Hypothetical investigation of electron movement cross section at Metal-semiconductor

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Abstract

A theoretical studies and calculation the cross-section for electron transfer at metal/semiconductor interfaces material depending on quantum description . Cross sections of charge transfer for Ag with Si ,TiO_2 ,and ZnO were carried out using simplified models of the system at the Multi driving force energy at interaction in the devices interface . Investigation and evaluation of the cross section for electron transfer σ_{ET} at metal/semiconductor system is depending on the coefficient ; driving force energy $E(\vartheta)$, transfer energy orientation energy, wave number ϑ, mean Refractive index n , amplitude of electronic coupling coefficient $\langle|\overline{\Lambda(0)}|^2\rangle$and the lifetime of electron transferτ_{ET} . The cross section for electron transfer σ_{ET} at metal/semiconductor system evaluated using MATLAP program. The result of cross section show that cross section increases with increasing the driving force energy and coupling coefficient and vice versa .

Key words: Electron transfer ,Cross section ,Metal -Semiconductor , Lifetime,

1. Introduction

Many researchers had been studied and investigation of the movement of electron through metal/semiconductor interface in the past years ago . These interfaces play a key role in many emerging fields, creating a need for a better theoretical treatment of the interfacial electron transfer . Electron transfer (ET) is the simplest interaction: an electron is transferred from a donor to an acceptor without the breaking or the creation of chemical bonds [1]. The investigation of the electron transfer processes in collisions is of great importance not only in basic atomic collision physics, e.g. for understanding the interactions between charged particles, but also in such diverse fields as controlled-thermonuclear-fusion research, development of x-ray laserm, electronic devices and astrophysics[2]. The transfer of a single

electron from an atom or a molecule to another is considered to be the most elementary [3]], and one of the most ubiquitous and fundamental phenomena in chemistry, physics, biology processes and technology [1], involves an oxidation of donor state and reduction of an acceptor state . In such processes, several electrons could be simultaneously transferred to excited states with significantly large cross sections, and finally the product ions are stabilized by emission of photon(s) or electron(s) or both,[2].

Since the late 1940s, the field of electron transfer processes has grown enormously. The development of the field, experimentally and theoretically, as well as its relation to the study of other kinds of reactions been brought together. The early experiments in the electron transfer field were on 'isotopic exchange reactions' (self-exchange reactions) and, later cross reactions [4]. The electron transfer cross sections have been expressed by the classical over-barrier model (ECBM)[5]. Around 1950 ,the theoretical description of ET reactions was mainly triggered by Marcus , who was awarded the Nobel prize in 1992 "for his contributions to the theory of electron transfer reactions in chemical systems".

Marcus realized the importance of nuclear configuration changes between reactants and products to the ET rate[6]. 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 the metal /semiconductors interfaces [7]. Metal/ semiconductor contact from interfaces that give basic features of many metal /semiconductor devices In 2009 [8], .To construct the diagram of a metal/ semiconductor contact; we consider the energy band diagram of metal /semiconductor , align with each other these ET systems 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 [9]. The energy levels in the two materials are rearranged relative to the new common Fermi level. However, the Fermi energy of the metal and semiconductor do not change right away [10]. Fundamental studies, as performed in this theses are expected to provide guidelines for design of such practically useful ET system In this theses, our main theoretical model can be study of electron transfer at metal/semiconductor interface system .There orientation energy and the probability rate of electron transfer constant are calculated according to this model. In this paper, we performed to undertake a theoretical study and calculation the cross section of electron transfer reaction the metal/semiconductor interface system using quantum consideration .

2. Theory

One of the most important parameter for the study the properties of many material is the cross section that's defined as the number of particles passing in a time unit through the unit of area of a beam and may be represented as[11].

$\sigma_{ET} = \sum_{i=1}^{n} \sigma_{et(i)}$.....(1)

The effective stimulated cross section of electron transfer depended on the lifetime and given by [12].

$\sigma_{ET} = \frac{E(\vartheta)}{8\pi n^2 c \vartheta^2 \tau_{ET}}$.....(2)

Where $E(\vartheta)$is the driving force energy , ϑ is the wave number $\vartheta = \frac{1}{\lambda}$, n is the mean refrective index , c is velocity of light and $\tau_{ET}$is the lifetime of electron transfer

The lifetime of electron transfer is related to the rate of electron transfer is given by [13].

$\tau_{ET} = \frac{1}{\mathbb{R}_{et}}$.....(3)

Where the $\mathbb{R}_{et}$ is the probability of electron transfer at metal/semiconductor that's depending exponentially on distance with a decay constant and may be write [14].

$$\mathbb{R}_{et} \approx \frac{2\pi}{\hbar} \frac{N_{in} V_{sem}}{\beta \sqrt{4\pi \mathrm{E}_{\mathrm{met}}^{\mathrm{sem}} \mathrm{k_B T}}} \exp - \frac{(\Phi_{met} - \chi_{sem})}{\mathrm{k_B T}} \langle \left|\overline{\Lambda(0)}\right|^2 \rangle \left[[\pi \mathrm{k_B T} - \frac{1}{4\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}} \mathrm{k_B T}} \left(\frac{(\pi \mathrm{k_B T})^3}{4} \right) \right] \text{.....(4)}$$

Here , Φ_{met} is the work function of metal, χ_{sem} is affinity of semiconductor, N_{in}consentration of electron, V_{sem} volume of unit cell for semiconductor, β penetration factor and the coupling matrix element coefficient$\langle \overline{\Lambda(0)} \rangle$for metal and semiconductor interface .

Inserting Eq.(4) in Eq(3) results

$$\tau_{ET} = \frac{1}{\mathbb{R}_{et}} = \frac{\hbar}{2\pi} \frac{\beta \sqrt{4\pi \mathrm{E}_{\mathrm{met}}^{\mathrm{sem}} \mathrm{k_B T}}}{N_{in} V_{sem}} \exp \frac{(\Phi_{met} - \chi_{sem})}{\mathrm{k_B T}} (\langle \left|\overline{\Lambda(0)}\right|^2 \rangle)^{-1} \left[[\pi \mathrm{k_B T} - \frac{1}{4\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}} \mathrm{k_B T}} \left(\frac{(\pi \mathrm{k_B T})^3}{4} \right) \right]^{-1} \text{.....(5)}$$

Then the cross section of electron transfer can obtained by substituting Eq.(5) in Eq.(2) to gate

$$\sigma_{ET} = \frac{N_{in} V_{sem}}{4\hbar n^2 c \vartheta^2} \frac{E(\vartheta)}{\beta \sqrt{4\pi \mathrm{E}_{\mathrm{met}}^{\mathrm{sem}} \mathrm{k_B T}}} \exp \frac{-(\Phi_{met} - \chi_{sem})}{\mathrm{k_B T}} \langle \left|\overline{\Lambda(0)}\right|^2 \rangle \left[[\pi \mathrm{k_B T} - \frac{1}{4\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}} \mathrm{k_B T}} \left(\frac{(\pi \mathrm{k_B T})^3}{4} \right) \right] \text{.....(6)}$$

However the quantum driving force energy $E(\vartheta)$ is satisfy the energy that needed to drive an electron to transfer from donor state to an acceptor state when a light is incident on the donor acceptor system, and given by [15]

$E(\vartheta) = hf - \mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}$.....(7)

Where h is Planck constant, f is the frequency, $f = \frac{c}{\lambda}$ Where c is the velocity of light, λ is the wavelength and $\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}$ is transfer energy orientation .

The transfer energy orientation $\mathrm{E}_{\mathrm{met}}^{\mathrm{sem}}$ 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/semiconductor interface is given by [16]

$$E_{semi.}^{met} = \frac{e^2}{4\pi\varepsilon_0}\left[\frac{1}{2R_{met}}\left(\frac{1}{n_{met}^2} - \frac{1}{\varepsilon_{met}}\right) + \frac{1}{2R_{semi}}\left(\frac{1}{n_{semi}^2} - \frac{1}{\varepsilon_{semi}}\right) - \frac{1}{4D_{semi}}\left(\frac{n_{met}^2 - n_{semi}^2}{n_{met}^2 + n_{semi}^2}\frac{1}{n_{semi}^2} - \frac{\varepsilon_{met} - \varepsilon_{semi}}{\varepsilon_{met} + \varepsilon_{semi}}\frac{1}{\varepsilon_{semi}}\right) - \frac{1}{4D_{met}}\left(\frac{n_{semi}^2 - n_{met}^2}{n_{semi}^2 + n_{met}^2}\frac{1}{n_{met}^2} - \frac{\varepsilon_{semi} - \varepsilon_{met}}{\varepsilon_{semi} + \varepsilon_{met}}\frac{1}{\varepsilon_{met}}\right) - \frac{1}{R_{met-semi}}\left(\frac{1}{n_{met}^2 + n_{semi}^2} - \frac{1}{\varepsilon_{semi} + \varepsilon_{met}}\right)\right] \text{.....(8)}$$

Where 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 semiconductor ,metal to interface and metal-semiconductor , n_{met} , ε_{met} are the optical and 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 a spherical approach [17].

$R = \left(\frac{3M}{4\pi N\rho}\right)^{\frac{1}{3}}$..... (9)

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

3. Results

Investigation and description of the cross section for electron transfer σ_{ET} at metal/semiconductor system theoretically is depending on many coefficient , one of these important parameters is the driving force energy $E(\vartheta)(eV)$. The driving force energy $E(\vartheta)(eV)$ is the energy required to the electron transfer interaction at the system. Its can be evaluated using Eq(7) with calculated the transfer energy orientation energy using Eq.(8) .

The calculation of the transfer energy orientation $E_{met}^{sem}(eV)$) may be fullfiled with estimation the radi of Ag by Eq,(9) with inserting the values of Avogadro's constant $N = 6.02 \times 10^{23} \frac{Molecule}{mol}$,molecular weight $M = 107.87$[18]and density masses $\rho = 10.43$[18] for Ag, the radi results is 1.44 A . The transfer energy orientation $E_{met}^{sem}(eV)$) have been estimation by inserting the raadi Ag valus 1.44 A with the refrective index and dielectric constant for Si, ZnO ,TiO_2 from table(1) in Eq.(8).

Table (1): Common properties of semiconductor.

Properties	Si[19]	TiO_2	ZnO
Atomic weigh	28.09	79.866 [20]	81.38
Crystal structu	Diamond	Tetragonalrut	Wurtzite[23
Density (g/cm	2.328	4.23[20]	5.66 [23]
Refractive ind	3.3	2.609[20]	2.00337[24
Dielectric const	11.9	10.2[20]	8.5 [23]
Effective densit states in conduc band, N_C (cm	2.8 x 10^{1}	1.163× 10^{19}[	2.22*10^24
Energy gap (eV 300K	1.12	3.02[22]	3.4[23]
Lattice constant	5.4310	a = 4.5936 c =2.9587[2	a=0.32495,c= 5206[23]
Melting point (	1415	1.843°C[20	1975°C
Radius(Å)	1.920	1.95612	3.8025
Electron affinity,	4.05	4.2[22]	4.5[25]

The results of transfer energy orientation E_{met}^{sem}(eV)) are 0.9839 for Ag / Si, 0.6094 for Ag / TiO_2 and 0.4326 for Ag / Zno semiconductor interface. The driving force energy $E(\vartheta)(eV)$ evaluated using Eq(7) with results of the transfer energy orientation 0.9839, 0.6094 and 0.4326 eV for Ag / Si, Ag / TiO_2 and Ag / Zno system respectively and results are shown in table(2)

Table (2): Results of Driving force energy for Ag metal with Si , TiO_2 and ZnO semiconductor.

System	Driving force energy				
	400nm	500nm	600nm	700nm	800nm
Ag-Si	2.10985	1.4911	1.0786	0.7839	0,5629
Ag- TiO_2	2.48435	1.8656	1.4531	1.1584	0.9374
zno -Ag	2.66115	2.0424	1.6299	1.3352	1.1142

The probability of cross section for electron transfer σ_{ET} have been evaluated according on Eq.(6) that's a results of a simple model derived due to quantum consideration with continuum state level for Ag metal and Si,$TiO_2$and ZnO semiconductors state levels . Cross section is calculated depending on the estimation of the driving force energy $E(\vartheta)$, transfer energy orientation, wave number ϑ, mean refrective index n , amplitude of electronic coupling coefficient $\langle\left|\overline{\Lambda(0)}\right|^2\rangle$and the lifetime of electron transferτ_{ET} coefficients . The lifetime of electron transferτ_{ET} was eva;iated according on the transfer energy orientation energyE_{met}^{sem}, ,work function of metal Φ_{met}, affinity of semiconductor χ_{sem},concentration of electron n_{in},volume of unit cell for semiconductor V_{sem},penetration factor β, temperature T(K) .

The results of cross section of electron transfer can be obtained using the expression (6) and inserting the transfer energy orientation $E_{met}^{sem}(eV)$ data for twelve Ag /Si, Ag /TiO_2 and Ag /ZnO systems, concentration of electron n_{in},volume of unit cell for semiconductor V_{sem} from table(1) ,penetration factor β=$1\times10^{-10}\,m^{-1}$, and the coupling matrix element 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 $0.8\text{x}10^{-11}(\,eV)^2$[4] for metal and semiconductor and calculation of the driving force energy $E(\vartheta)$ from table(2) with A MATLAB program has been formulated to evaluation the probability of cross section for electron transfer at metal/semiconductor interface system .

Results data of evaluation are listed in tables (3),(4), and (5), for Ag /Si, Ag /TiO_2 and Ag /ZnO systems respectively.

Table (3): Results data of the cross section for electron transfer σ_{ET} at Ag / Si devices due to variety coupling coefficient $\langle|\overline{\Lambda(0)}|^2\rangle$,at 300 K

Cross section for electron transfer $\sigma_{ET}(m^2)$									
Wave lengt (nm)	*Coupling matrix element* $\langle|\overline{\Lambda(0)}|^2\rangle$ x$10^{-11}(eV)^2$								
	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8
400	1.903E-16	2.1415E-16	2.3795E-16	2.6172E-16	2.855E-16	3.0933E-16	3.3313E-16	3.570E-16	3.8084E-16
500	2.101E-16	2.3648E-16	2.6276E-16	2.8901E-16	3.152E-16	3.4158E-16	3.6786E-16	3.942E-16	4.2055E-16
600	2.189E-16	2.4633E-16	2.7370E-16	3.0104E-16	3.284E-16	3.5580E-16	3.8318E-16	4.106E-16	4.3806E-16
700	2.189E-16	2.436E-16	2.7075E-16	2.9780E-16	3.248E-16	3.519E-16	3.7905E-16	4.062E-16	4.3339E-16
800	2.031E-16	2.2854E-16	2.5360E-16	2.7930E-16	3.047E-16	3.3011E-16	3.5551E-16	3.810E-16	4.0643E-16

Table (4): Results data of the cross section for electron transfer σ_{ET} at at Ag / TiO_2 devices due to variety coupling coefficient $\langle|\overline{\Lambda(0)}|^2\rangle$,at 300 K

Cross section for electron transfer $\sigma_{ET}(m^2)$									
Wave Length (nm)	*Coupling matrix element* $\langle|\overline{\Lambda(0)}|^2\rangle$ x$10^{-11}(eV)^2$								
	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8
400	1.843E-14	2.074 E-14	2.3045 E-14	2.5346 E-14	2.765 E-14	2.9956 E-14	3.2261 E-14	3.456 E-14	3.6871 E-14
500	E-142.573	2.8955E-14	3.2173E-14	3.5385E-14	3.8603E-14	4.1821E-14	4.5039E-14	4.8257 E-14	5.1475E-14
600	2.886E-14	3.247 E-14	3.6085E-14	3.9688 E-14	4.3298 E-14	4.6907 E-14	5.0516E-14	5.4126 E-14	5.7735E-14
700	3.132E-14	3.523 E-14	3.9155E-14	4.3065 E-14	4.6981 E-14	5.0897E-14	5.4814E-14	5.8730 E-14	6.26466E-14
800	3.3106E-14	3.7246 E-14	4.1385E-14	4.5517 E-14	4.9656 E-14	5.3795 E-14	5.7935E-14	6.20744 E-14	6.6213E-14

Table (5): Results data of the cross section for electron transfer σ_{ET} at at Ag / Zno devices due to variety coupling coefficient $\langle|\overline{\Lambda(0)}|^2\rangle$,at 300 K

Cross section for electron transfer $\sigma_{ET}(m^2)$									
Wave length (nm)	*Coupling matrix element* $\langle|\overline{\Lambda(0)}|^2\rangle$ x$10^{-11}(eV)^2$								
	0.4	0.45	0.5	0.55	0.6	0.65	0.7	0.75	0.8
400	9.1766E-1	1.0322 E-9	1.1467 E-9	1.2613E-9	1.3764 E-9	1.4910 E-9	1.6055 E-9	1.7201 E-9	1.8346 E-9
500	1.1004E-9	1.2378 E-9	1.3751 E-9	1.5125E-9	1.6506 E-9	1.7880 E-9	1.9254 E-9	2.0627 E-9	2.2001 E-9
600	1.2639E-9	1.4216 E-9	1.5794 E-9	1.7372E-9	1.8958 E-9	2.0536 E-9	2.2114 E-9	2.3691 E-9	2.5269 E-9
700	1.4100E-9	1.5860E-9	1.1.7620 E-	1.9380E-9	2.1150 E-9	2.2910 E-9	2.4671 E-9	2.6431 E-9	2.81911 E-9
800	1.5368E-9	1.7287E-9	1.9205 E-9	2.1123E-9	2.3053 E-9	2.4971 E-9	2.6889 E-9	2.8808 E-9	3.07265 E-9

4. Discussion

A simple model have been used to investigation the cross section for electron transfer at Ag /Si ,Ag/TiO_2,and Ag/ZnO devices system depending on the quantum theory. Due to this model, we assume the wave function for electron transmission interaction was satisfied all Hilbert space properties . According on this model, the electron transfer interaction has been occurring due to tunnelling region from the overlapping wave functions at interface state **.**

At the interface ,one assumes the two material energy levels state are continuum for system to alignment energies to happen the electron transfer between two material different structures electron state in metals, and also its electronic density on various metal surfaces has more than in conduction band of semiconductor. These electronic states are brought into resonance by fluctuations of wave function of metal and semiconductor system and this resonance is the transition state of electron transfer reaction. The probability of cross section $\boldsymbol{\sigma_{ET}}$ in Eq.(6)indicates that the interaction of electron depending on the driving force energy $E(\vartheta)$, wave number ϑ, mean refrective index n , amplitude of electronic coupling coefficient $\langle|\overline{\Lambda(0)}|^2\rangle$and the lifetime of electron transferτ_{ET} that's depending on the transfer energy orientation energy, concentration of electron n_{in},volume of unit cell for semiconductor V_{sem}, penetration factor β, and temperature T(K). First of all the evaluation of cross section parameter requires us to evaluation the driving force energy $E(\vartheta)$ that's important parameter

to enables us to evaluation the cross of section of electron at metal/semiconductor system. It is estimation depending on the spectrum of devices and the transfer energy orientation for system .A driving force energy $E(\vartheta)$in Eq.(7) refers to the basic physical relations for the interaction of light with the metal/semiconductor system[19-23] .

The results of the cross section in tables (3 to 5) for Ag/semiconductor systems are effected by the driving force energy. The cross section is large for large driving force energy and vice versa, this indicates that the cross section are dependent on the driving force energy and its support the energy to interaction.

The cross section increases with the increases of the driving force energy ,this indicates that Ag/ZnO, are more reactive to electron transfer interaction compare with Ag/ TiO_2 and Ag/Si systems . On the other hand, the factor related to the cross section for electron transfer is related to the coupling coefficient term $\left|\overline{\Lambda(0)}\right|$(eV) that has been controlled to the electron transfer interaction between the metal and semiconductor system. Electronic coupling is evidently reflected that the capability to electron transfer interaction and determine by the alignment of the levels state of semiconductor with respect to the metal Fermi energy. Hence, the coupling coefficient have been used in the range from $(0.4-\ 0.8)$(eV) depending on the typical results of experimental data [4]. Cross section of electron become increasing when the coupling coefficient matrix element between metal and semiconductor system will be increasing that's shown from data in tables (3 to 5) for Ag/ZnO, Ag/ TiO_2 and Ag/Si systems.

Afterwards a theoretical analysis of the cross section evaluation data sets has to be performed for the joint determination of the driving force energy, transfer energy orientation,coupling coefficient and life time into the cross section expression in Eq.(6). The probability of cross section $\boldsymbol{\sigma_{ET}}$ results data are large for Ag/ZnO system compare with Ag/Si and Ag/TiO_2 system, this refers that there is Ag is reactive to ZnO semiconductor than TiO_2 and Si and electron transfer reaction occurs.

5. Conclusion

The cross section for electron transfer in metal/semiconductor system has been studies theoretically depending on quantum considerationand one can conclusions that simple model was good tool enable us to described the cross section in the metal, semiconductor interface system.

On the other hand the data results of cross section for electron transfer at metal/semiconductor system enable to elective the system to use or not in many applied physical . Cross section for electron transfer related to the driving force energy and coupling coefficient and the cross section is increases with increases the driving force energy and coupling coefficient and vice versa.

6. References

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