Resonance Electron Capture Calculation in Atom-Surface Scattering :H^- Formation at Au(100) and Ag(110) Thin Films

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Abstract

In this work, electron capture by H- projectiles in grazing scattering from Au (100) and Ag (110) thin films is studied theoretically using Perturbative method. The resonance charge transfer (RCT) on thin film appears to be quite different from that on a semi - infinite free- electron approximation metal, due to the quantization of electron movement perpendicular to the surface plane. Some of the features of RCT on thin films have already been discussed based on CAM studied , so we treat the same systems using CAM method for comparison.

1- Introduction

Charge exchange phenomena between ions and solid surfaces have been studied extensively (Guan et.al., 2000; Riccardi et.al.,2000; Edre et.al., 2001; Souda, 2002; Casagrande et.al., 2001; Almulhem, 2003). Many experimental studies on charge exchange between atom (ion) and metal surfaces have been performed by scattering fast atoms or ions off clean surfaces under grazing angle of incident (Zimny et.al.,1989; Wyputta et.al., 1991; Kimmel et.al.,1993; Geerling et.al.,1990; Brako et.al.,1989). In these studies, the electron exchange depends essentially on the quantity of the parallel velocity $v_{//}$ of the projectile .

This dependence is explained by the fact that electron structure of solid change in system of coordinate relative to the projectile moving parallel to the surface and affects character and intensity of charge exchange process.

Most of the experimental studies on the formation of negative ion of metal surfaces has been described by the small binding energies like H^- (Van Wunnik et.al.,1981; Zimny et.al., 1990). and Li^- (Geerlins

et.al.,1987; wears et.al., 1996) the affinity level of these projectiles are always lying over the Fermi- level of metals, so the RCT process will take place with the unoccupied states of the metal, then the electron will loss from atom to the surface results in a small negative ion yield.

In order to increase these yields we must, either lowering the surface work function, or using grazing scattering with small indecent angle. In the 2nd case the kinematics affect of parallel velocity bridges the energy gap between the affinity level of the projectile and the occupied states of the metal surface "$v_{//}$ effect" (Geerlings et.al.,1989; Van Wunnik et.al. 1983).

Perturbative method has been widely used for calculation of the transition rates and negative ion fraction of atomic levels at large distance in front of metal surface. Last investigation years, some nonperturbative methods was successfully employed for of charge exchange under grazing scattering , for example (CAM) Coupled Angular mode method (Teillet et.al., 1990) was used for treatment of experimental results for formation of negative – ion under grazing scattering from metal surface (Borisov et.al.,1996).

2- Quantum Size Effect (QSE)

The field of surface science has developed very quickly during past few years, along with advances in fabrication and measurement technologies at nanometer length scales. The dramatic reduction in size brought along the concepts of reduced dimensionality , reduced symmetric and change in structural geometry (Borisov et.al.,1993; Burgdorfer et.al., 1982).

A good example to (QSE) is a thin metallic film grown by depositing a metal layer on a dielectric substrate with large band gap lying on the conduction band of the metal.

When the thickness of a metal film reaches nanoscale dimensions , QSE can cause many material properties which differ greatly from those of the bulk (Winter ,2002; Jennings et.al.,1988; Smith, 1960 ; Stolterfoht, 1994).

The electron gas within a film is confined in the direction perpendicular to the plane of the film, these confined states called quantum well (QW), with energy levels , where $E(k_{//})$ is the energy $E = E_n + E(k_{//})$ measured from the bottom of the well associated with motion parallel to the film surface and,

$$E_n = (\frac{\hbar^2}{2m})(\frac{n\pi}{L})^2 \quad \text{.....(1)}$$

The change of these energies as a function of film thickness (L) have been linked to many unique properties of ultra thin films and multilayer.

charge exchange process between the incoming partcle and thin metal films is differ from charge exchange with semi-infinite metal (Burgdorfer et.al., 1982), this distinction is related to the difference of the electron structure of thin- metal films and the semi-infinite metal. The size quantization in

this metallic films allows through the variation of the film thickness.

In the present work, the influence of $v_{//}$ on electron exchange process is consider in case of grazing scattering at thin Au and Ag films using Perturbative method and CAM method.

The probability of H^- ion outer shell electron transfer from n- th level of the film is calculated during approach of H-atom to the film from infinity ,with different thickness of the metal film (L) as a function of atom-surface distance (d) and the atom velocity parallel component ($v_{//}$). These results show a pronounced dependence of the negative- ion fraction on the method we applied , on velocity component parallel to the surface and on the film thickness.

We choose Au and Ag thin films for their experimental importance where these thin films are used for studies of ultra thin over layers such as self- assembled monolayer SAS_s. The SAS_s are the most elementary form of nanometer scale organic thin film material. Thin film of these metals also used for scanning probe microscopy (SPM) for educational purpose.

3- Electron Structure of Metal Film / Model Potential

Electron structure of Au and Ag thin films is described by free electron model (jelly model) (Jennings et.al., 1982), it depends only on distance between electron and surface (z) " where z correspond to vacuum". $z\rangle 0$ calculated from image surface

$$V_{e-film(z)} = V_j(|z| - L/2) \qquad \ldots\ldots(2)$$

Where $V_j(z)$ defined the potential of semi-infinite metal , L is film thickness , z is the distance between electron and middle of the thin film.

For thin film, the electron is moving freely along parallel to the surface ,so the interaction potential in equation 2 is electron's coordinate parallel to the surface independent .

Within the potential in equation 2 electrons of the film have discrete set of energy state in the perpendicular to the surface direction, which correspond to proper value of energies of the potential well (equation 1).

5- Wave Functions Definition

The Proper function of the film (thickness of several monolayer) are given by

$$\phi_{n,k_{11}} = e^{i\vec{k}_{11}\cdot\vec{r}_{11}}\Psi_n(z)$$

$$\phi_{n,k_{11}} = e^{ik_x x}e^{ik_y y}\Psi_n(z) \qquad \ldots\ldots..(3)$$

$e^{ik_x x}, e^{ik_y y}$ Chosen as traveling waves with k_x and k_y for x and y coordinates parallel to the surface, however , the wave function dependence on z is given by $\psi_n(z)$, where $\psi_n(z)$ are normalized wave function with discrete energies E_n .

To described a thin metal film, it is useful to consider a deep potential well with a

thickness L is small while the two other dimensions are very large, then $\psi_n(z)$ are calculated using elementary quantum mechanics (Shestakov et.al., 2009)

$$\Psi_n(z) = A_n \cos\sqrt{2E_n(z)} \quad \text{.....(4)}$$

A_n is the normalization constant which is function of the film thickness (L) and equal to $(2\pi/\sqrt{L})$ .The wave functions of metal electrons are:-

$$\langle r|k\rangle = e^{ik_{//}.r_{//}}\psi_{k_z}(Z) \quad \text{.....(5)}$$

$$\Psi_k(z) = \sqrt{2}\cos(k_z z) \quad \text{.....(6)}$$

In the range distance z from the center of the film to $+\infty$, $V_{e\text{-film}}(z) \equiv V_{e\text{-metal}}(z)$ (Borisov et.al., 1992). So by made a comparison between the wave function in equations 4 and 6 then the wave function of the film will take the form;

$$\Psi_n(z) = \frac{A_n}{\sqrt{2}}\ \Psi_{k_z^n}(z) \quad \text{.....(7)}$$

$$k_z^n = \sqrt{2E_n} \quad \text{.....(8)}$$

6- CAM- method

In this work, we put a simple outline on CAM method and for more details read the ref. (Whinter,2002). The coupled angular mode method is a scattering method allowing for calculating atomic or molecular levels, and it can applied to neutral, positive and negative ions (Jennings et.al., 1988: Smith ,1960). So it is a well suited for our problem, where the CAM method is applied here to the case of H^- -ion formation in H/Au (100) and H/Ag (110) systems.

If $|\sigma_i(\theta,\phi,d)|^2$ is defined as the angular distribution of the transition probability, and it could obtained from the eigenvector $Q_{l\ m}$ of the time-delay matrix (Newns ,1970)

$$|\sigma(\theta,\phi,d)|^2 = \left|\sum_i Q_{lm}^i(d)Y_{lm}(\theta,\phi)\right|^2 \quad \text{.....(9)}$$

$Y_l^m(\theta,\phi)$ are the spherical harmonics of the effective electron wave functions i refer to the states n_s , n_p respectively, In our calculation , we take the eigen vector Q_{lm} as an approximate formula which is function of z.

$$Q_{lm} = q_o e^{(-\alpha z/4)} \quad \text{.....(11)}$$

q_o taken as an adjustable parameter and α is parameter related to the ionization level of the incoming ion.

7- The Transition Matrix Elements for Thin Film Using Perturbative method

The transition matrix elements between metallic states $\langle\phi_{n,k_{//}}|$ of thin film and the atomic state $|a\rangle$ for H^-/metal system are defined by,

$$M^{e-film}(n,k_{//}\to a:d) = \langle\phi_{n,k_{//}}|V_{e-a}|a\rangle \quad \text{.....(12)}$$

Where $k_{//} = \sqrt{2(E_n - E_a(d)}$ at the resonance condition, E_n are the discrete energies for thin film, $d = v_z t$.

Following the argument of (Gadzuk,1987) and assuming the perturbation to be between a pure atomic and metallic state (e^- -atom

interaction). V_{e-a} is unperturbed core potential of the neutral atom, and it can be replaced by some constant value, $V_{e-a} = -\lambda$ then equation 12 is replaced by

$$M^{e-film}(n, k_{//} \to a : d) = -\lambda \langle \phi_{n,k_{//}} | a \rangle \quad \ldots.(13)$$

This introduced an overlap integral multiple by a scaling constant. This reduction is particularly valid for atom – surface distance larger than about $3a_o$.

The corresponding bound state wave function for bound state of the $H^- - ion$, is taken from (Waghmare, 1996)

$$\langle a | = \frac{1}{\sqrt{4\pi}} \frac{[2\alpha\beta(\alpha+\beta)]^{1/2}}{(\beta-\alpha)} \frac{e^{-\alpha r} - e^{-\beta r}}{r} \quad \ldots..(14)$$

α *and* β are the effective core charge and they are chosen such that the binding energy of H^- and the effective range of the $e^- - H$ interaction are reproduced. for

H^-- ion , $\alpha = 0.2355,\ \beta = 0.5315$ and $\lambda = \frac{(\alpha+\beta)^2}{2} = 0.5315$.

The wave functions in equations 3 and 14 are brought into equation 19 to compute the matrix elements of the perturbing potential,

$$M^{e-film}_{a,k_{//},n}(d) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi_a \,.\,-\lambda.\phi_{n,k_{//},}\, dx\ dy\, dz \quad \ldots(15)$$

The calculation of $M^{e-film}_{a,k_{//},n}(d)$ can be partially performed analytically (the integral of x and y) such as;

$$M^{e-film}_{a,k_{//},n}(d) = -A_o \int_{-\infty}^{\infty} \psi_n(z)\, \frac{e^{-C_o[z-d]}}{C_o}\, dz \quad \ldots.(16)$$

And for a fixed distance from the film (z-d) is calculated from the image plan z_{img}

Where $A_o = \lambda\sqrt{2\pi}\sqrt{\frac{\alpha\beta}{\alpha+\beta}}$, $C_o = (k_{//}^2 + \beta^2)^{1/2}$

and the wave function associated to the energy E_n for the quantized states in the film $\psi_n(z) = A_n \cos\sqrt{2E_n(z)}$.

8 - The Transition Matrix Elements for Thin Film Using CAM method

In this section we will discuses how we could estimated the transition matrix semi - infinite metal. by using the CAM calculation of for thin film

Following the work of (Winter et.al., 1996), where he calculated the transition matrix elements for semi- infinite metal using CAM method such as;

$$\left|M^{e-metal}(k_{//}, \theta; d)\right|^2 = \frac{\pi}{k_{//}} \Gamma(d) \left|\sigma(\theta, \phi, d)\right|^2 \quad \ldots\ldots(17)$$

$\left|\sigma(\theta, \phi, d)\right|^2$ is the angular distribution , Γ(d) is the total width of atomic state in front of the metal, $k_{//} = \sqrt{2\varepsilon_a(d)}$,

$\varepsilon_a(d)$ is the energy of the incoming atom and it is assumed to be the same for the film and for semi- infinite metal .

If we take a film of several monolayer from the same metal and assume that the response of this film to the external charge is the same as for meta (Jennings et.al., 1988; Newns, 1970) , and $V^{e\text{-film}} = V^{e\text{-metal}}$,then the transition matrix for thin film will be;

$$M^{e-film}(n,k_{//};d)=\langle\phi_{n,k_{ll}}\left|V^{e-met}\right|a\rangle \quad \ldots\ldots(18)$$

$V^{e\text{-metal}}$ represent the interaction potential between incoming atom and the metal Surface, $\phi_{n,k_{//}}$ is the metallic film states and $|a\rangle$ is the atomic state. By using the definition in equations 3 and 7 then,

$$M^{e-film}_{n,k_{ll}\to a}(d)=\frac{A_n}{\sqrt{2}}\langle e^{i\vec{k}_{ll}\cdot\vec{r}_{ll}}\ \Psi_{k_z^n}(z)\left|V^{e-met}\right|a\rangle \quad \ldots..(19)$$

$\Psi_{k_z^n}(z)$ is the wave function for metal electron and the term $\langle e^{i\vec{k}_{ll}\cdot\vec{r}_{ll}}\ \Psi_{k_z^n}(z)\left|V^{e-met}\right|a\rangle$ will represents the matrix elements for the semi –infinite metal :-

$$\left|M^{e-film}_{n,k_{ll}\to a}(d)\right|^2=\frac{A^2_n}{2}\ \left|M^{e-met}(k,\theta,\phi)\right|^2 \quad \ldots(20)$$

$\left|M^{e-met}(k,\theta,\phi)\right|^2$ is calculated for semi-infinite metal so, the transition matrix elements for thin film is introduced from equation 20.

get use of equation 17 , then the matrix elements for thin film will be:-

$$\left|M^{e-film}_{n,k_{ll}\to a}(d)\right|^2=\frac{A^2_n}{2}\frac{\pi}{\sqrt{2\varepsilon_a(d)}}\Gamma(d)\left|\sigma(\theta_n,d)\right|^2 \quad \ldots..(21)$$

Γ(d) is equal to summation of loss and capture rates, then equation 21 be equal to ,

$$\Gamma(d)=\left|M^{e-film}_{n,k_{ll}\to a}(d)\right|^2=\frac{A^2_n}{2}\frac{\pi}{\sqrt{2\varepsilon_a(d)}}\Gamma(d)\left|\sigma(\theta_n,d)\right|^2 \ldots(22)$$

9- H^- Fraction Calculation

Let's now consider scattering under grazing angle of H- atom on gold and silver thin films with perpendicular to the surface velocity v_z and parallel velocity $v_{//}$ and with using the rates for electron loss and capture for thin film which is defined by equations similar to that for semi-infinite metal (Hech et.al., 2002)

$$\begin{Bmatrix}\Gamma_c^{film}(d)\\ \Gamma_\ell^{film}(d)\end{Bmatrix}=\frac{1}{2\pi}\sum_n\left|M^{\text{e-film}}{}_{(n,k^{res}_{l//},d)}\right|^2\int_0^{2\pi}d\phi\begin{Bmatrix}f(E_F-E_n-\frac{(\vec{k}^{res}_{//}+\vec{V}_{ll})^2}{2})\\ 1-f(E_F-E_n-\frac{(\vec{k}^{res}_{//}+\vec{V}_{ll})^2}{2})\end{Bmatrix} \quad \ldots..(23)$$

While the master equation for the evaluation of the negative ion population P^- along the outgoing part of the trajectory can be computed by integrating the following rat equation:-

$$\frac{dP^-}{dt}=-\Gamma_L(Z(t))\ P^-(t)+\Gamma_C\ (Z(t))\ (1-P^-(t)) \quad \ldots\ldots\ldots(24)$$

$$P^-(z)=P^-\ e^{\int_{-\infty}^{\infty}\frac{[\Gamma_l(z')+\Gamma_c(z')]}{V_z}dz'}+\int_{-\infty}^{\infty}\frac{\Gamma_c(z')}{V_z}\ e^{\int_{-\infty}^{\infty}\frac{[\Gamma_l(z'')+\Gamma_c(z'')]}{V_z}dz''}\ dz \quad \ldots..(25)$$

This equation is solved numerically and the integration is solved for $Z(t) = v_z.t$ V_z is the normal component of the atom velocity and we take the experimental value 0 .015a.u. for the hydrogen atom , this condition is equivalent to an energy for the normal motion of about 5eV. (Borisov et.al., 1992).

10- Results and Discussions

With theoretical concepts outlined in the previous section, the matrix elements $M^{e-film}_{n,k_{||}\to a}(d)$, the transition rates Γ_c , Γ_l , $\Gamma^{film}_{total}(d)$ and finally the negative hydrogen ion fractions at Au(100) and Ag(110) thin films are calculated for different thickness (1ML, 2ML , 3ML, 4ML, 5ML, 6ML and 9ML).

The Fermi energy and the metal work function differs from one of semi- infinite metal and depends upon thickness of the film, based on condition that in the volume $L\times L\times L$ of film and semi- infinite metal is located equal quantity of electrons (Shestakov et.al.,2009),

$$E_F = \frac{1}{n_{\max}}\left\{\frac{L}{\pi}.\frac{k_F^3}{3} + \sum_{n=1}^{n_{\max}} E_n\right\} \qquad \text{.....(26)}$$

$E_n \langle E_F$ and $n = 1,2,3,....n_{\max}$, k_F is the Fermi vector in the case of semi- infinite metal.

Table (1) contain the calculated Fermi energy E_F, Work function W and the film thickness "which can be taken as discrete set of values corresponding to different amount of atomic plane within Au(100) and Ag(110)" .

Table(1): The calculated Fermi energy , work function and the film thickness for Au(100) and Ag(110)metals

		1Ml	2Ml	3Ml	4Ml	5Ml	6Ml	Experi..
Au(100)	*Thickness*(a.u.)	5.04	11.08	15.12	20.16	25.20	30.24	
	$E_{F(eV.)}$	6.02	6.197	5.985	5.469	5.722	3.49	5.53
	W(eV.)	5.96	6.13	5.92	5.41	5.66	5.43	5.47
Ag(110)	*Thickness*(a.u.)	3.94	7.90	11.84	15.78	19.73	23.68	
	$E_{F(eV.)}$	5.06	4.58	4.72	4.63	4.60	4.59	4.64
	W(eV.)	4.93	4.46	4.60	4.51	4.48	4.46	4.52

Fig.(1) and fig.(2) we presents the square resonance matrix elements for H^- ion infront of Au(100) and Ag(110) thin films with different thickness (1Ml- 9Ml), as a function of the distance between ion and film [measured from the image plane $z_{im} = \pm(\frac{L}{2} + 1a.u)$ (Jennings et.al., 1988)] . The figures also include comparison with the similar results obtained for semi- infinite metals " our calculation too" .

In the static situation (fixed ion- surface distance) it is important to find the ion Level width (the total transition rates) $\Gamma^{film}(d)$ calculated from the summation of Γ_l Γ_l with Γ_c or $\Gamma^{film}(d) = \frac{\Gamma_c}{g^-} + \frac{\Gamma_l}{g^o}$, and we use the statistical factors equal $g^o = 1$ and $g^- = \frac{1}{2}$ so fig. (3) and fig.(4) presented the results of $\Gamma^{film}(d)$ for $H^- - ion$ on Au (100) and Ag (110) with different thickness (1ML-9ML) calculated by the two different methods, these results include also $\Gamma^{film}(d)$ for semi –infinite free electron metal surface.

We notice here that these results differ from the case of film, this distinction is associated with the different of electron structure of metal film from semi- infinite metal . With increasing the film thickness the width $\Gamma^{film}(d)$ converge towards the results for the semi- infinite metal, this means, by increasing the film thickness one should recover the limit of a semi- infinite free- electron surface, i.e. the density of quantized states in the 2D-film increases leading to 3D traveling states in the semi-infinite limit. Also these figures shows a different in shape of dependencies on distance in case of $\Gamma^{film}(d)$ calculated from CAM- method and the calculated by perturbing metod .

The level width for all films and for the systems H^-/Au(100) and H^-/ Ag(110) displays an exponential behavior with the ion- film surface reaching very large values in eV. range at small distances. No step structures in the $\Gamma^{film}(d)$ dependence on the distance is observed, the same behavior exists in Na^+-ion neutralization at Al films (Borisov et.al., 1996).

11-H^- Fraction under Grazing Angle Scattering on Au(100) and Ag(110) Thin Films/ Dynamical Calculations.

The dependence of H^- ion formation probability upon value of parallel to the surface velocity ($v_{//}$) during scattering from thin metal film was calculated numerically using the Perturbative method (equation 25). This dependence is calculated for film of different thickness (1ML- 9ML), and presented in fig.5 for Au(100) metal ,with atom normal velocity (v_z =0.015 a.u.) . The

figure also represent our calculation for the semi infinite metal.

These calculations are also carried out for $H^- / Ag(110)$ and $H^- / Au(100)$ system using CAM method and the results are plotted in fig. 6 and fig.7. It is interesting to remark that H^--fraction yield in both Perturbative and CAM method during scattering on the films (1ML- 6ML) thickness is more than ion yields in case of thick films and for both systems, this is due to the lower work function for thin film which is related to the quantization of the states in thin film.

Dependence of 9ML thickness is very close to the one of semi- infinite target. The H^- ion fractions shows the dependence of a kinematics resonance, where the small affinity level (-0.75eV.) for H^- -ion compared to the work function of the metal leads to small fractions ($P^- = 10^{-2}$).

During increase of film thickness the maximal value of negative ions fraction decreases to be approached the maximal value of semi- infinite metal, where during increase the film thickness the density of it's two dimension levels increases, and reaches the case of three dimensional band of metal .

Moreover, during increase of film's thickness the maximum of dependency for both systems shifted toward higher values of $v_{//}$, which is connected with the dependence of Fermi energy on the film thickness.

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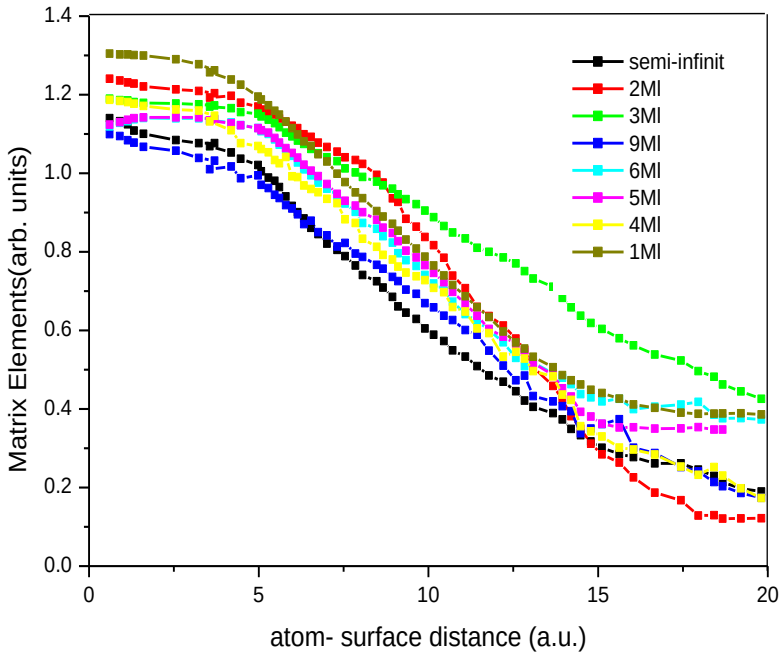

Fig.1: Matrix elements for H⁻ - ion in front of Ag(110) thin films using the

Perturbative method.

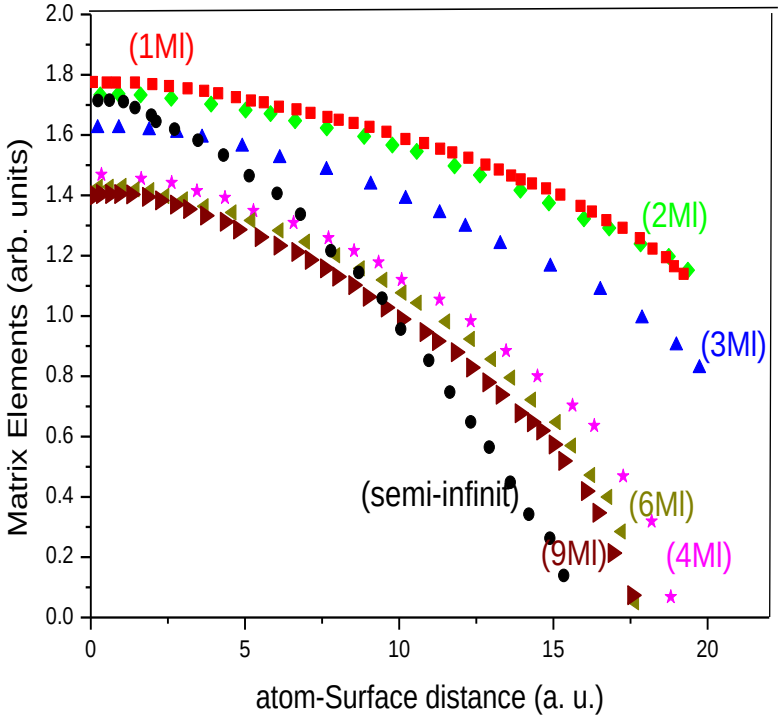

Fig.2: Matrix elements for H⁻ - ion in front of Au(100) thin films using CAM method.

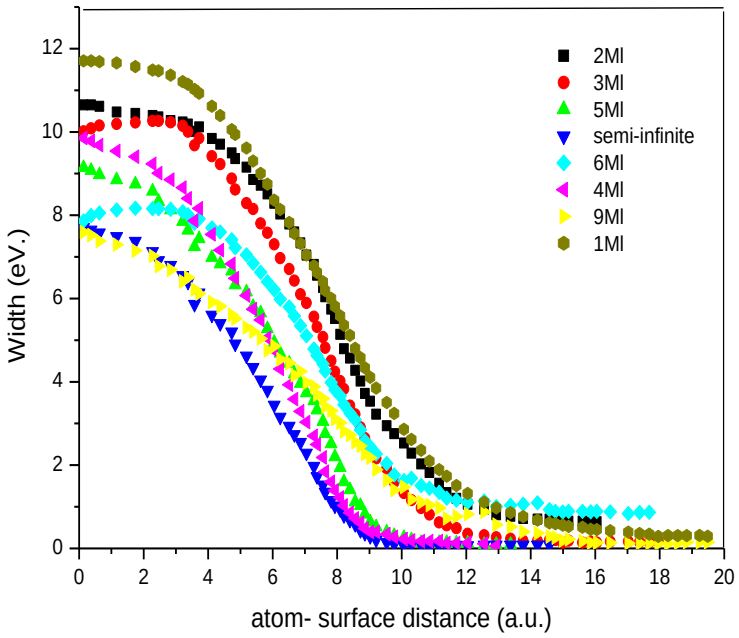

Fig.3: Total transition rates for H⁻ / Au(100) thin films using the Perturbative method.

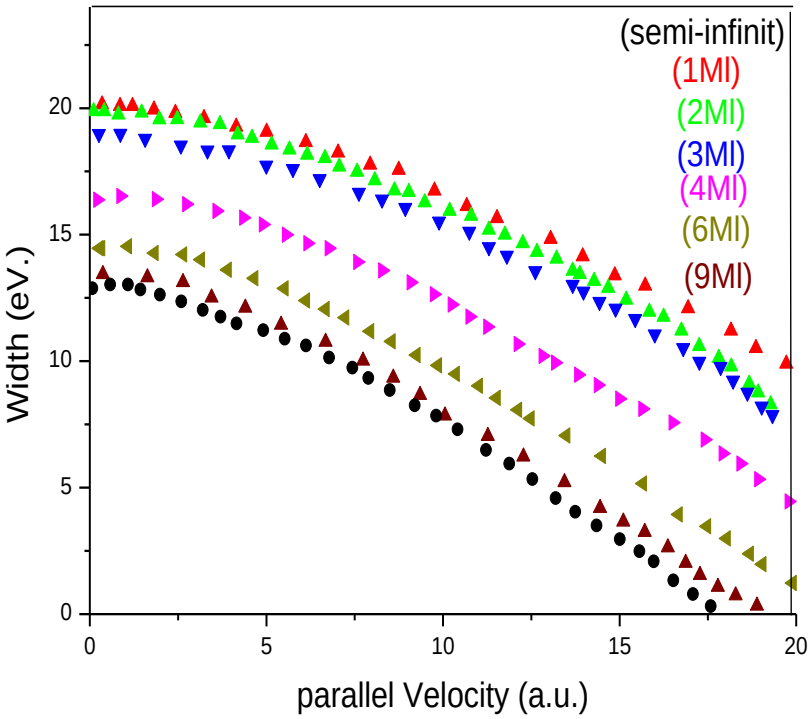

Fig.4: Total transition rates for H^- / Ag(110) thin films using CAM method.

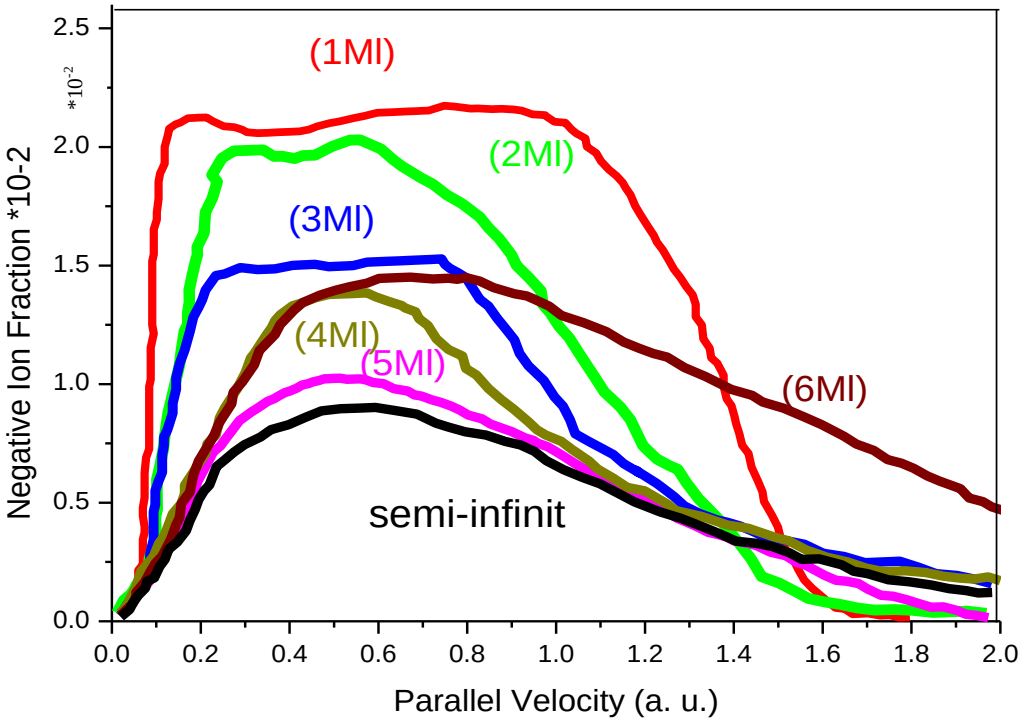

Fig.5: Negative ion fraction for H^- / Au(100) thin films using the Perturbative method.

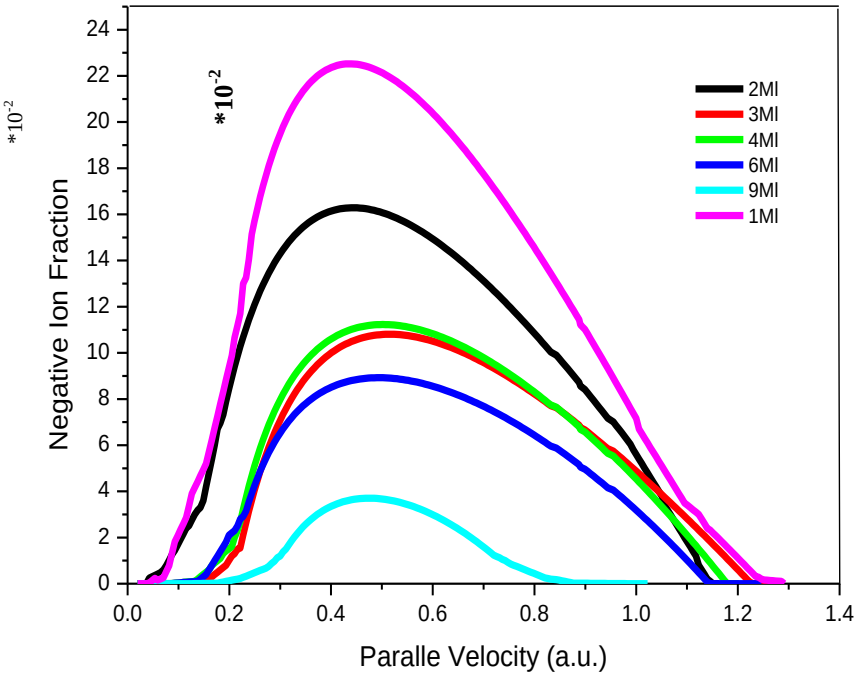

Fig.6: Negative ion fraction for H^- / Au(100) thin films using CAM method.

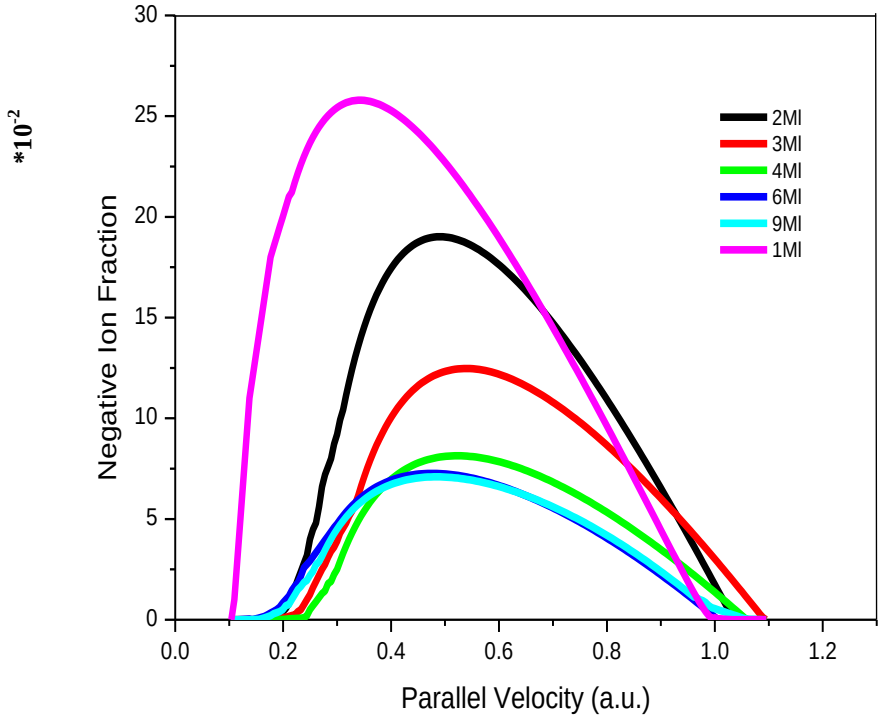

Fig.7: Negative ion fraction for H^- / Ag (110) thin films using CAM method.

دراسة في اقتناص الالكترون وتنبأ في استطارة ذرة غشاء رقيق : تكوين H^- عند أغشية رقيقة من Au(100) و Ag(110)

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المستخلص:

في هذا العمل تمت دراسة اقتناص الألكترون عند استطارة ذرة الهيدروجين من أغشية رقيقة ذات سمك متغيرمن سطوح Au (100)و Ag (110) باستخدام الطريقة المضطربة . وقد بدا واضحا ان عملية انتقال الشحنة الرنيني (RCT) للغشاء تكون مختلفة عند استخدام تقريب الإلكترون الحر للمعدن شبه اللانهائي وذلك بسبب التكميم بحركة الإلكترون باتجاه العمود على الغشاء . أن الكثير من التطبيقات على الأغشية الرقيقة قد تمت دراستها سابقا باستخدام نمط ازدواج الزخم الزاوي الغير مضطرب (CAM) ، ولهذا قمنا أيضا بتطبيق الطريقة الغير مضطربة لنفس الانظمة المستخدمة في هذا البحث للمقارنة.