Analysis of photoassisted field emission current in Iridium and Titanium by using Kronig-Penney potential model and transfer Hamiltonian method

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Abstract. We present here a model calculation of photoassisted field emission current (PFEC) by using transfer Hamiltonian method. Matrix element for the transition probability is calculated by using the wavefunctions which are deduced by applying the Kronig-Penney potential model PFEC is calculated for Iridium and Titanium, and the results are compared with experimental data.

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1. Introduction

Photoassisted field emission is a technique in which a metal is irradiated by an incident laser radiation of photon energy (ℏω). Photon energy is usually less than the work function (φ) of the metal. The incident radiation photoexcites the electrons to states which lies between the Fermi level and the vacuum level, hence these electrons are confined within the metal surface. A strong static electric field (~ 10¹¹ Vm⁻¹) when applied to the surface of the metal causes the photoexcited electrons to tunnel through the surface potential barrier into the surrounding vacuum. These electrons which are now emitted into the vacuum region constitute the measurable current called photoassisted field emission current (PFEC). One attractive application of photoassiated field emission (PFE) is to allow short time modulation of laser to combine photoemission and field emission which can control the duration of emission and increase the emitted peak current. This had been possible in the case of ZrC single tip and nanoscale current pulses have been emitted with laser pulses at 1064 nm illuminating a ZrC tip under high DC electric field [1]. We present here the calculation of PFEC from Iridium and Titanium by using the transfer Hamiltonian method. Matrix element for transition \( M_{fi} = \langle f | A \cdot p + p \cdot A | i \rangle \) had been evaluated by using the Kronig-Penney periodic potential [2] for photoemission studies. The calculated result of PFEC from Iridium and Titanium are compared with the experimental data as measured by [3] and [4].

2. Theory

The transfer Hamiltonian (TH) is based on the division of the tunnelling system into two subsystems. The transfer of electrons between the two subsystems is described by a term called the
transfer Hamiltonian, from which the method derived its name. The separation of the system into two subsystems is only possible if the coupling between the two subsystems is weak and the probability of an electron tunnelling through the potential barrier is small [5]. The transfer Hamiltonian method is the approximate separation of the Hamiltonian for the tunnelling system into its components which is treated as a perturbation, leading to a total Hamiltonian. The total Hamiltonian of electrons in one dimension is

\[ H = T + V_m\theta(-z) + V(z) - eFz\theta(z) \]  

(1)

Here, \( T \) is one electron kinetic energy operator, \( V_m \) the periodic metal potential, \( V(z) \) the outside potential in the absence of field and \( F \) is the high static electric field. Here \( V(z) = V_o - eFz - (e^2 / 4z) \) where \( V_o \) is the height of the potential barrier and \( -e^2 / 4z \) is the image potential.

A p-polarized radiation of photon energy \( \hbar\omega \) is incident on an electron lying at energy \( E_i \) below the Fermi level as shown in figure 1. This incident radiation, usually a laser beam causes the transition of electron from the initial state \( \psi_i \) to the final state \( \psi_f \). As this electron still lies below the vacuum level, a high electric field (~ 10^{11} \text{ Vm}^{-1}) will now cause the electron to be transmitted through the potential barrier to vacuum region thereby causing photoassisted field emission.

\[ M_{\mu} = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \left[ \psi_f^* \frac{\partial \psi_f}{\partial z} - \psi_i^* \frac{\partial \psi_i}{\partial z} \right] dz - \frac{\hbar^2 e^2}{8m} \int_{-\infty}^{\infty} \left[ \psi_f^* \left( \frac{1}{z} \right) \psi_i \right] dz \]

\[ + \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \psi_f^* \left( A_o(z) \frac{d}{dz} + \frac{1}{2} \frac{dA_o(z)}{dz} \right) \psi_i \]  

(2)

One dimensional Kronig-Penney potential is used [2] to deduce \( \psi_i \) in equation (2). In one dimension, this is given by

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**Figure 1.** Model potential used for PFE calculations for describing the band states with a surface of width \( a \).
\[ \psi_f(z) = \begin{cases} \left( \frac{m}{2\pi^2 q} \right)^{1/2} \frac{2q}{q^2 + k_f^2} (1 - iP \exp(-i\delta) \sin \delta \exp(ik_f z)) \exp(-\chi z), & \text{for } z \leq 0 \\
 + \left( \frac{m}{2\pi^2 q} \right)^{1/2} \frac{2q}{q^2 + k_f^2} (1 + iP \exp(i\delta) \sin \delta \exp(-ik_f z)) \exp(\chi z), & \text{for } z > 0 
\end{cases} \] (3)

The reflection and the transmission coefficients across the boundary plane \( P \) and \( T \) are deduced by using boundary condition and are
\[ P = -\left( \frac{\chi - ik_f}{\chi - ik_f} \right) \exp(i\delta) \sin \delta \exp(ik_f z) \]
and
\[ T = \left( \frac{2k_f \sin 2\delta}{\chi - ik_f + (k_f - \chi) \exp(i\delta)} \right) \]
where \( \delta = -\tan \left( \frac{\hbar^2 k_f}{mg} \right) \) is the phase shift introduced in the transmitted wave and \( g \) is the strength of the potential. The one dimensional final state wave function used in equation (2) is
\[ \psi_f(z) = \begin{cases} \left( \frac{m}{2\pi^2 q} \right)^{1/2} \frac{2q}{q^2 + k_f^2} \exp(ik_f z) \exp(-\alpha |z|), & \text{for } z \leq 0 \text{ (Bulk and surface)} \\
 + \left( \frac{m}{2\pi^2 q} \right)^{1/2} \frac{2q}{q^2 + k_f^2} \exp(ik_f z) + \left( \frac{q - k_f}{q + k_f} \right) \exp(-iz), & \text{for } z > 0 \text{ (Vacuum)} 
\end{cases} \] (5)

Here, \( k_i = \left( \frac{2mE_i}{\hbar^2} \right)^{1/2} \), \( k_f = \left( \frac{2mE_f}{\hbar^2} \right)^{1/2} \), \( q = \left( \frac{2m}{\hbar^2} \right)(E_f - V_o) \), \( \chi = \left( \frac{2m}{\hbar^2} \right)(V_o - E_i) \) (6)

where, \( E_f = E_i + h\omega \alpha \) and, \( V_o = E_f + \phi \).

The term \( e^{-\alpha |z|} \) is responsible for the inelastic scattering of the electrons on the surface and bulk side. The one dimensional form of vector potential of interest used in equation (2) for the bulk \((z < -a)\), surface \((-a \leq z \leq 0)\) and vacuum \((z > 0)\) regions are given by [8]
\[ A_o(z) = \begin{cases} A_i, & \text{for } z \leq -a \text{ (Bulk)} \\
 + \frac{A_i e(\omega) a}{(a + [1 - e(\omega)] |z|)}, & \text{for } -a \leq z \leq 0 \text{ (Surface)} \\
 A_i e(\omega), & \text{for } z \geq 0 \text{ (Vacuum)} 
\end{cases} \] (7)

where, \( A_i = -\sin 2\theta_i \left[ \frac{e(\omega) - \sin^2 \theta_i}{e(\omega) \cos \theta_i} \right]^{1/2} \) is a constant depending on the dielectric function \( e(\omega) \) and angle of incidence \( \theta_i \).

Photoassisted field emission current density can be calculated by using the formula [6]
\[ \frac{d\tilde{j}(E)}{dE} = \left( \frac{2\pi e}{h} \right)^2 |M_{\beta}|^2 D(W) \delta(E_f - E_i) \delta(E - E_i) f(E_i) \] (8)
The transmission probability $D(W)$ used in equation (8) had been calculated by [7] which is

$$D(W) = \left[ \frac{W^{1/4} \pi^{1/2}}{(\hbar e F)^{1/6}} \right] \left[ \frac{2i k_i}{(ik_i + \chi)} \right] \left( 2m \right)^{1/2} \times \exp \left[ -i \left( \frac{2W^{3/2} (2m)^{1/2}}{3\hbar e F} + \frac{\pi}{4} \right) \right].$$

(9)

As the expansion in equation (8) cannot be solved analytically, PFEC is evaluated by writing FORTRAN programs.

3. Results and discussions

Formalism developed for calculating the photoassisted field emission current (PFEC) by using the transfer Hamiltonian method is applied to the case of Ir and Ti. We have calculated PFEC as a function of applied field, location of electron states with reference to a Fermi level for surface width $a = 10$ a.u. and narrow surface width ($a \approx 0$). As it is a theoretical calculation, we have assumed the following data both for Ir and Ti.

- Potential barrier height ($V_0$) = 15 eV,
- Work function ($\phi$) = 4.928 eV,
- Fermi energy ($E_F$) = 10.06 eV,
- Scattering factor ($\alpha$) = 0.35
- Angle of incidence = 45°

The experimental values of dielectric constants $\varepsilon(\omega)$ had been used for evaluating the vector potential $A_\omega(z)$ given by equation (7).

3.1 Iridium

Plot of PFEC as a function of applied electric field for $a = 10$ a.u., is shown in figure 2. Here we have shown the plots of PFEC for the photon energies $\hbar \omega = 1.96$ eV and 2.70 eV. It is found that as the values of applied field is increased, PFEC decreases from a high value in an exponential manner for both the values of photon energies 1.96 eV and 2.70 eV respectively. The exponential decrease in the PFEC is due to the presence of exponential term in transmission probability [3] have also experimentally measured PFEC in the case of Iridium and compared with their calculated true photocurrent results. It was found that PFEC decreases from a high value towards zero when the applied field is increased both for photon energies 1.96 eV and 2.70 eV respectively. The measured PFEC decreases but not exponentially in both the cases [3].

Figure 2. Plot of PFEC against applied field $F$ in Iridium for photon energies 1.96 eV and 2.70 eV. Initial state energy $E_i$ = 1 eV below Fermi level, and angle of incidence of photon radiation is 45°, surface width $a = 10$ a.u.
Plot of PFEC as a function of initial state energy of the electron with respect to the Fermi level is shown in figure 3. PFEC is plotted for $a = 10$ a.u. for photon energies 1.96 eV and 2.70 eV respectively. For both the photon energies, peak in PFEC occurs at initial state energy $-9$ eV below $E_F$ (Fermi level). It is seen from the figure that peak is higher for 1.96 eV photon energy than 2.70 eV. Also occurrence of peaks for both photon energies at the same location of initial state energy i.e., $-9$ eV below $E_F$. This is attributed to the contribution from the $d$-electron states in the valence band.

In figure 4, we have shown the plots of matrix element $M_{f|i} = \langle f | A | p + p_{A} | i \rangle$ and calculated PFEC as a function of incident photon energies. Both $M_{f|i}$ and PFEC increases as photon energy of the incident laser radiation increases and then showed a maxima at 2 eV photon energy. Beyond 2 eV, both showed decrease in the magnitude for $M_{f|i}$ and PFEC.

At 3.5 eV, a second peak is observed this is due to the effect of applied field in the surface. Similar trends in the behaviour of $M_{f|i}$ and PFEC is expected because $M_{f|i}$ is involved directly in the formula for calculating PFEC in equation (8).

### 3.2 Titanium

Plot of variation of PFEC as a function of applied field for surface width $a = 10$ a.u. is shown in figure 5. Plot is shown in the case of photon energies 1.96 eV and 2.70 eV respectively. Here also we find that just like in the case of Iridium, the PFEC decreases from a high value as applied field increases. The decrease in PFEC is exponential in nature as in the case of Iridium. Reference [4] has also shown experimentally that PFEC decreases from high value toward minimum as applied field is increased. Calculated results as obtained by [4] also showed similar trends.
Figure 5. Plot of PFEC against applied field $F$ in Titanium for photon energies 1.96 eV and 2.70 eV. Initial state energy $E_i = 1.0 \text{ eV}$ below Fermi level, and angle of incidence of photon radiation is $45^\circ$, surface width $a = 10 \text{ a.u.}$

Figure 6. Plot of PFEC against initial state energy $E_i$ below Fermi level ($E_F = 0.0$) in Titanium for photon energies 1.96 eV and 2.70 eV. Here value of applied field $F = 3.08 \times 10^{11} \text{ Vm}^{-1}$ and angle of incidence of photon radiation is $45^\circ$, surface width $a = 10 \text{ a.u.}$

In figure 6, plot of PFEC against initial state energies of electron are shown for two photon energies 1.96 eV and 2.70 eV respectively. Similar features in the variation of PFEC is observed with the occurrence of single peak in PFEC at initial state energy $-2 \text{ eV}$ below $E_F$ both for photon energies 1.96 eV and 2.70 eV. For the same photon energies, peaks in PFEC is also obtained at $-8 \text{ eV}$ below $E_F$, but of lower heights than at $-2 \text{ eV}$ energy below $E_F$.

The surface density of states for Ti as measured experimentally [4] for p-polarized photon energy 1.96 eV showed several peaks below $E_F$ with a maximum at $-0.15 \text{ eV}$ below $E_F$. Occurrence of peaks in PFEC at $-2 \text{ eV}$ agrees qualitatively with the experimental results of [4]. In figure 7, plots of $M_{\beta}$ and PFEC as a function of photon energy is shown. Just like in the case of Ir, variation of $M_{\beta}$ and PFEC showed similar behaviour as photon energy increases. Peaks in $M_{\beta}$ and PFEC occurs at 0.8 eV, after which plots in $M_{\beta}$ and PFEC decreases with the further increase of photon energies. The similar behaviour found in the plot of $M_{\beta}$ and PFEC as a function of photon energy in both the metals is due to the inclusion of vector potential $\mathbf{A}$ in the matrix element.
We have also checked the effect of inclusion of surface width on PFEC. For this purpose we have included a narrow surface width ($a \approx 0$) and calculated PFEC as a function of applied field. It is seen that PFEC increases drastically to a high value without showing exponential type of variation as in the case of results obtained with surface width $a = 10$ a.u.

4. Conclusions

We have shown the variation of PFEC as a function of applied electric field and photon energy by considering the transfer Hamiltonian method. Exponential decrease in PFEC both in the case of Ir and Ti shows features which were also found in the case of tungsten [9]. Calculated results of PFEC also showed similar behaviour [3] in the case of Ir and [4] in the case of Ti. Here we have calculated band structures of Ti by using the FP-LAPW method [6] which is implemented in the WIEN2k code [10].

In the case of Ir, occurrence of peaks at $-9$ eV below Fermi level is shown in figure 3. This is attributed to the surface related features. Due to the high value of work function of Iridium; it was difficult to obtain accurate data at the lower photon energies.

Further increase in applied field does not bring any change in PFEC but instead keeps it minimum. As evidence of our calculations, we find that matrix element when plotted as a function of photon energies is not constant [11]. We have also not found oscillations in PFEC as shown by [12] in their experimental results.

There are drawbacks in the method of calculations which must be taken into considerations. For example, the wavefunctions $\psi_i$ chosen are too simple. For this, we must derive $\psi_i$ with correct type of potential for the bulk and the surface regions. The wavefunctions appropriately chosen should have the symmetry well defined. Same wavefunction is used for bulk and surface regions. Further, vector potential used should be correctly defined for both the bulk and surface regions. However, even with all these shortcomings, results obtained are comparable to other results [13].

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