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Heavy Electrons in Nano-Structure Clusters of Disordered Solids

Dimiter Alexandrov
Lakehead University, Thunder Bay, Ontario, Canada

Abstract

The existence of heavy electrons is found theoretically in nano-structure clusters of disordered solids. The basis of the investigation is the electron band structures of disordered semiconductors previously determined by the author. The existence of electron energy pockets is found for the electrons in the conduction bands of these semiconductors that are nano-confining potential valleys of dimensions in the range of the primitive cell. The electron wave function of the confined electron is determined in when the electron interacts with local electrical field that is external for the energy pocket, and the average velocity of the electron is found. An expression for electron mass of an electron localized in pocket is derived. It is found that this electron mass is greater than the electron mass at rest and the confined electrons are designated heavy electrons. The possibility of interactions of protons with heavy electrons is discussed.

Introduction

The problem about the electron effective mass in solids is important with regard to both electron and optical properties of solids. The usual methods of determining the electron effective masses are connected with preliminary calculations of corresponding electron band structures and further computations of electron mass values. These approaches assume there are no external radiations (laser, etc.) that interact with the electrons in solids leading to electron mass renormalizations according to a determined rule [1, 2]. Generally it can be considered that all effective mass calculations about the charges (electrons and holes) in solids are based on the corresponding electron band structures ignoring the rule given in [1, 2]. However, recently some authors [3, 4] have considered the impact of interaction of external electro-magnetic field with electrons in solids on the electron effective mass, and they have found that increase of this mass can be expected. Although the authors of [3] in comparison with the authors of [4] give different estimation of the impact of an external electro-magnetic field interacting with electrons on the electron mass both works [3] and [4] can be considered as contributions in the theory of the effective mass of heavy electrons. Both works assume the existence of heavy electrons in nano-layers on the electrode surface.

The author's research progress [5-8] in determining the electron band structures of disordered semiconductors is the basis of this paper. Previously calculated electron band structures of disordered nitride semiconductor compound alloys are used and the existence of energy pockets for electrons in conduction bands is found. These energy pockets are found to be potential energy valleys in the conduction bands having dimensions in the range of the primitive cell. Interaction of external electrical field with electron located in energy pocket is investigated and the

corresponding electron wave function of the confined electron in a free electron approximation is determined. Formula for effective mass of a confined electron in pocket is derived and conclusions are drawn about the existence of heavy electrons. The interaction of the heavy electrons with protons is discussed.

Electron band structures of disordered solids and electron energy pockets

Disordered solids having common formula $A_xB_{1-x}C$ ($0 \leq x \leq 1$, A and B have equal valences) are called multinary crystals. A multinary crystal is considered to be a periodical crystal having a large primitive super-cell, containing a finite number of quasi-elementary cells. It is found [5] that the electron energy in a primitive super-cell of the multinary crystal can be presented in the following way:

$$E(\mathbf{r}) = \sum_{\mathbf{q}} \delta(\mathbf{r} - \mathbf{R_q})\, E(\mathbf{q}) \qquad (1)$$

Where **r** is the radius-vector of the electron, E(**q**) is electron energy in the quasi-elementary cell **q** and $\delta(\mathbf{r} - \mathbf{R_q})$ is a delta-function. The electron band structure of the multinary crystal can be determined on the basis of local interactions within the primitive super-cell, which determine the corresponding sub-bands. As a matter of fact the electron band structure of the multinary crystal determined in this way contains the same sub-bands as those determined for the primitive super-cell of the same multinary crystal without consideration of the localizations of the interactions. However the sub-bands determined by (1) are localized in the corresponding quasi-elementary cells. Linear combination of atomic orbitals (LCAO) method is used by the author for electron band structure calculations for disordered solids in case of nitride semiconductors.

After detailed investigation, the author found [5-8] that the properties of a disordered semiconductor can be determined if it is taken only a part of the calculated LCAO electron band structure corresponding to configuration of quasi-elementary cells giving the deepest energy pocket for the electrons in the conduction band, deepest energy pocket for the holes in the valence band, and that these energy pockets are at the shortest distance. To satisfy these three conditions, a configuration of five different types of wurtzite quasi-elementary cells taken in the following order must be used for $In_xGa_{1-x}N$ (Fig. 1):

(1) Pure GaN quasi-elementary cell containing two atoms of Ga and two atoms of N surrounded by second neighboring Ga cations
(2) Mixed In-GaN quasi-elementary cell containing half atoms of In, one and half atoms of Ga and two atoms of N, having second neighboring cations In and Ga
(3) Mixed In-GaN quasi-elementary cell containing one atom In, one atom Ga and two atoms of N, having second neighboring cations In and Ga
(4) Mixed In-GaN quasi-elementary cell containing half atoms of Ga, one and half atoms of In and two atoms of N, having second neighboring cations In and Ga
(5) Pure InN quasi-elementary cell containing two atoms of In and two atoms of N, having second neighboring cations In. Each type of quasi-elementary cell forms sector υ of the corresponding electron band structure ($\upsilon = 1, 2, 3, 4, 5$)

The same method can be used for calculation of energy band structures of other disordered semiconductors – nitrides, arsenides, etc. The author has made LCAO electron band structure calculations [5 – 8] for $In_xGa_{1-x}N$ (Fig. 1), for $In_xAl_{1-x}N$, for $Ga_xAl_{1-x}N$, for InO_yN_{1-y} and for non-

stoichiometric InN:In .The energy levels Γ^{υ}_{c1} are the bottom of the conduction band, and the energy levels Γ^{υ}_{v15} are the top of the valence band. All energies are determined by taking the energy of the vacuum as being equal to zero. (The values shown in Fig. 1 correspond to a ratio of 1:1 between the surrounding atoms of different sorts.) The energy difference $E^{\upsilon}_{g} = (\Gamma^{\upsilon}_{c1} - \Gamma^{\upsilon}_{v15})$ gives the energy band gap of sector υ. The energy level Γ^{4}_{c1} for $In_xGa_{1-x}N$ (Fig. 1) is below the neighboring levels Γ^{3}_{c1} and Γ^{5}_{c1}, which means that an electron occupying this level is confined in local potential valley Γ^{4}_{c1} of the conduction band of $In_xGa_{1-x}N$. In addition the dimensions of this valley are equal to the dimensions of the quasi-elementary cell of $In_xGa_{1-x}N$ containing half atoms of Ga, one and half atoms of In and two atoms of N, having second neighboring cations In and Ga, and these dimensions are in the range of the primitive cell – i.e. one can consider that Γ^{4}_{c1} forms an electron energy pocket. The same consideration can be done for the level Γ^{3}_{v15} in regard to holes in the valence band of $In_xGa_{1-x}N$, however in this paper it is assumed that the valence band is fully occupied in term of electrons, i.e. there are no holes, and there are no inter-band electron transitions.

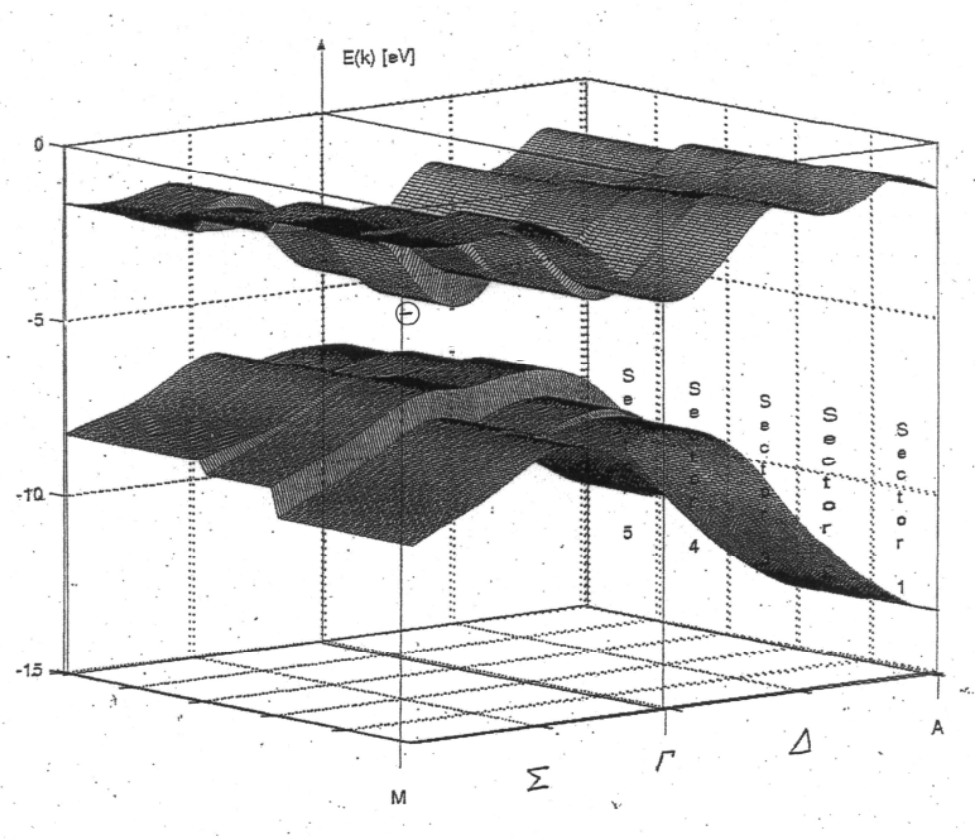

Figure 1. Electron band structure of $In_xGa_{1-x}N$. The electron energy pocket is designated.

Effective mass of confined electron in pocket

If an electron occupies the state Γ^{4}_{c1} in $In_xGa_{1-x}N$ it will be confined in the pocket and its further participation in a charge transfer along the solid will require its removing from the level Γ^{4}_{c1}. One considers this removing to be done by electrical filed in order the results to be applicable in case of interaction of other charged particles such as protons and deuterium nuclei

with confined electrons. An applied electrical field can remove the confined electron by quantum tunneling trough potential barrier [9]. In this case one can write:

$$\Psi_{out}(x_\mu) = D^{1/2}\ \Psi_{in}(x_\mu) \tag{2}$$

Where $\Psi_{in}(x_\mu)$ is the wave function of the confined electron, $\Psi_{out}(x_\mu)$ is the wave function of the electron after the barrier, and D is transmission coefficient. The applied electrical field has strength ξ_μ acting in direction x_μ. According to [9] one can write (k is electron wave vector):

$$\Psi_{in}(x_\mu) = A \exp(i\, k_\mu\, x_\mu) \tag{3}$$

$$\Psi_{out}(x_\mu) = C \exp(i\, k_\mu\, x_\mu) \tag{4}$$

The process of quantum tunneling of an electron confined in pocket Γ^4_{c1} in $In_xGa_{1-x}N$ is schematically described in Fig. 2. In fact the line Γ^υ_{c1} is the bottom of the conduction band at point Γ in the electron band structure in Fig. 1, and Γ^υ_{v15} is the top of valence band at point Γ of the same electron band structure. The shifts of the lines Γ^υ_{c1} and Γ^υ_{v15} in Fig. 2 are due to influence of the electrical filed ξ_μ having designated direction on this figure as well.

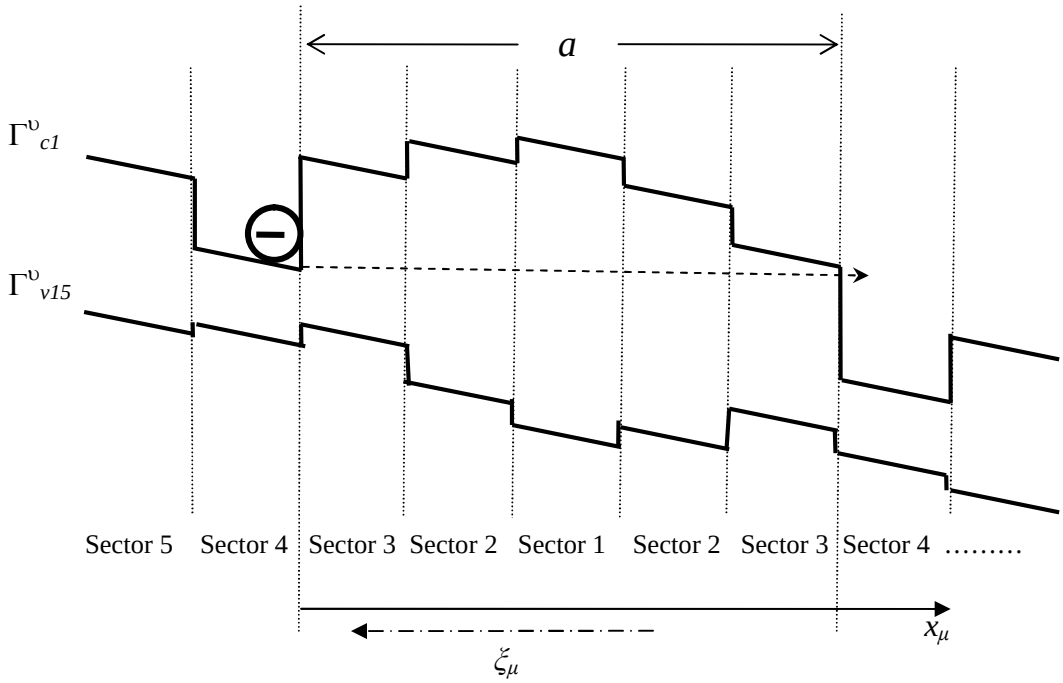

Figure 2. Electron band structure of $In_xGa_{1-x}N$ in external electrical field (not in scale). The tunneling from level Γ^4_{c1} is shown.

According to both [9] and Fig. 2 the transmission coefficient of quantum tunneling trough a potential barrier of with a is

$$D = \exp\{- (2/\hbar) \int_0^a [2m(U(x) - E)]^{1/2} dx \} \quad (5)$$

Where E is the electron energy, $U(x)$ is the potential function of the barrier, m is electron mass on level Γ^4_{c1}, and $x = x_\mu$. Also $m = m^* m_0$ where m^* is electron zone mass and m_0 is the electron mass in rest. The author assumes that the bottom of the conduction band in a pocket has the same behavior as the bottom of the same band of pure semiconductor built by the same chemical elements as these presented in the corresponding sector. In this way the author assumes that $m^* \neq 1$. Using Fig. 2 one can write for $U(x)$ ($x = x_\mu$):

$$U(x) = U_0 - q\xi_\mu x_\mu \quad (6)$$

Where q is electron charge and U_0 is average height of the potential barrier for $\xi_\mu = 0$.

It can be considered a free electron having mass m moving after the barrier. According to [10] the average value of the velocity $\overline{v_\mu}_{out}$ of this electron in direction x_μ is:

$$\overline{v_\mu}_{out} = (\hbar / 2 m i) \int \{ \Psi^*_{out}(x_\mu) \partial \Psi_{out}(x_\mu) / \partial x_\mu - \Psi_{out}(x_\mu) \partial \Psi^*_{out}(x_\mu) / \partial x_\mu \} d x_\mu \quad (7)$$

Considering (2) and (5) one can write

$$\overline{v_\mu}_{out} = (\hbar / 2 m D^{-1} i) \int \{ \Psi^*_{in}(x_\mu) \partial \Psi_{in}(x_\mu) / \partial x_\mu - \Psi_{in}(x_\mu) \partial \Psi^*_{in}(x_\mu) / \partial x_\mu \} d x_\mu \quad (8)$$

or

$$\overline{v_\mu}_{out} = (\hbar / 2 m_{eff} i) \int \{ \Psi^*_{in}(x_\mu) \partial \Psi_{in}(x_\mu) / \partial x_\mu - \Psi_{in}(x_\mu) \partial \Psi^*_{in}(x_\mu) / \partial x_\mu \} d x_\mu \quad (9)$$

Where m_{eff} is defined to be effective mass of the electron confined in an energy pocket and

$$m_{eff} = m D^{-1} = m^* m_0 \exp\{(2/\hbar) \sqrt{2m^* m_0} \int_0^a [U_0 - q\xi_\mu x - E]^{1/2} dx \} \quad (10)$$

Where the condition $U_0 - q \xi_\mu x - E \geq 0$ must be obeyed. The meaning of (10) is that one can treat a confined electron as a free electron having electron effective mass m_{eff}. The expressions (7) – (10) can be used in case of interactions of a confined electron with local fields of strength ξ_μ – for example with charged particles (other electrons, protons, deuterium nuclei, etc.). The author considers that these expressions can be used for description of currents using confined charges in disordered solids however corresponding corrections accounting other phenomena must be made as well.

The expression in the exponent of (10) is positive and therefore $m_{eff} \geq m^* m_0$. It is the reason that the author to consider that the confined electrons are heavy. The formula (10) provides that if $E \rightarrow U_0$ or/and $a \rightarrow 0$ then $m_{eff} \rightarrow m^* m_0$. This expression includes parameters a, U_0, E and m^*,

i.e. m_{eff} depends on the properties of the electron band structure and for ξ_μ = const. (or weak ξ_μ) further change of m_{eff} is possible only by change of m^*. As it was mentioned above the electron effective mass m_{eff} can be used in case of interaction of heavy electron with other charged particles including protons and deuterium nuclei. In this way it is useful the effective Bohr radius [9] to be determined

$$a_{B\,eff} = \hbar^2 / m_{eff}\, q^2 \tag{11}$$

Using the author's previous results [5 – 8] for LCAO electron band structure calculations and expressions (10) and (11), the parameters m_{eff} and $a_{B\,eff}$ for heavy electrons in $In_xGa_{1-x}N$, in $In_xAl_{1-x}N$, in InO_yN_{1-y} and in non-stoichiometric InN:In are found for: *i)* weak local electrical fields $\xi_\mu << (U_0 - E) / (q\, a)$; and *ii)* strong local electrical fields $\xi_\mu = (U_0 - E) / (q\, a)$. It is accepted that $m^* = 0.18$ for all nitride semiconductor materials. It is assumed that a corresponds to shortest possible distance between two nearest electron energy pockets. This situation is shown in Fig. 2 and it can be achieved technologically in nano-layers. The results are summarized in Table 1. It is important to be noted that the impact of the heavy electrons on the electrical properties can be expected to be significant in nano-structures having low concentrations of light electrons. Also this impact is higher in wide energy band gap disordered materials because the influence of the defects on the conductivity is small. Existence of heavy electrons in non-metal nano-layers – for example in nano-structures of metallic hydrides on metal surfaces – can be expected as well.

Table 1. Effective masses and effective Bohr radii of heavy electrons in several disordered solids

	m_{eff}, in m_0 units		$a_{B\,eff}$, Å	
	weak field	strong field	weak field	strong field
$In_xGa_{1-x}N$	851.02	50.89	$0.62*10^{-3}$	0.0104
$In_xAl_{1-x}N$	3.41	1.28	0.1553	0.4134
InO_yN_{1-y}	11.96	2.96	0.0442	0.1788
InN:In	286.41	24.61	0.0018	0.0215

Discussion about possible interactions of protons with heavy electrons

It can be seen in Table 1 that the effective mass of the heavy electrons can reach high values in some materials. However it depends on the local field. Therefore the necessary and sufficient condition that the heavy electrons to behave as heavy negative particles in interactions with other charged particles is that the field of every interaction must be weak.

In the light of the above if this condition is fulfilled, a heavy electron e_h^- can participate in process [3, 11]:

$$e_h^- + p^+ \rightarrow n + \nu_l \tag{12}$$

Where p^+, n and ν_l designate proton, neutron and neutrino respectively. In order for this process to take place the following threshold condition about the effective mass of heavy electron e_h^- must be fulfilled [3]:

$$\beta = m_{eff} / m_0 > 2.531 \tag{13}$$

The effective masses from Table 1 even for strong field interactions (except for $In_xAl_{1-x}N$) fulfill the condition (13).

It must be noted that certain particles must reach the region where the heavy electron is localized for the interaction to occur; i.e., the probability of the interaction of heavy electron–particle is higher in nano-layers or in nano-structure clusters that are close to the surface.

Conclusion

This paper can be considered the author's first contribution in the field of interaction of charged particles with electrons localized in solids. Although the existence of heavy electrons in nano-structures is shown theoretically the author considers that the conditions about weak interaction in solids must be found in order further study of heavy electron-particle interactions to be performed. Finding of these conditions will be subject of a future work. Future work will also consider the role of heavy electrons in metallic hydride nano-layers.

References

1. L. D. Landau, E. M. Lifshitz, *The Classical Theory of Fields*, Pergamon Press, Oxford (1975)
2. V. B. Berestetskii, E. M. Lifshitz, L. P. Pitaevskii, *Quantum Electrodynamics*, Butterworth Heinmann, Oxford (1997)
3. A. Widom, L. Larsen, *Eur. Phys. Journal C*, **46**, 107 (2006)
4. P. L. Hagelstein, I. U. Chaudhary, *Electron mass shift in nonthermal systems* (D. Nagel, private communication)
5. D. Alexandrov, *Journal of Crystal Growth*, **246**, 325 (2002)
6. D. Alexandrov, S. Butcher, M. Wintrebert-Fouquet, *Journal of Vacuum Science and Technology*, **A22(3)**, 954 (2004)
7. D. Alexandrov, S. Butcher, T. Tansley, *Physica Status Solidi*, **203,** 25 (2006)
8. D. Alexandrov, S. Butcher, T. Tansley, *Journal of Crystal Growth*, **288**, 261 (2006)
9. A. S. Davydov, *Quantum Mechanics*, Pergamon Press, Oxford (1965)
10. K. F. Brennan, *The Physics of Semiconductors*, Cambridge University Press, Cambridge (1999)
11. R. E. Marshak, Riazuddin, C. P. Ryan, *Theory of Weak Interaction of Elementary Particles*, Interscience, New York (1969)