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Acoustic Phonon Limited Cross Section for the Capture of an Electron by an Attractive Trap in Semiconductor Inversion Layer

A. K. Ghorai

Physics Department, Kalimpong College, Darjeeling - 734301, West Bengal, India

Abstract: ***At low lattice temperature*** $(< 20\,\mathrm{K})$ ***a theory of recombination cross section of a conduction electron in semiconductor inversion layer has been developed here under the assumption that the electron is captured by excited states of Coulomb attractive centre due to a cascade of acoustic phonon transitions. It is found that in inversion layer the probability of capture of electron into the ground state is more with the lowering of lattice temperature and increase of binding energy of traps in comparison to what follows for the bulk material under the same prevalent conditions. The dependence of total capture cross section of electron in surface layers on lattice temperature as well as surface charge density is calculated and compared with the results of the bulk material.***

Keywords: Semiconductor inversion layer, recombination, acoustic phonon, capture cross section.

1. Introduction

The thermodynamic equilibrium with respect to the charge carrier concentration in semiconducting materials as contrasted to metals may significantly be deviated by means of external perturbations like illumination, injection through p-n junction. One of the most important kinetic processes that restores the equilibrium is the recombination (also generation) of the free charge carriers in semiconductors. The study of recombination mechanism is important both from theoretical as well as experimental aspects in view of understanding of a number of interesting phenomena observed in semiconductors. To mention in particular, the electrical non-linearity of the three dimensional electron gas (3DEG) system in bulk semiconductors may occur due to recombination effect [1]-[3].

In covalent and III-V compound semiconductors the transition of conduction electrons to some discrete levels produced in the forbidden band by various imperfections is usually described as the capture process and the relevant imperfections are called the recombination centres or traps. These traps may be created in the materials by impurities, vacancies or by dislocations. The traps may be either attractive or repulsive or neutral. The most important parameters that have to know for the calculation of the rate of recombination are the electron and hole capture cross section for the trap levels in question. Once the capture cross section is determined one may obtain the relevant dynamical information of carrier transport in semiconductors. Particularly, the useful facts and data on the directly observable quantity like life-time of the carriers could be worked out by the statistical theory using the results of the capture cross sections. However, a lot of theoretical investigations have been carried out on bulk germanium and silicon and the results obtained are reliable enough [4]-[9].

Of the different conceivable mechanisms of the non-radiative transitions, namely, the phonon, the impact, the exciton, the plasmon and the spin, the acoustic phonon mechanism plays the important role for the capture of an electron by a positive coulomb centre in semiconductors at lower lattice temperatures. At low lattice temperatures $(< 20\,\mathrm{K})$, as the process of electron-multiphonon interaction is improbable, Lax [10] developed the scheme of cascade electron capture. This model proposes that the excited levels due to the recombination centre are arranged quasi-continuously near the conduction band edge and the electron from the conduction band rolls down over the levels with a one acoustic phonon transition and is finally being captured. According to Lax the substantial contribution in recombination is due to the capture of the electrons having energy of the order of $k_B T_L$ (k_B is the Boltzmann constant and T_L is the lattice temperature) by levels having binding energy of the same order. Later on a minor correction was pointed out by Abakumov and Yassievich [11]. The cascade capture model, however, is efficient enough to derive the right order of magnitude of the experimentally observed trapping cross sections associated with coulomb attractive centres in bulk semiconductors at low temperatures ranging from 4K to 10K.

With the advent of Molecular Beam Epitaxy, Planer Technology, Metal-Oxide-Semiconductor Field Effect Transistor, Heterojunction Devices etc., the study of the electrical transport in two-dimensional electron gas (2DEG) formed in semiconductor inversion and accumulation layers evoked greater and greater attention. A good number of investigations on the electrical transport in 2DEG have been carried out in the light of 3DEG model [12]-[21]. The study of the recombination mechanisms would be interesting because the surface electric field and hence the thickness of the layer of lattice atoms in inversion and accumulation layers with which the charge carriers interact, is sensitive to the variation of the concentration of the charge carriers, the life-time of which is controllable by the prevalent recombination processes. In view of the important role played by the recombination effect in the electrical transport in semiconducting materials, the purpose of the article is to develop the theory of the cascade capture of electron by attractive traps in 2DEG at low lattice temperature. The expression for the sticking probability for a state of specific binding energy has been derived for 2DEG and it is then used to calculate the lattice temperature and carrier energy dependence of the capture cross section of an electron due to acoustic phonon in a 2DEG.

2. Theory

2.1 Sticking Probability

The sticking probability of an electron is the probability that the electron will enter the ground state before escaping. If the sticking probability be $P(U)$ for a state of binding energy U, then the capture cross section of an electron having energy ϵ can be written as [10]

$$\sigma(\epsilon) = \int \sigma(\epsilon, U) dU\, P(U), \qquad (1)$$

where $\sigma(\epsilon, U)dU$ is the cross section for capture into a state with binding energy between U and $U + dU$. Lax assumed that $P(U)$ depends only on the binding energy U and does not depend on how the electron falls into a state with such binding energy.

Using Fokker-Planck type of diffusion approximation, Lax obtained an expression for the sticking probability of an electron in 3DEG as

$$P_{3D}(\eta_{3D}) = 1 - \left(1 + \alpha + \tfrac{1}{2}\alpha^2\right) \exp[-\alpha], \qquad (2)$$

where $\alpha = (\eta_{3D} - 1)/\gamma_{3D}$. Here $\eta_{3D} = 2U/m^* u_l^2$ is the dimensionless binding energy and $\gamma_{3D} = 2k_B T_L/m^* u_l^2$ is the dimensionless lattice temperature. m^* is the conductivity effective mass of the electron in semiconductor at Γ −point and u_l is the acoustic velocity. The Eq.(2) is valid for $\eta_{3D} \geq \delta$ where the parameter δ depends upon γ_{3D} and the dependence is shown graphically in Fig.6 of Ref.[10]. To evaluate δ as a function of γ_{3D}, a nonlinear fitting procedure shows the dependence as

$$\delta = 3.3 + \frac{7.24}{1 + 100.78\, \gamma_{3D}^{-1.4}}. \qquad (3)$$

In the light of Lax model a detailed theory on the sticking probability of an electron in a 2DEG has been calculated here and the expression for the sticking probability can be given as

$$P_{2D}(\eta_{2D}) = 1 - \frac{\Gamma\left(-\frac{1}{3}, \frac{\eta_{2D}}{\gamma_{2D}}\right)}{\Gamma\left(-\frac{1}{3}, \frac{1}{\gamma_{2D}}\right)}. \qquad (4)$$

Here $\Gamma(a, b)$ are incomplete Gamma functions. The dimensionless binding energy $\eta_{2D} = 2U/m_\parallel^* u_l^2$ and the dimensionless lattice temperature $\gamma_{2D} = 2k_B T_L/m_\parallel^* u_l^2$ where $m_\parallel^*$ is the longitudinal effective mass of the electron. The Eq.(4) is defined for the range of the dimensionless binding energy $\eta_{2D} > 1$.

2.2 Capture Cross Section

Once the sticking probability of electron is known then the dependence of the cross section $\sigma(x)$ on dimensionless electron energy $x\ (= \epsilon/k_B T_L)$ can be calculated from Eq.(1). This dependence will lead to determine the total recombination cross section σ by the equation

$$\sigma = \int x\sigma(x) \exp[-x]\, dx\, . \, (5)$$

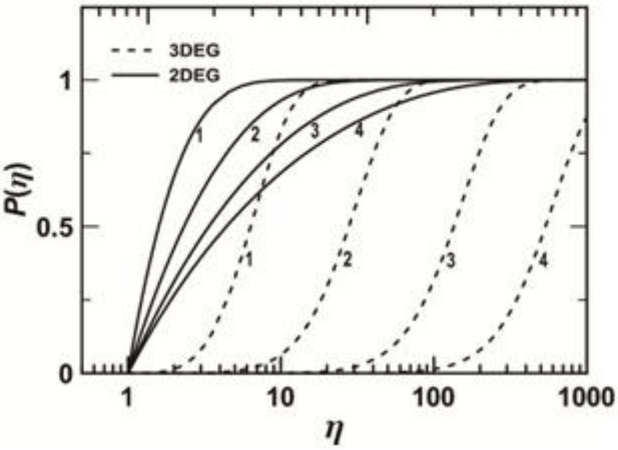

Figure 1: Dependence of sticking probability $P(\eta)$ on binding energy η. Curves marked 1, 2, 3 and 4 correspond to the dimensionless lattice temperature γ's equal to 2, 10, 50 and 200.

In bulk semiconductors the acoustic phonon limited cross section of electron energy for the physically important case of $k_B T_L \gg \frac{1}{2} m^* u_l^2$ i.e., $\gamma_{3D} \gg 1$ is seen to be [10]

$$x\sigma_{3D}(x) = \frac{4^6 \sigma_{3D}'}{\gamma_{3D}^4} F_{3D}(x), (6)$$

where

$$F_{3D}(x) = \frac{1}{24}\left(x + \frac{\delta}{\gamma_{3D}}\right)^{-1}. (7)$$

Here

$$\sigma_{3D}' = \frac{\varepsilon_1^2 m^{*3}}{3\hbar^4 \rho}\left(\frac{Ze^2}{\kappa m^* u_l^2}\right)^3,$$

ε_1 is the deformation-potential constant for the bulk material, Ze is the charge of the recombination centre, κ is the dielectric constant, ρ is the crystal density and ħ is the Dirac constant.
Then the total cross section is seen to be

$$\sigma_{3D} = \frac{4^5 \sigma_{3D}'}{6\gamma_{3D}^4}\left[\ln\left(\frac{\gamma_{3D}}{1.7818}\right) + \frac{\delta}{\gamma_{3D}}\right]. \qquad (8)$$

Using the expression for the sticking probability in 2DEG as given in Eq.(4) the electron energy dependence of the recombination cross section of an electron by a positive centre due to acoustic phonon can be given for physically important case of $\gamma_{2D} \gg 1$ as

$$x\sigma_{2D}(x) = \frac{4^6 \sigma_{2D}'}{\gamma_{2D}^5} F_{2D}(x), \qquad (9)$$

where

$$\sigma_{2D}' = \frac{4\sqrt{2}\varepsilon_a^2 m_\parallel^{*2}}{3\hbar^3 d\rho u_l}\left(\frac{Ze^2}{\kappa m_\parallel^* u_l^2}\right)^3.$$

Here d is the width of the layer of lattice atoms with which the electrons can interact. Under the condition of low lattice temperature the electrons occupy the lowest sub-band when d is given by $(\hbar^2\kappa/2m_\perp^* e^2 N_i)^{1/3}\gamma_0$, where $m_\perp^*$ is the effective mass of the electron perpendicular to the surface and γ_0 is the zeroth root of the Airy function $A_i(-\gamma_n)$ [16]. e is the electronic charge and ε_a is the deformation-potential constant in quantized surface layer and it can be given in terms of bulk value ε_1 and surface charge density N_i (in cm^{-2} unit) as [22]

$$\varepsilon_a = \varepsilon_1 + 2.5 \times 10^{-8} \times N_i^{2/3} \text{ eV}.$$

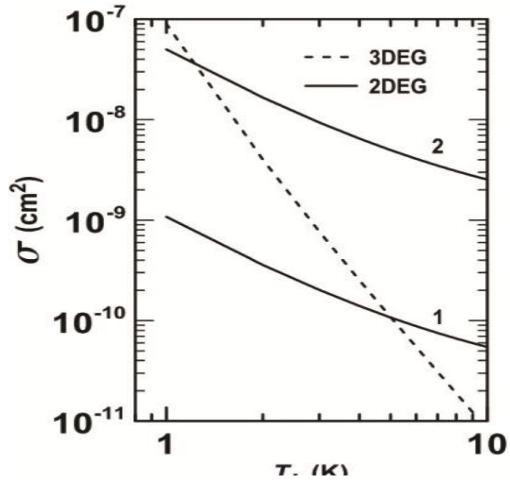

Figure 2: Dependence of cross section σ on lattice temperature T_L for 3DEG in Si and 2DEG in Si(100) layer. Curves marked 1 and 2 are for $N_i = 1 \times 10^{11}$ cm^{-2} and $N_i = 1 \times 10^{12}$ cm^{-2} respectively.

The function $F_{2D}(x)$ is of the form

$$F_{2D}(x) = \int_{1/\gamma_{2D}}^{\propto} \frac{\left\{1 - \frac{\Gamma(-1/3, y)}{\Gamma(-1/3, 1/\gamma_{2D})}\right\}\{32y + \gamma_{2D}(x+y)^2\}}{32y(x+y)^5\{1 - \exp[-(x+y)]\}} dy. \quad (10)$$

Here $y = U/k_B T_L$. The Eq.(10) cannot be solved analytically and as such it has been evaluated numerically [23]. The evaluated results are used to obtain the dependence of $F_{2D}(x)$ on x by nonlinear fitting and the expression for $F_{2D}(x)$ can be given empirically as

$$F_{2D}(x) = a(x+b)^{-c}. \quad (11)$$

The parameters a, b and c are dependent upon γ_{2D} and can be given to a good approximation as

$$a = \frac{1}{12}\gamma_{2D}^{0.579}, b = \frac{22}{25}\gamma_{2D}^{-0.969} \text{ and } c = 3.388\gamma_{2D}^{0.059}.$$

Now using Eqs.(5), (9) and (11) one can calculate the total capture cross section of a conduction electron in a 2DEG semiconducting system by a positive trap due to acoustic phonon and the result can be given as

$$\sigma_{2D} = \frac{4^6\sigma_{2D}'}{\gamma_{2D}^5}[ae^b\Gamma(1-c, b)]. \quad (12)$$

3. Results and Discussion

From Eqs. (2) and (4) it turns out that the sticking probability of an electron obtained here for a 2DEG system depends upon the binding energy of positive traps and lattice temperature in a very complex manner in comparison to the results of bulk materials. To obtain the qualitative as well as quantitative estimation, in Fig.1, we plot the binding energy dependence of sticking probability both for 2DEG and 3DEG systems at different lattice temperatures. The figure shows that in both cases the sticking probability depend upon lattice temperature more or less in a same qualitative manner but quantitatively in 2DEG the same probability increases rapidly with the slight increase of the binding energy of the charge centre. At lower lattice temperatures the sticking probability in 2DEG is seen to attain its maximum value for a slight increase in binding energy. So the capture of a conduction electron by the positive centre in 2DEG is more probable in comparison to that in 3DEG and the probability is more with the lowering of lattice temperature.

For an application of the above theory to find out the acoustic phonon limited electron capture cross section by a positive trap in semiconducting surface layer, an n-channel (100) oriented Si inversion layer is considered with the material parameter values [20] : $\varepsilon_1 = 9.8$ eV, $u_l = 9.037 \times 10^5$ cm s^{-1}, $\rho = 2.329$ gm cm^{-3}, $\kappa = 11.9$, effective mass $m^* = 0.32m_0$, longitudinal effective mass $m_l^* = 0.96m_0$, transverse effective mass $m_t^* = 0.19m_0$, m_0 being the free electron mass. For the (100) surface of Si the six valleys are not equivalent. At low lattice temperatures one may consider presumably the electrons occupy only the lowest subband and then two equivalent valleys for which $m_\parallel^* = m_t^*$ and $m_\perp^* = m_l^*$ occupy the lowest subband.

From Eqs.(8) and (12) it is seen that, in contrast to 3DEG, the electron capture cross section in 2DEG depends upon carrier concentration of the semiconducting system. To facilitate a comparison the dependence of the capture cross section on the lattice temperature as obtained for 3DEG and 2DEG systems are plotted in Fig.2. It is seen from the figure that in 3DEG the cross section increases sharply with the lowering of the lattice temperature in comparison to what follows in 2DEG. In case of 2DEG the electron capture cross section increases slowly with the lowering of lattice temperature. This apart, the figure reveals that in 2DEG the cross section increases appreciably with the increase of the surface charge density without any qualitative change in the cross section due to the increase of the surface charge density.

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