Theoretical Estimation of Electronic Flow Rate at Al-TiO₂ Interfaces System

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Abstract. The mechanism of the electronic flow rate at Al-TiO₂ interfaces system has been studied using the postulate of electronic quantum theory. The different structural of two materials lead to suggestion the continuum energy level for Al metal and TiO₂ semiconductor. The electronic flow rate at the Al-TiO₂ complex has affected by transition energy, coupling strength and contact at the interface of two materials. The flow charge rate at Al-TiO₂ is increased by increasing coupling strength and decreasing transition energy.

Key words: Electronic Flow Rate, Al-TiO₂ and Interface.

1. Introduction
The reactions of an electronic transfer are a simple process that occurs in donor-acceptor media and it is an elementary electronic transition from an atom to atom system. It is one of the main reaction in physics devices involves oxidation-reduction state systems. It is developed since the beginning of the twentieth century [1]. Electronic transfer over distances has been investigated extensively in both experimental and theoretical studies in different inhomogeneous devices and through monolayers on the electrode system [2]. Nowadays, structure evaluations of electronics are important tools to investigate the physical properties of materials [3]. The electronic transfer due to metal/semiconductor interface has been devoted to investigate the origin of the potential barrier height at interface and effect on the electrical characteristics of this device [4]. Titanium dioxide (TiO₂) produces by low cost and higher stability and has very attractive research for mechanical, electronic and optical properties material. TiO₂ is used in many electronic applications such as adsorbents and catalytic systems [5-6]. Generally, the transition reaction at metal/semiconductor interfaces is a considerable inhomogeneous quantity of states. Therefore, the flow rate of transfer improves the performance of metallic junction devices; the transfer of electron continues across the interface above the potential junction [7]. In this work, we study the electronic flow rate at Al-TiO₂ System with coupling, electronic reorientation energies and potential coefficients. We investigate the transition rate for Al-TiO₂ structure with concerning to driving force and transition energy of the system.
2. Theory

The electronic flow rate (EFR) refers to the electronic transfer current through donor-acceptor system. It is evaluated according to quantum theory for continuum energy levels. The flow rate EFR from metal to semiconductor interface in the medium of Al - TiO₂ is given by [8].

\[
EFR_{Al}^{TiO₂} = \frac{2\pi}{h} \left| \Psi_{Al}^{TiO₂} \right|^2 \Lambda_{Al}^{TiO₂}
\]

(1)

Where \( \left| \Psi_{Al}^{TiO₂} \right|^2 \) is squaring coupling and \( \Lambda_{Al}^{TiO₂} \) is Franck-Condon factor. The Franck-Condon \( \Lambda_{Al}^{TiO₂} \) can be evaluated due to perturbation approximation according to potential and can be written as [9].

\[
\Lambda_{Al}^{TiO₂} = (\frac{G_{D}}{G_{S}}) \cdot \frac{1}{\sqrt{\varepsilon}} \exp \left( -\frac{(\phi_{Al}^{TiO₂} + G_{D})^2}{G_{D}^2} \right)
\]

(2)

Where \( G_{D} \) is reorientation energy, \( \kappa = 4\pi k_B T \) (where \( k_B \) is Boltzmann constant, \( T \) is room temperature, and \( \phi_{Al}^{TiO₂} \) is activity energy). Substitute Eq.(2) in Eq.(1) and integrate over space of system gives:

\[
EFR_{Al}^{TiO₂} = \frac{2\pi}{h} \int_{-\infty}^{\infty} \left| \Psi_{Al}^{TiO₂} \right|^2 \left( \frac{G_{D}}{G_{S}} \right) \cdot \frac{1}{\sqrt{\varepsilon}} \exp \left( -\frac{(\phi_{Al}^{TiO₂} + G_{D})^2}{G_{D}^2} \right) d\varepsilon
\]

(3)

Under the condition of electrons above the Fermi level due to the activity energy (E) for system is reduced:

\[
\phi_{Al}^{TiO₂} = \phi_{Al}^{TiO₂} - E
\]

then potential must be written as [10].

\[
\Psi_{Al}^{TiO₂} = \left( \frac{\phi_{Al}^{TiO₂} + G_{D} + E}{G_{S}} \right)^{\frac{1}{2}}
\]

(4)

Due to continuum levels material, Eq.(3) must be formed according to density function \( F(\varepsilon) \):

\[
EFR_{Al}^{TiO₂} = \frac{2\pi}{h} \int_{-\infty}^{\infty} \left| \Psi_{Al}^{TiO₂} \right|^2 \left( \frac{G_{D}}{G_{S}} \right) \cdot \frac{1}{\sqrt{\varepsilon}} \exp \left( -\frac{(\phi_{Al}^{TiO₂} + G_{D} - E)^2}{G_{D}^2} \right) F(\varepsilon) d\varepsilon
\]

(5)

Where \( F(\varepsilon) \) is the Fermi density of electrons at Al/TiO₂ system and may be written as [11]:

\[
F(\varepsilon) = \frac{1}{e^{\frac{\varepsilon + \phi_{Al}^{TiO₂}}{kT}} + 1}
\]

(6)

The exponential term in Eq.(5) simplified to:

\[
\exp \left( -\frac{(\phi_{Al}^{TiO₂} + G_{D} - E)^2}{G_{D}^2} \right) = \exp \left( -\frac{\phi_{Al}^{TiO₂} + G_{D}^2}{G_{D}^2} \right)^2 2E(\phi_{Al}^{TiO₂} + G_{D}) - E^2
\]

(7)

And must be approximated to:

\[
\exp \left( -\frac{(\phi_{Al}^{TiO₂} + G_{D} - E)^2}{G_{D}^2} \right) \approx \exp \left. \frac{\phi_{Al}^{TiO₂} + G_{D}^2}{G_{D}^2} \right) \exp \frac{-E^2}{G_{D}^2}
\]

(8)

The potential of Al/TiO₂ system interfaces at powering term in Eq.(5) can be reformed to:

\[
\Psi_{Al}^{TiO₂} = \left( \frac{\phi_{Al}^{TiO₂} + G_{D}}{G_{S}} \right)^{\frac{1}{2}} \approx \left( \frac{\chi_{Al} - \chi_{TiO₂}}{kT} \right)\frac{1}{G_{S}}
\]

(9)

Where \( \chi_{Al} \) is work function for Al and \( \chi_{TiO₂} \) is electron affinity for TiO₂.

Inserting Eq.(9) and (8) in Eq.(5) result [12].

\[
EFR_{Al}^{TiO₂} = \frac{2\pi}{h} \int_{-\infty}^{\infty} \left| \Psi_{Al}^{TiO₂} \right|^2 \left( \frac{G_{D}}{G_{S}} \right) \cdot \frac{1}{\sqrt{\varepsilon}} \exp \left( -\frac{\chi_{Al} - \chi_{TiO₂}}{kT} \right) F(\varepsilon) \exp \frac{-E^2}{G_{D}^2} d\varepsilon
\]

(10)

The Eq.(10) has reformed to:

\[
EFR_{Al}^{TiO₂} \approx \frac{2\pi}{h} \left( \frac{G_{D}}{G_{S}} \right) \cdot \frac{1}{\sqrt{\varepsilon}} \exp \left( -\frac{\chi_{Al} - \chi_{TiO₂}}{kT} \right) \int_{-\infty}^{\infty} F(\varepsilon) \exp \frac{-E^2}{G_{D}^2} d\varepsilon
\]

(11)
The integral in Eq.(11) could be solved using mathematical physics to get [13]:
\[
\int_{-\infty}^{\infty} F(\epsilon) \exp \left( -\frac{\epsilon^2}{\kappa T} \right) d\epsilon \approx \left[ \pi \kappa T - \frac{(\pi \kappa T)^2}{16\pi \sigma_S^2} \right]
\]
(12)
The average of flow rate electronic current EFR is given by:
\[
\frac{EFR_{\text{Al}}^{\text{TiO}_2}}{n} = \frac{V_{\text{TiO}_2}}{n} EFR_{\text{Al}}^{\text{TiO}_2}
\]
(13)
Then Eq.(12) with Eq.(13) becomes:
\[
\frac{EFR_{\text{Al}}^{\text{TiO}_2}}{n} = \frac{2\pi V_{\text{TiO}_2}}{h} (\kappa g_S^D)^{-1} \exp \left( \frac{1}{kT} \right) \left[ \kappa_{\text{Al}}^{\text{TiO}_2} \right]^2 \left[ \pi \kappa T - \frac{(\pi \kappa T)^2}{16\pi \sigma_S^2} \right]
\]
(14)
The electronic reorientation energies for Al/TiO\textsubscript{2} system is [14]
\[
G_{\text{Al}}^D (eV) = \frac{e^2}{8\pi\epsilon} \left( \frac{1}{2R_{\text{Al}}} \frac{1}{d_{\text{Al}-\text{TiO}_2}} \right) \left( n_{\text{Al}}^2 e_{\text{Al}} + n_{\text{TiO}_2}^2 e_{\text{TiO}_2} \right) - \frac{1}{4R_{\text{Al}}} \left( n_{\text{Al}}^2 - n_{\text{TiO}_2}^2 \right) - \frac{1}{d_{\text{Al}-\text{TiO}_2}} \left( n_{\text{Al}}^2 + n_{\text{TiO}_2}^2 \right)
\]
(15)
Where e is electronic charge, \(e^*\) is space permittivity, \(\mathfrak{f}(n_{\text{Al}}^2, e_{\text{Al}}) = \left( \frac{1}{n_{\text{Al}}^2} - \frac{1}{\epsilon_{\text{Al}}} \right)\) and \(\mathfrak{f}(n_{\text{TiO}_2}^2, e_{\text{TiO}_2}) = \left( \frac{1}{n_{\text{TiO}_2}^2} - \frac{1}{\epsilon_{\text{TiO}_2}} \right)\) are the polarity function of two material system respectively, \(n_{\text{Al}}^2\) and \(e_{\text{Al}}\) are the refractive index and dielectric constant of metal(Al), \(n_{\text{TiO}_2}^2\) and \(e_{\text{TiO}_2}\) are the refractive index and dielectric constant of TiO\textsubscript{2}, \(R_{\text{Al}}\) is Aluminum radius, and \(d_{\text{Al}-\text{TiO}_2}\) is the distance between TiO\textsubscript{2} and Al. Then the radii of any material estimates are [15]:
\[
R_{\text{mat}} = \left( \frac{3}{4\pi} \frac{M_{\text{mat}}}{N_{\text{mat}}} \right)^{\frac{1}{3}}
\]
(16)
Where \(M_{\text{mat}}\) is the molecular weight, \(N\) is Avogadro's number, and \(\rho_{\text{mat}}\) is the matter density.

3. Results and discussion
The electric flow rate has been estimated by using a simple numerical model for transfer in Al-TiO\textsubscript{2} system, it has been discussed and predicted by experimental results. It assesses to explained the effect of transition energy parameters on the performance of transfer in metal-semiconductor interfaces. The performance of transfer can be discussed in terms of electronic flow rate of the device. In order to evaluate the transition flow rate, we can estimate the transition energy according to Eq (15) with the estimation of the radii of Al and TiO\textsubscript{2} using Eq (16) by inserting atomic density and molecular weight from Tables 1 and 2 of Al and TiO\textsubscript{2} material and resulted in Tables 1 and 2, respectively.

**Table 1. Properties of Al Metal.**

| Properties                  | Values               |
|-----------------------------|----------------------|
| Atomic weight               | 26.982 [16]          |
| Crystal structure           | cubic                |
| Lattice constant (nm)       | 0.405 [17]           |
| Dielectric constant         | 1.6-1.8              |
| Refractive index            | 0.2 to 1.20 [18]     |
| Density (g/cm\textsuperscript{3}) | 2.70 [16]          |
| Work function               | 4.05 [19]            |
| Calculated radius (nm)      | 0.143                |
Table 2. Characteristic of TiO$_2$ semiconductor.

| Properties                        | Values                      |
|-----------------------------------|-----------------------------|
| Chemical Formula                  | TiO$_2$                     |
| Atomic weight                     | 79.866 [20]                 |
| Density (g/cm$^3$)                | 4.23[20]                    |
| Crystal structure                 | Tetragonal rutile[20]       |
| Melting point (°C)                | 1843°C[20]                  |
| Refractive index                  | 2.609[20]                   |
| Dielectric constant               | 15.10 [21]                  |
| Volume (Å$^3$)                    | 62.432[22]                  |
| Energy gap (eV) at 300K           | 3.02[22]                    |
| Lattice constant (Å)              | a=4.5936                    |
|                                   | c =2.9587[22]               |
| Electron affinity (eV)            | 4.2[22]                     |
| Calculated Radius(Å)              | 1.95612                     |
| Effective density of states in conduction band, N$_C$ m$^{-3}$ | $1.163 \times 10^{25}$[4] |

The transition energy is calculated using the values of primary input refractive index and dielectric constant and radii of Al and TiO$_2$ parameters which are listed in Tables 1 and 2 and inserting in Eq.(15). The results are listed in Table 3.

Table 3. Results of transition energy for Al-TiO$_2$ system.

| Refractive index($n_{Al}$) | Dielectric constant($\varepsilon_{Al}$) | Transition energy $g_s^D$ (eV) | Refractive index($n_{Al}$) | Dielectric constant($\varepsilon_{Al}$) | Transition energy $g_s^D$ (eV) |
|----------------------------|----------------------------------------|-------------------------------|----------------------------|----------------------------------------|-------------------------------|
| 0.2                        | 1.8                                    | 43.5806                       | 0.2                        | 1.6                                    | 43.4568                       |
| 0.4                        | 1.8                                    | 10.2653                       | 0.4                        | 1.6                                    | 10.1415                       |
| 0.6                        | 1.8                                    | 4.0937                        | 0.6                        | 1.6                                    | 3.9699                        |
| 0.8                        | 1.8                                    | 1.9315                        | 0.8                        | 1.6                                    | 1.8077                        |
| 1                          | 1.8                                    | 0.9285                        | 1                          | 1.6                                    | 0.8047                        |
| 1.2                        | 1.8                                    | 0.3817                        | 1.2                        | 1.6                                    | 0.2579                        |

From Table 3, it can be seen that the transition energy decreased with increasing the refractive index and stable dielectric constant for the same Al metal. It also increases with increasing the dielectric constant of Al metal for same refractive index and dielectric constant for TiO$_2$ semiconductor. It means that energy as a function of the polarity of Al metal dependent on energy absorption by the system because the refractive index depends on energy.

On the other hand, Eq. (14) outlined in theory can be applied to calculate and studied the electron transfer flow rate in Al-TiO$_2$ system. To investigate the electronic transfer cross interface of Al-TiO$_2$ using quantum theory, we have considered continuum energy levels for two materials. All parameters of Al metal and TiO$_2$ are taken from Tables 1, 2 and 3 and take the strength coupling from literature.
In order to show the effect of polarity of metal, we take two different dielectric constants for Al metal. Tables 4 and 5 show that the flow rate increased with decreasing of transition energy for two dielectric constant 1.8 and 1.6 respectively, in a way that flow rate increases with coupling strength for two Table 4 and 5; this indicates that the energy levels for two materials must be closed to each other with high electrons concentration closed interface of the system. Similar behaviors of flow rate in Table 4 and 5 at dielectric constant with $\varepsilon_{Al}$=1.8 and 1.6 indicate that the structure and properties of Al metal is important effect on the behavior of flow rate of system. Specifically, we have considered the same properties of TiO$_2$ semiconductor with Al metal to avoid the effects of polarity of TiO$_2$ on the flow rate. However; the results were obtained from two tables (4-5) which show that flow rate increased with decreasing dielectric constant of Al metal.

### Table 4. Electronic Flow Rate at Al-TiO$_2$ Interfaces System with dielectric constant $\varepsilon_{Al}$=1.8.

| Transition Energy $G^B_0$ (eV) | Electronic Flow Rate $\overline{EF}_{Al}^{TiO_2}$ (eV) | Strength Coupling (eV) |
|-----------------------------|---------------------------------|---------------------|
|                            | $4 \times 10^{-2}$              | $8 \times 10^{-2}$  | $12 \times 10^{-3}$ | $16 \times 10^{-3}$ | $2 \times 10^{-4}$ |
| 43.5806                    | 1.4455E-12                     | 2.8910E-12          | 4.3365E-13          | 5.7820E-13          | 7.2274E-15         |
| 10.2653                    | 2.9346E-12                     | 5.8926E-12          | 8.8038E-13          | 1.1738E-12          | 1.4673E-14         |
| 4.9397                     | 4.5104E-12                     | 9.0209E-12          | 1.3531E-12          | 1.8042E-12          | 2.2552E-14         |
| 1.9315                     | 6.1961E-12                     | 1.2392E-11          | 1.8588E-12          | 2.4784E-12          | 3.0980E-14         |
| 0.9285                     | 7.8424E-12                     | 1.5068E-11          | 2.3531E-12          | 3.1377E-12          | 3.9221E-14         |
| 0.3817                     | 7.5341E-12                     | 1.5068E-11          | 2.2602E-12          | 3.0136E-12          | 3.7671E-14         |

### Table 5. Electronic Flow Rate at Al-TiO$_2$ Interfaces System with dielectric constant $\varepsilon_{Al}$=1.6.

| Transition Energy $G^B_0$ (eV) | Electronic Flow Rate $\overline{EF}_{Al}^{TiO_2}$ (eV) | Strength Coupling (eV) |
|-----------------------------|---------------------------------|---------------------|
|                            | $4 \times 10^{-2}$              | $8 \times 10^{-2}$  | $12 \times 10^{-3}$ | $16 \times 10^{-3}$ | $2 \times 10^{-4}$ |
| 43.4568                    | 1.4475E-12                     | 2.8951E-12          | 4.3426E-13          | 5.7901E-13          | 7.2376E-15         |
| 10.1415                    | 2.9518E-12                     | 5.9035E-12          | 8.8553E-13          | 1.1807E-12          | 1.4759E-14         |
| 3.9699                     | 4.5730E-12                     | 9.1460E-12          | 1.3719E-12          | 1.8292E-12          | 2.2865E-14         |
| 1.8077                     | 6.3551E-12                     | 1.2710E-11          | 1.9065E-12          | 2.5420E-12          | 3.1776E-14         |
| 0.8047                     | 8.0784E-12                     | 1.6157E-11          | 2.4235E-12          | 3.2314E-12          | 4.0392E-14         |
| 0.2579                     | 4.5048E-12                     | 9.0096E-12          | 1.3514E-12          | 1.8019E-12          | 2.2524E-14         |

In order to show the effect of polarity of metal, we take two different dielectric constants for Al metal. Tables 4 and 5 show that the flow rate increased with decreasing of transition energy for two dielectric constant 1.8 and 1.6 respectively, in a way that flow rate increases with coupling strength for two Tables 4 and 5; this indicates that the energy levels for two materials must be closed to each other with high electrons concentration closed interface of the system. Similar behaviors of flow rate in Table 4 and 5 at dielectric constant with $\varepsilon_{Al}$=1.8 and 1.6 indicate that the structure and properties of Al metal is important effect on the behavior of flow rate of system. Specifically, we have considered the same properties of TiO$_2$ semiconductor with Al metal to avoid the effects of polarity of TiO$_2$ on the flow rate. However; the results were obtained from two tables (4-5) which show that flow rate increased with decreasing dielectric constant of Al metal.

### 4. Conclusion

In this study, we first conclude that the transition energy is a function of the refractive index of Al, and it decreased with increasing refractive index and increased with increasing the dielectric constant of Al metal with constant refractive index and dielectric constant for TiO$_2$ semiconductor. In fact we can conclude that transition energy is a function of polarity of Al metal. The Al-TiO$_2$ devices exhibit a continuous transition of electrons across the interface; the flow rate increased with decreasing of transition energy and increased of coupling strength. Here, we assumed continuum energy levels for
Al and TiO\textsubscript{2} material to direct transfer over closed space for two materials with high electrons concentration near interface of system. Aggregation, the transition energy and contact at interface with coupling strength coupling of Al metal with TiO\textsubscript{2} surface are key factors affected on the quantity of electronic flow rate.

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