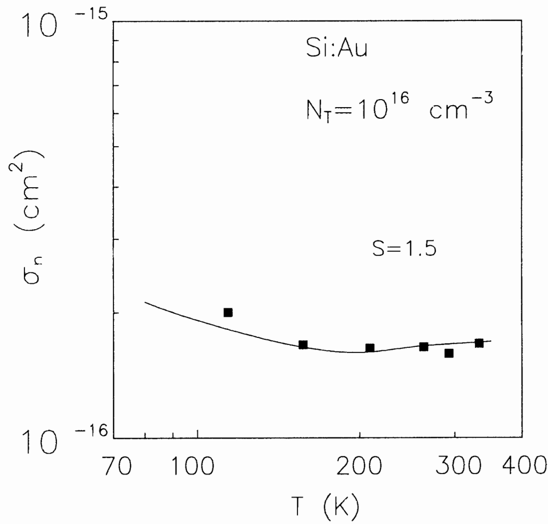

Figure 2: Comparison between experimental[4] (symbols) and numerical (line) σ_n of electrons for Au acceptor level in Si

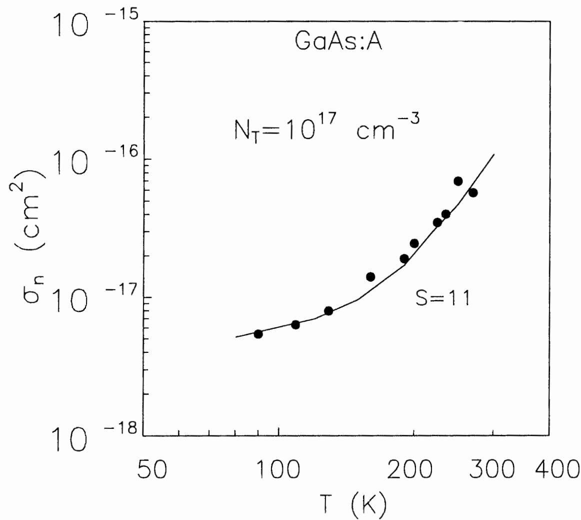

Figure 3: Experimental[5] (symbols) and numerical (line) σ_n for A center in GaAs

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