

## INTRODUCTION TO LOW FREQUENCY LOCAL PLASMONS IN BULK EXTRINSIC SEMICONDUCTORS

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**Abstract.** *It is shown that restoring force acts on the electronic cloud of the outer electrons of a neutral or charged impurity atom when it is shifted relative to the inner charged core (or expanded). Because of this the dipole oscillations arise which influence considerably the dispersion law of the plasma oscillations in bulk extrinsic semiconductors. Assuming that only one transition of electron from the ground state to the first excited state is essential, the dispersion law is calculated. It is shown that the calculated dispersion law consists of two separate branches, one of them originates from the regular plasma oscillations of the free electrons of a conductivity band, and the other one stems from the local oscillations of the outer electrons bounded to the impurity atoms.*

### 1. INTRODUCTION

The mass of an impurity atom in a crystal is different from that of the host atoms. In case of impurity the atom is heavier than the host atom as it oscillates with lower frequency. When this frequency is found outside the phonon spectrum of a crystal, the oscillation is called a local oscillation [1]. In case of impurity the atom is lighter than the host atom it oscillates with higher frequency, which could be found inside the phonon spectrum of a crystal. This oscillation is called a quasilocal oscillation [1]. Local and quasilocal oscillations of phonon modes in crystals, containing light and heavy impurity atoms are well known and studied in details [1]. Local oscillations manifest themselves also in plasmon modes of semiconductor superlattices. Bulk and surface local plasmon modes of the semiconductor superlattices were studied in [2-4]. Let us consider here local low frequency oscillations of the electronic cloud around donor or acceptor impurity atoms in bulk not heavily doped semiconductors and their interaction with regular plasma oscillation of the current carriers. The regular plasma oscillation of the current carriers is accompanied by the oscillating electric field, which influences other oscillations in a sample. This interaction changes significantly the dispersion law of the collective

electron oscillations. The interaction of the local oscillation of the electronic cloud around impurity atoms with the regular plasma one is the simplest example of the interaction between different modes of oscillations.

## 2. HYDROGEN ATOM MODEL FOR DONOR IMPURITY ATOM

The donor impurity atom has usually one more outer electron than the host atom of a semiconductor (e. g., the silicon atom). Therefore a positively charged core and one electron could model it. When the impurity atom is ionized, the electron moves to the conductivity band. When this extra electron is bound to the donor impurity atom, the hydrogen atom in a dielectric media could model it. This approximation is reasonable when the size of the electronic cloud is large enough, and it is so for semiconductors with dielectric constant  $\epsilon_0$  larger than 5 (quite typical value of  $\epsilon_0$  is about 10). In this case the size of the atom  $2R$  comprises several lattice parameters. At the same time to consider the approximation discussed reasonable one should assume that the screening (Debye for the Boltzmann statistics or Thomas-Fermi for the degenerated current carriers) radius is much larger than  $R$ . In this case the current carries do not influence significantly the formation of a "hydrogen atom". In such a model wave function of the electron in the ground state is [5]

$$\psi(r) = [\exp(-r/2R)]/2(2\pi)^{1/2}R^{3/2}, \quad (1)$$

where  $r$  is the radius-vector and  $R$  is related to either equilibrium or not to the size of the electronic cloud.

The energy of the ground state is considerably smaller for the atom in a dielectric media ( $\epsilon_0^2$  times) and it is described by the following equation [5]:

$$E_0 = -(me^4/2\epsilon_0^2\hbar^2), \quad (2)$$

where  $e$  is the electron (negative) charge,  $m$  is the effective electron mass and  $\hbar$  is the Planck constant divided by  $2\pi$ .

The electrostatic field created by the electron cloud, whose electric charge density is

$$\rho(r) = e\psi^*(r)\psi(r) = (e/8\pi R^3)\exp(-r/R), \quad (3)$$

can be calculated using Gauss's theorem. The corresponding electrostatic potential,

$$\varphi(r) = (e/\epsilon_0 r) - (e/2\epsilon_0 R)[(2R/r) + 1]\exp(-r/R), \quad (4)$$

in the vicinity of  $r = 0$  has the following form:

$$\varphi(r) \approx (e/2\epsilon_0 R) - (e/12\epsilon_0 R^3)r^2 + \dots \quad (5)$$

The kinetic energy of the electron is a quantum mechanically averaged value of its operator,

$$T = -(\hbar^2/2m)\Delta, \quad (6)$$

and it is described by the following relation:

$$\langle T \rangle = \hbar^2/8mR^2. \quad (7)$$

So the total energy of the electronic cloud and the positively charged core placed in the center of the electronic cloud is as follows:

$$E(R) = (\hbar^2/8mR^2) - (e^2/2\epsilon_0 R). \quad (8)$$

The electrostatic energy of the electronic cloud itself should not be taken into account as it represents a so-called self-interaction. Energy, described by Eq. (8), has a minimum at  $R = R_e = \epsilon_0 \hbar^2 / 2me^2$ , as is well known [5]. The minimum value of the energy is given by Eq. (2).

In order to see the nature of the restoring forces let us expand the energy  $E(R)$  (Eq. 8) in a series around  $R = R_e$  and  $x = 0$  ( $x$  is the shift of the electronic cloud as a whole relative to the positively charged core. Using Eqs. (5,8), one can see that this expansion has the following form:

$$E(x, R - R_e) = -(me^4/2\epsilon_0^2 \hbar^2) + (e^2/2\epsilon_0 \alpha)x^2 + (2m^3 e^8/\epsilon_0^4 \hbar^6)(R - R_e)^2 + \dots, \quad (9)$$

where  $\alpha$  is the polarizability of the hydrogen atom.

In classical mechanics the model of the movement of the electronic cloud as a whole relative to the charged core does not yield the correct value of the polarizability [6,7]. It yields  $\alpha = 6R_e^3 = 3\epsilon_0^3 \hbar^6 / 4m^3 e^6$ . This value represents that part of the polarizability, which is coming from the bulk of the electronic cloud (from the core of it) [6]. As to the experimentally observed polarizability, the tail of the electronic cloud gives the main contribution to it, which is not described correctly by this classical model. The correct quantum mechanical value is  $\alpha = 9\epsilon_0^3 \hbar^6 / 2m^3 e^6$  [5].

The first term in the left-hand part of Eq. (9) is the energy of the ground state. The second term describes the oscillatory movement of the electronic cloud as a whole around the positively charged core (the dipole oscillations) in terms of classical mechanics. The third term describes in the same framework the so-called breathing mode, that is the isotropic oscillations of the radius of the electronic cloud  $R$  around its equilibrium value, or oscillations of the atomic size [6,7]. Being of a spherical symmetry, such motion is not accompanied by the creation of a time-dependent dipole, quadrupole or any other multipole moments and therefore cannot emit electromagnetic radiation.

### 3. INTERACTION OF BULK AND LOCAL PLASMA OSCILLATIONS

In quantum mechanics the breathing mode for the hydrogen atom does not exist. In many electron atoms it could be realized as a collective motion of many electron system [6]. In quantum mechanics the only energy levels of the electron in a hydrogen atom are

$$E_v = -(me^4/2\epsilon_0^2 v^2 \hbar^2), \quad v = 1, 2, 3, \dots \quad (10)$$

The transitions between these levels cause the polarization of the impurity atom when the external electric field is applied [5]. The alternative external electric field excites regular plasma oscillation of the current carriers in a semiconductor. In a semiconductor regular plasma oscillation of the current carriers is accompanied by the oscillation of the electric field of the same frequency. This field acts on the impurity atoms along with the external one. Thus regular plasma oscillation of the current carriers interacts with the polarization of the impurity atoms. This interaction leads to a modification of the dispersion law of the oscillation. Let us assume further that the frequency is not too high,

so that only one transition, the transition from the ground level to the first excited one, should be taken into account, and that the other transitions could be neglected.

The dielectric permeability of a semiconductor sample as a function of the angular frequency  $\omega$  and the wave vector  $k$  is usually regarded to be as follows [8]:

$$\varepsilon(\omega, k) = 1 - (\omega_{pi}/\omega)^2 + 4\pi\chi, \quad (11)$$

where  $\omega_{pi}^2 = (4\pi e^2 n/m) + a_0 k^2$  is the initial plasma frequency of the electronic gas of the conductivity electrons of a density  $n$  without taking into account the specific polarizability of the substance of a sample  $\chi$  (without the contribution of the free electrons of a conductivity band). When the oscillation frequency of the electrons is much higher than the collision frequency then, as was shown in [9], the oscillations of the electrons are essentially one-dimensional and adiabatic. In this case factor  $a_0 = 3(k_B T/m)\varepsilon_0$  for the case of the Boltzmann statistics, but  $a_0 = 1.2(E_F/m)\varepsilon_0$  for a degenerated electronic gas ( $k_B$  is the Boltzmann constant,  $T$  is the absolute temperature, and  $E_F$  is the Fermi energy). When the oscillation frequency of the electrons is much lower than the collision frequency then  $a_0 = (k_B T/m)\varepsilon_0$  for the case of the Boltzmann statistics, but  $a_0 = (2E_F/3m)\varepsilon_0$  for a degenerated electronic gas [9].

Taking into account that  $1 + 4\pi\chi = \varepsilon_0$ , and that the polarizability of the bound electrons of the donor impurity atoms which are not ionized [8],

$$\alpha_i = f n_d e^2 / m (\omega_0^2 - \omega^2) \quad (12)$$

( $f$  is so called oscillatory force,  $n_d$  is the number of the neutral, not ionized, donor atoms per unit volume of a semiconductor, and  $\omega_0 = 3me^4/8\varepsilon_0^2 \hbar^3$  is the frequency of the transition from the ground state to the first excited state, due to which the polarizability arises), one can come to the following expression for the dielectric permeability as a function of the angular frequency and the wave vector:

$$\varepsilon(\omega, k) = \varepsilon_0 \{ 1 - (\omega_p/\omega)^2 + [b/(\omega_0^2 - \omega^2)] \}, \quad (13)$$

where  $\omega_p^2 = (4\pi e^2 n/\varepsilon_0 m) + ak^2$  is the regular plasma frequency of the free conductivity electrons in a semiconductor,  $a = a_0/\varepsilon_0$ ,  $b = 4\pi f n_d e^2/m$ , and  $\varepsilon_0$  is the low frequency limit of the dielectric constant.

As was mentioned above, in Eq. (13) only one transition from the ground state to the first excited state was taken into account.

The dispersion law, that is the dependence of the angular frequency on the wave vector is determined in quantum mechanics by a well known condition  $\varepsilon(\omega, k) = 0$  [8]. From this and Eq. (13) follows that there are two branches of the oscillations:

$$\omega_{1,2}^2 = 0.5(\omega_{p0}^2 + \omega_0^2 + b + ak^2) \pm 0.5[(\omega_{p0}^2 - \omega_0^2 + ak^2)^2 + b(2\omega_{p0}^2 + 2\omega_0^2 + b + 2ak^2)]^{1/2}. \quad (14)$$

At  $b = 0$  one has  $\omega_1 = \omega_p = [(4\pi e^2 n/\varepsilon_0 m) + ak^2]^{1/2}$  and  $\omega_2 = \omega_0$ . This means that at a low concentration of neutral donor impurity atoms one has two separate modes of the oscillations considered: a regular plasma oscillation of the free electrons in a conductivity band and a local plasma oscillation of the outer electrons bounded to the donor impurity atoms. When  $b = 0$  and  $\omega_0$  is larger than  $\omega_{p0}$  the two branches of the oscillations cross at some  $k$ . But when  $b$  is not zero, one can see from Eq. (14) that the two branches never

cross. One of them goes below the other. This means that at higher concentrations the dispersion law changes considerably. Typical dispersion curves are shown in Fig. 1. They were calculated using Eq. (14) for  $\omega_0 = 1.1\omega_{p0}$  and  $b = 0.1\omega_{p0}$ .

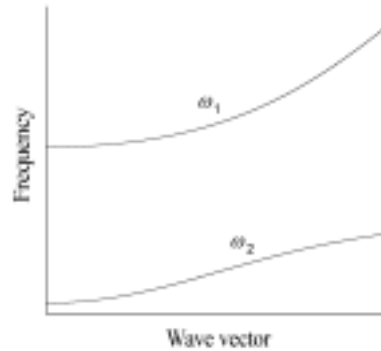


Fig. 1. Two branches of a typical dispersion curve, calculated using Eq. (14) for  $\omega_0 = 1.1\omega_{p0}$  and  $b = 0.1\omega_{p0}$ .

At high enough concentrations the impurity levels of the oscillation form the so-called impurity band [1]. When there are no free electrons in the conductivity band and there are no regular plasma oscillations, Eq. (14) yields that the local mode only is present.

#### 4. CONCLUSION

As one can see from the results in Section 3, the interaction between a regular bulk mode of the plasma oscillation and local plasma oscillation around donor impurity atoms leads to the creation of low frequency branch of plasma oscillations.

The acceptor impurity atom may have also one or two outer electrons, which contribute to the formation of a local mode of the plasma oscillations in the same manner as was considered above. Only the factors in equations have their specific values.

So, it is worthwhile to mention that the dipole oscillations of the electronic cloud of the impurity atoms in bulk semiconductors interact with the regular plasma oscillations of conductivity electrons. This leads to a significant modification of the dispersion law of the plasma oscillations. It was shown that as a result of this interaction two branches of the plasma oscillations appear in the bulk extrinsic semiconductor.

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## **UVOD U NISKOFREKVENTNE LOKALNE PLAZMONE UNUTAR PRIMESNIH POLUPROVODNIKA**

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*Pokazano je da povratna sila deluje na elektronski oblak spoljašnjih elektrona neutralnog ili naelektrisanog atoma nečistoća, kada je on pomeren u odnosu na unutrašnji naelektrisani ostatak. Dipolne oscilacije koje proizilaze utiču značajno na zakon disperzije u poluprovodnicima. Pretpostavljajući de jedino jedan prelaz elektrona iz osnovnog u prvo pobuđeno stanje je značajan, izračunat je zakon disperzije. Takođe je pokazano da zakon disperzije sadrži dve grane, jedna od njih potiče od regularnih oscilacija, a druga potiče od lokalnih oscilacija spoljašnjih elektrona vezanih za atome nečistoća.*