Probability of charge transport through al/GaAs interfaces system using quantum model

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احتمالية انتقال الشحنة خلال سطح نظام Al/GaAs باستعمال انموذج كمي

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ألمستخلص

تمركز هذا البحث على تحقيق ودراسة احتمالية الانتقال للشحنة عند سطح معدن /شبة موصل بالاعتماد على حسابات معدل الانتقال ..لهذا النظام افترضنا حالتين كميتين متمركزتين هما حالة المانح. $\langle\varphi_D^{et}$ لحزمة التوصيل لشبه الموصل وحالة المستقبل $|\varphi_A^{et}>$ للالكترون في حزمة التوصيل للمعدن وعلى التتابع والتي تزدوج مع بعظها البعض وفقا لمصفوفة العناصر. علاقة ثابت معدل الانتقال الالكتروني عند سطحي نظام معدن/شبه موصل أعتمد على النضرية الكمية ونظرية الاضطراب للانتقال بين حالتي$\langle\varphi_D^{et}$ و φ_A^{et} عندما يكون الازدواج اقل من k_BT .احتمالية ثابت معدل الانتقال اللشحنة لنظام سطح معدن/ شبه موصل تصف حاجز الجهد للنظام بين المادتين. احتمالية معدل الانتقال الالكتروني حسبت مع الطاقة الحرة لاعادة الترتيب باستعمال برنامج ماتلاب. النتائج النظرية لحسابات معدل الانتقال الالكتروني اظهرت ازدياد الانتقال بزيادة طاقة اعادة الترتيب.

الكلمات المفتاحية: احتمالية انتقال الشحنة , سطح نظام Al/GaAs , انموذج كمي

Abstract

The focus of this paper is on the investigation and the understanding of transition probability of charge at the metal/semiconductor interface depending on the calculation of the rate constant. For this system we can suppose two localized quantum vector states system with a conduction electron state vector $l\varphi_D^{et}\rangle$ interacting with an acceptor state vector $l\varphi_A^{et}\rangle$ of electron in band of metal with the interacting described by the coupling matrix element. Expression of rate constant of charge transfer for metal/semiconductor system derived upon the quantum model and perturbation theory for transition between $l\varphi_D^{et}\rangle$ and $I\varphi_A^{et}$ state when the coupling matrix element coefficient smaller than k_BT . The probability of the charge transfer rate constant for the metal/semiconductor interface in this context, is basically defined as a relatively to potential barrier between a metal and a semiconductor The probability of charge transfer rate constant evaluated with reorganization energy using a matlap program. Theoretical results obtained for our mode show that the probability of charge transfer is more probable with decreasing the reorganization energy.

Key Word: Probability of Charge transport, Al/GaAs interface, Quantum model

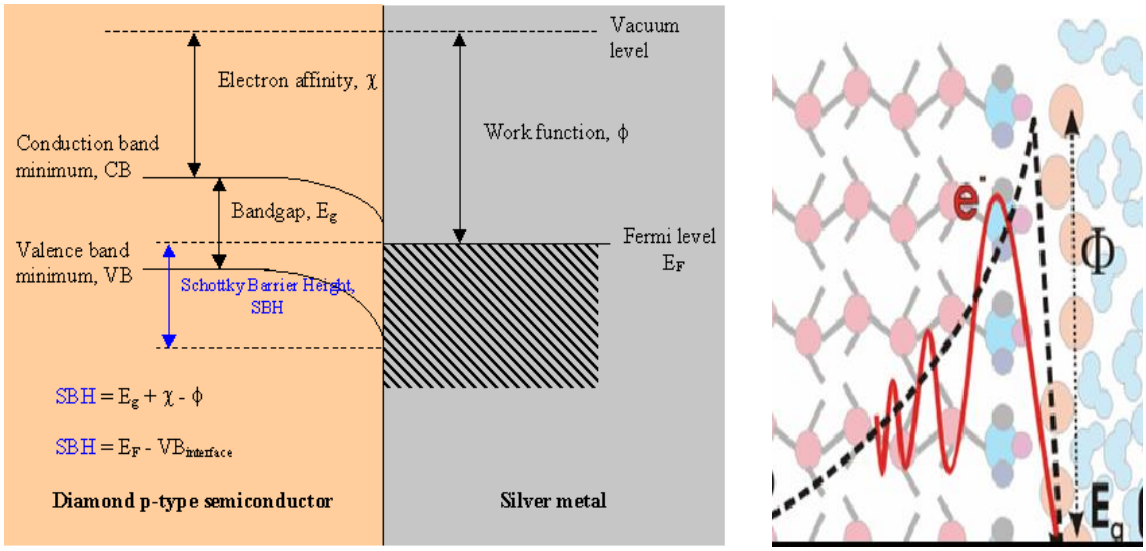
Introduction

Electron transfer reactions represent a simple process which occurs in donor-acceptor system molecules. The transfer of a single electron from an atom or a molecule to another is considered to be the most elementary reactions (1). Electron transfer is one of the most important reactions in physical chemistry and biophysics involves an oxidation of donor state $|D\rangle$ and reduction of an acceptor state $|A\rangle$.

The theory of electron transfer reaction is the subject of persistent interest in chemical and biological physics. Over the past several decades, researchers have investigated the transfer of electron through molecule and solid state structure at molecule/ metal interfaces (2) , and metal semiconductors interfaces (3) .They showed that the electron transfer from semiconductor to metal in the bleaching of surface Plasmon band and occur within the time frame of incident pulse laser in 2009 (4). Since the seminal work predicting dynamical of ET reaction in the early 1980's, a great deal of theoretical effort has gone into clarifying the dynamics of the electron transfer.(5). Rudolph Marcus described electron transfer between two states, a model which was the basis for the classical theory of electron transfer .Latter, this model was extended to describe electron transfer from a single donating state to a continuum of accepting state (6) .The field of electron transfer has been greatly advanced by the detailed analytical theory in the past half century ago depending on the standards Marcus theory and also by the introduction of new technology, such as photochemical initiation (7).Metal semiconductor contact from interfaces that give basic features of many metal –semiconductor devices .To construct the diagram of an metal/ semiconductor contact ,we consider the energy band diagram of metal /semiconductor , and align .These ET systems are seen important from technological and biological , where a metal is placed in intimate contact with a semiconductor , the electrons from the conduction band in one material ,which have higher energy ,flow into the other material until the Fermi level on the two sides are brought into coincidence (8-9) .The energy level in the two material are rearranged relative to the new common Fermi level (10) however ,the Fermi energy of the metal and semiconductor do not change right away. In this paper a theoretical description and studied of electron transfer at metal/semiconductor interface and will be calculated theoretically the rate constant for this transfer of electrons depending on the results of reorganization energy and coupling matrix element coefficient.

Theoretical model

Charge transport probability across metal/semiconductor interface system happens between the localized quantum states for the donor state vector $l\psi_D^{et}\rangle$and acceptor state vector $l\psi_A^{et}\rangle$ in Hilbert space .It perturbs the energy between the metal state electron and semiconductor conduction electron state and the electron have been tunneling from donor state to an acceptor state as shown in figure (1).



a b

Figure (1): Schematic illustration of (a) model potential of electron transfer at band probability at the metal/semiconductor (11), and (b) tunneling process (12).

The exchange of charge occurs mainly at interface near equilibrium, but a reduced species can denote charge to any empty level on the metal . The probability of the charge transfer at the semiconductor acceptor to the metal donor relation is given by [13]

$$\Gamma_{ET} = \frac{2\pi}{\hbar}\sum_{-\infty}^{\infty}|T_{DA}(E)|^2(4\pi E_{met}^{sem}k_BT)^{\frac{-1}{2}}exp\frac{-(E_{met}^{sem}+\Delta V)^2}{4E_{met}^{sem}k_BT}F_{(E)}\ldots\ldots\ldots\ldots\ldots(1)$$

where ħ is the Planck constant, $|T_{DA}(E)|^2$ is the coupling coefficient between the electronic state of the metal and the conduction band at semiconductor ,E_{met}^{sem} is the reorganization energy ,k_B is the Boltzmann constant , T is absolute temperature ,and $F_{(E)}$ is the Fermi-Dirac probability distribution of the electrons in the electron metal-semiconductor interface and given by(14).

$$F_{(E)} = (1 + exp^{\frac{E}{k_BT}})^{-1}\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

On the other hand, the charge transfer probability depends on the barrier height created between two material interfaces (metal and semiconductor). Near metal/semiconductor interface, due to energy level difference the barrier is formed with properties of two metal and semiconductor system, for large height barrier and caused impedance of charge transport. The ability of charge to transfer across the barrier height or the tunneling between metal/semiconductor when brought the barrier energy, this scale is the of electron transfer probability. The barrier height which is equal to the difference of metal work function and semiconductor electron affinity, is given by (15).

$$\Delta\mathbb{V}^{*} = \frac{(\varphi_m - \chi_{\mathrm{se}})^2}{\mathrm{k_B T}} \quad \text{.....(3)}$$

Where φ_m the work is function of metal, and χ_{se} is the electron affinity of semiconductor.

The probability of the charge transport rate constant at metal/semiconductor interface system can be calculated by inserting

Eq.(2) ,and Eq.(3) in Eq.(1),and evaluating Eq.(1) ,then results [16].

$$\Gamma_{ET} = \frac{2\pi}{\hbar}(4\pi \mathrm{E_{met}^{sem} k_B T})^{\frac{-1}{2}} \frac{n_{in} V_{sem}}{\beta} \exp - \frac{(\Phi_{met} - \chi_{sem})}{\mathrm{k_B T}} \langle \left|\overline{\Lambda(0)}\right|^2 \rangle \left[[\pi \mathrm{k_B T} - \frac{1}{4\mathrm{E_{met}^{sem} k_B T}} \left(\frac{(\pi \mathrm{k_B T})^3}{4}\right) + \frac{1}{32 \mathrm{E_{met}^{sem\,2} k_B{}^2} T^2} \left(\frac{5(\pi \mathrm{k_B T})^5}{16}\right) - \frac{1}{384 \mathrm{E_{met}^{sem\,3} k_B{}^3} T^3} \left(\frac{61(\pi \mathrm{k_B T})^7}{64}\right) \ldots\ldots + \frac{1}{\mathrm{n!}\left(4\mathrm{E_{met}^{sem} k_B T}\right)^{\mathrm{n}}} (\propto (\pi \mathrm{k_B T})^{2\mathrm{n}+1}) \right] \text{.....(4)}$$

where n_{in} concentration of electron, V_{sem} volume of unit cell for semiconductor, β petration factor and the coupling matrix element coefficient $\langle \left|\overline{\Lambda(0)}\right|^2 \rangle$ for metal and semiconductor.

The reorganization energy $\mathrm{E_{met}^{sem}}$ contribution arises from the reorientation of the charge in the system .Its magnitude dependent on the radius of the donor and acceptor site, on its distance (d) ,and on the dielectric properties of the metal and the semiconductor . Its due to the electron transfer reaction for metal/liquid interface is given by [17].

$$E_{semi.}^{met} = \frac{q^2}{4\pi\varepsilon_0} [\frac{1}{2R_{met}} \left(\frac{1}{n_{met}^2} - \frac{1}{\varepsilon_{met}}\right) + \frac{1}{2R_{semi}} \left(\frac{1}{n_{semi}^2} - \frac{1}{\varepsilon_{semi}}\right) - \frac{1}{4D_{semi}} \left(\frac{n_{met}^2 - n_{semi}^2}{n_{met}^2 + n_{semi}^2} \frac{1}{n_{semi}^2} - \frac{\varepsilon_{met} - \varepsilon_{semi}}{\varepsilon_{met} + \varepsilon_{semi}} \frac{1}{\varepsilon_{semi}}\right) - \frac{1}{4D_{met}} \left(\frac{n_{semi}^2 - n_{met}^2}{n_{semi}^2 + n_{met}^2} \frac{1}{n_{met}^2} - \frac{\varepsilon_{semi} - \varepsilon_{met}}{\varepsilon_{semi} + \varepsilon_{met}} \frac{1}{\varepsilon_{met}}\right) - \frac{1}{R_{met-semi}} \left(\frac{1}{n_{met}^2 + n_{semi}^2} - \frac{1}{\varepsilon_{semi} + \varepsilon_{met}}\right)] \text{.....(5)}$$

Where $q = q_D - q_A$ the difference of energy in donor and acceptor , R_{met} and R_{semi} are the radius of metal and semiconductor , $D_{semi} = R_{semi} + 1A^{\circ}$, $D_{met} = R_{met} + 1A^{\circ}$,and $R_{met-semi} = R_{met} + R_{semi}$ are the distance between

metal,metal to interface and metal-semiconductor , n_{met}, $\varepsilon_{met}$are the optical, statistical dielectric constant and n_{semi} and ε_{semi} are the optical and statistical dielectric constant for semiconductor.

The radius of the molecule can be estimated from the apparent molar volume using spherical approach [18]

$$R = (\frac{3M}{4\pi N\rho})^{\frac{1}{3}} \quad \text{(6)}$$

Where M is the molecular weight, N is Avogadro's number, and ρ is the mass density.

Results

A theoretical studies of charge transfer probability due to interface of the metal/semiconductor system depends on several parameters such that; transition rate constant Γ_{ET}, reorganization energy E_{met}^{sem}, electronic coupling coefficient $\langle|\overline{\Lambda(0)}|^2\rangle$,

height barrier ,volume unit cell V_{sem},concentration of electron charge n_{in},and penetration constant β . The rate constant of charge transport Γ_{ET} have been calculated depending on the Eq. (4) to know the behavior of charge transfer across interface of metal/semiconductor

The one of the most important parameter for charge transfer of the calculated probability rate constant of charge transfer in Al/ GaAs interface system is the reorganization energy$E_{met}^{sem}(eV)$.

It can be calculated theoretically depending on Marcus– Hush semi classical in Eq.(5).,that's must be estimated radius for metals ,and semiconductors from Eq.(6) by inserting the values of Avogadro's constant $N = 6.02 \times 10^{23}\ \frac{Molecule}{mol}$,molecular weight M=26.982 g/mole, and density $\rho = 2.7 g/cm^3$ (19),for Al metal and M =144.36 , , and $\rho = 5.32 g.cm^{-3}$ for GeAs semiconductor[20] in Eq.(6), we can estimate the values of radii for metals and semiconductor respectively. Reorganization energies for metal/semiconductor interface can be calculated using Eq.(5),with the values of the static dielectric constant ε , and optical dielectric constant$n$,for metal and semiconductor from table (1), and radii estimated radii of the metal and semiconductor, result are tabulated in table(2).

Next we can calculate the rate of charge transport Γ_{ET}, for Al/GaAs system interface using Eq.(4) with a Matlab program and depending on results of reorganization energy $E_{met}^{sem}(eV)$, ,concentration of electron n_{in},volume of unit cellfor semiconductor

V_{sem},petration factor β , the coupling matrix element coefficient$\langle\left|\overline{\Lambda(0)}\right|^2\rangle$for metal and semiconductor and calculation of height barrier through on values of work function of metalΦ_{met} and affinity of semiconductorχ_{sem} . Substituting values of the reorganization

energies data from table(2) ,and the matrix element coupling coefficient$\langle\left|\overline{\Lambda(0)}\right|^2\rangle =$ 0.4, 0.45, 0.5, 0.55, 0.6, 0.65, 0.7, 0.75, and $0.8\text{x}10^{-11}(\ eV)^2$ [21], height barrier and temperature is taken depending on experimental T=,300 K ,results are shown in table(3).

Table (1): Common properties of semiconductor. (20)

Properties	GaAs
Atoms/cm^3	4.42×10^{22}
Atomic weight	144.63
Breakdown field (V/cm)	4×10^5
Crystal structure	Zincblende
Density (g/cm^3)	5.32
Refractive index	3.4
Dielectric constant	13.1
Effective density of states in conduction band, N_C (cm^{-3})	4.7×10^{17}
Effective density of states in valence band,N_v (cm^{-3})	7×10^{18}
Energy gap (eV) at 300K	1.424
Intrinsic carrier concentration	1.7×10^6
Intrinsic Debye length (μm)	2250
Lattice constant (Å)	5.6533
Melting point (ºC)	1238
Minority carrier lifetime (s)	10^{-8}
Optical-phonon energy (eV)	58
Specific heat (J/gºC)	0.35
Electron affinity, (eV)	4.07

Table(2): The results of the reorganization energy $E_{met}^{sem}(eV)$ for electron transfer at interface system

Material	Refractive index	Dielectric constant	Reorganization energy(eV)
GaAs semiconductor	3.4[20]	13.1[20]	
Al metal	1.02[20]	1.6[20]	1.229492949665298
	0.77		3.808930471692719
	1.01		1.297565734849107
	1.00		1.367685007183577

Table (3): Data of the rate constant calculation for electron transfer at Al / Si semiconductor interface with variety coupling coefficient $\langle|\overline{\Lambda(0)}|^2\rangle$, at T= 300 K

$Rate\ constant\ of\ electron\ transfer\ \Gamma_{ET}$ (Sec − 1)										
$Coupling\ matrix\ element\ \langle|\overline{\Lambda(0)}|^2\rangle$ x$10^{-11}(\ eV)^2$										
System		0.4	0.45	0.5	0.55	0.6	0.65	**0.7**	0.75	0.8
Al/ GaAs	1.2294	0.9008X1(	1.0134 × 10^{10}	1.1260 × 10^{10}	1.2386 × 10^{10}	1.3512 × 10^{10}	1.4638 × 10^{10}	1.5764 × 10^{10}	1.6890 × 10^{10}	1.8016 × 10^{10}
	3.8089	0.5160 × 10^{10}	0.5805 × 10^{10}	0.6450 × 10^{10}	0.7095 × 10^{10}	0.7740 × 10^{10}	0.8385 × 10^{10}	0.9030 × 10^{10}	0.9675 × 10^{10}	1.0320 × 10^{10}
	1.2975	0.8774 × 10^{10}	0.9871 × 10^{10}	1.0967 × 10^{10}	1.2064 × 10^{10}	1.3161 × 10^{10}	1.4258 × 10^{10}	1.5355 × 10^{10}	1.6451 × 10^{10}	1.7548 × 10^{10}
	1.3676	0.8551 × 10^{10}	0.9620 × 10^{10}	1.0689 × 10^{10}	1.1758 × 10^{10}	1.2827 × 10^{10}	1.3896 × 10^{10}	1.4965 × 10^{10}	1.6034 × 10^{10}	1.7102 × 10^{10}

For our research, we have applied the quantum theory to investigation and study the charge transfer across metal/semiconductor interface system.

In this research , we have assuming that the wave function for transfer of charge from donor to acceptor state are overlapping at interface to transfer the transfer of charge across ,,when the metal is brought to contact with semiconductor. Fermi level for tow material must be coincident at equilibrium state and describe by Fermi distribution function. The electron upon driving force energy has to be rapidly transfer into the metal before it can fall back to its ground state.

The probability of charge transport rate constant in tables (3) for system Al/ GaAs refer that rate constant is function of reorganization energy $E_{met}^{sem}(eV)$,and height barrier. Height barrier for system depending on the work function $\varphi_m(eV)$,of metal and affinity of semiconductor $\chi_{se}(eV)$.

Rate constant of charge transport across metal/semiconductor system in table (3) showed that increasing with decreasing reorganization energy and vice versa. This indicates that the reorganization energy is large for large dielectric constant for semiconductor, and the system have more energy to reorient before transport. Also the rate constant increasing with increasing the coupling matrix element, this refers to that the transport increases at overlap of two wave for donor and acceptor system. On the other hand, the theoretical result show an agreement with result in (22), and this gives us more facility to be applied in devices technology.

Conclusion

It can be summarized, depending on our results of calculation that the charge transfer is more probable and stronger depending on the reorganization energy, height barrier, and coupling coefficient.

It has been shown that the theoretical model for charge transport across metal/semiconductor interface has given a good model that describe the fundamental electron transfer process depending on the agreement of our result with experimental. On the other hand the increase of refractive index leads to small depending on the optical properties of molecule.

The rate constant of charge transport increases with decreasing the reorganization energy because the electron have more driving force energy to transport across interface when the system need small part of reorganization energy that is necessary to alignment and oriented of the configuration system . This mean that reorganization energy limits the ability of transport of electron cross interface of metal/semiconductor system.

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