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Scattered atom energy effect on determination interaction appearances of the system (scattered atom – adatom/surface)

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Abstract
Order to study initial energy effect of scattered atom when interaction with Adatom on determination of the interaction appearances. The atomic level locate was determined for the scattered atom according to the Fermi level as a function of the initial energy. The classical path was determined of the scattered atom and their related to the initial energy in the nearest neighbour to the surface. The interaction behaviour between orbitals of scattered atom and adatom was studied as a function of the initial energy of the scattered atom. The effect of external force of scattered atom on the adatom was studied as well. Also, we study the relation of the atomic level locate for scattered atom with respect to the Fermi level and the system temperature. Finally, value of occupation number on atomic level for scattered atom was studied when increase the coupling force in the system.

1. Introduction

The measuring of the relation between the translation, oscillation and rotation energies of the incident particle and the final energy of the product after scattering provides important information about the dynamic of system interaction (particle-surface). Many experimental and theoretical [1-3] studies have shown that the majority of hyper thermal particles transfer 75% of their initial energies to the surface, and the renaming energy distributed to translation, oscillation and rotation degree of freedom of the particle emerges from scattering region. Many experimental studies [4] have shown that when light atom scatters from the metal surface, the final translation energy of the scattered product regardless of its charge states, this energy increased with collision energy. The majority of experimental studies of hyper thermal scattering focused on the contribution of translation energy of an incident particle on the reaction's dynamic. The binary collision model (BCM) is the most commonly used to calculate the amount of the translated kinetic energy at a high collision energy. Additionally, this model treats the single collision between the incident particle and the target's atom while the energy and momentum are conserved. Comprehensive physical and chemical understanding of solid surfaces demands a wide knowledge about the atomic forces connecting atoms within and on the surface, where the bonding on a surface is different from solid. The measuring of force constants among the atoms on a surface provides significant entrance toward an accurate modelling [5] and clear understanding of various surface properties and the included processes.

The light atoms with low energies are very convenient to study surfaces in general and

surface vibration in specific. If the scattered atom has a lightweight such as helium and lithium, it does not penetrate the surface toward the bulk. The information obtained from the scattered atom either about the structure or dynamic are connected only with the external shell of the crystal. In addition, the helium band for instance, provides chemical, electrical, magnetic and dynamic probe if the energies of the band are within the range of thermal energy [6]. The Translation motion for incident and scattered band is the only one that is required to obtain further information about the exchange of energy and momentum [7]. For the studying of inelastic scattering, the exchanged energy and momentum of the light atoms are within a range of the surface's phonon. When the cross sections of inelastic scattering are low to specific range of temperature and scattering angles, only the surface phonons are excited ore moderated. This leads to obtain inelastic gained or loosed energy diagram described as a function of oscillated frequency and wavelength. It is worth mentioning that, low intensities can be obtained by controlling the conditions of inelastic scattering process. The mode of excitation could be recognized in the scattering process taking into account the surface deformation caused by incident particles band. The particles used as probe either those move with high velocity (such as electrons, ions and photons) or those interact with low range forces (neutrons) generate local deformation. In contrast, displacement of the lattice generated by the collision of atom with surface, varies slowly with the time and space [14].

2. The Model Calculation

The aim of this paper to study the effect of initial energy for scattered ion or atom on surface solid is covered with atoms (low covering).first, must identify classic path scattered atom $Z(t)$ that interact with surface atom in potential function $W(Z(t))$ which cause appearance of force between them, this force gives:

$$F=-\frac{dW(Z(t))}{dZ(t)} \tag{1}$$

We use the Born-Mayer potential [8]

$$W(Z(t)) = A\ \exp(-2a'Z(t)) \tag{2}$$

a' and A are parameters Born-Mayer potential that dependent on type of surface atom and scattered atom. We can describe motion of scattered atom during scattering [9].

$$E(t) = E_o - W(Z) \tag{3}$$

And

$$E_o = (1/2)M_p v_0^2 \tag{4}$$

$$E(t) = (1/2)M_p v_\perp^2 \tag{5}$$

M_p, v_0 are mass and initial velocity for scattered atom respectively, $v_\perp$ represented vertical velocity at all time (t) and when compensation relations (2),(4) in (3) and solution the resulting equation , can be obtained classic path for scattered atom:

$$(\frac{v_\perp}{v_0})^2 = 1-\frac{1}{\eta}\exp(-2a'Z(t)) \tag{6}$$

And $\eta=\frac{E_0}{A}$

And after solution equation (6) we obtain:

$$Z(t) = \frac{1}{2a'}\ln[\frac{1}{\eta}\cos^2(a'v_0 t) \tag{7}$$

This relation of **Z(t)** is a function of time to be linear with the large value of time, but its smooth for all value of time (time corresponding to the zone nearest to neighbour) in reveres to the linear path:

$$Z(t) = R_0 + v_0|t| \tag{8}$$

Which used usually in situation of elastic scattering where R_0 represent the distance for nearest neighbour .but in the location of atomic level for scattered atom(Li) with respect to the Fermi level is given by:

$$E_a(t) = \varphi + V_i + \frac{e^2}{4(z(t)+4.5a_0)} \tag{9}$$

Where V_i represent the ionic potential for scattered atom (Li) which is equal (-5.392eV) and the final term from relation (9) represented image shift resultant from effect of image forces which affect to shift of atomic level to upper. The value of ($4.5a_0$) [9] represent of blocking length. The interaction $V(Z(t))$ which called hopping integral between orbitals scattered atom and adatom is given by [10]:

$$V(Z(t)) = V_0 \exp(-\mu Z(t)) \tag{10}$$

The formula of $V(t)$ which we used in our treatment is taken from reference [11] and it equal to:

$$V(t) = V_0 \eta^{\mu/2a'} \sec h^{\mu/a'}(a'v_0 t) \tag{11}$$

The coefficients of Born-mayer potential are taken from the reference [12] and it equal to:

$$a' = 1.065\,\text{A}^{\circ -1}\ ,\ A = 149.59\text{eV}$$

The scattered atom effect on oscillator (adatom in surface) by external force given by the formula [13]:

$$g(t) = -(2M\omega)^{1/2} 2a'E_o \sec h^2(a'v_0 t) \tag{12}$$

When calculate number of occupation on the atomic level, for scattered atom, adatom and number of phonons on the harmonic oscillator as a function of the time. The present study uses the equations system:

$$\dot{C}_a = iE_a(t)C_a - iV(t)C_d \tag{13}$$

$$\begin{aligned} C_d^{\bullet} &= [-iE_d - 2\pi\gamma^2\rho - i\lambda(b^+ + b)]\, C_d(t) - iV(t) \\ &\quad C_a(t) - i\gamma\rho \int_{u_o}^{\phi} \sqrt{f(E,T)}\, \exp(-iE(t-t_o))\, dE \end{aligned} \tag{14}$$

$$\dot{b} = -i\omega b - i\lambda C_d^{+} C_d - ig(t) \tag{15}$$

These relations above include system of equations (13, 14 and 15) and which solved numerically with atomic unit system ($m=\hbar=e=1$) and all energy measurements are related to Fermi level $E_F = 0$ and given the initial conditions [14]:

$$\begin{aligned} C_a(t_o) &= (1,0) \\ C_d(t_o) &= (0,0) \\ \tilde{C}_k(t_o) &= \sqrt{f(E,T)} \end{aligned} \tag{16}$$

3. Results

In this study the initial energy for the scattered atom was chosen (1-50 eV) because the scattered atom effect on the surface obvious in this range of energy. In order to determine the appearances of scattering as atomic level locate for the scattered atom with respect to the Fermi level in the nearest neighbour (Fermi level E=0). In this study the atomic level locate for the scattered atom depend on the path Z(t) and the atomic level locate for scattered atom $E_a(t)$ as function of the initial energy for the scattered atom. $E_a(t)$ has been found locate at lower than Fermi level for all initial energy level (1-50 eV), and then when the initial energy for the scattered atom increased, $E_a(t)$ becomes high than Fermi level, see fig(1).

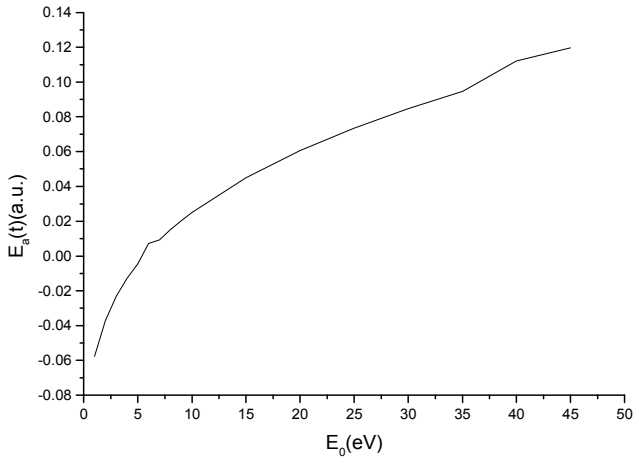

Fig (1). *Location of atomic level for scattered atom with respect Fermi level as function for its initial energy.*

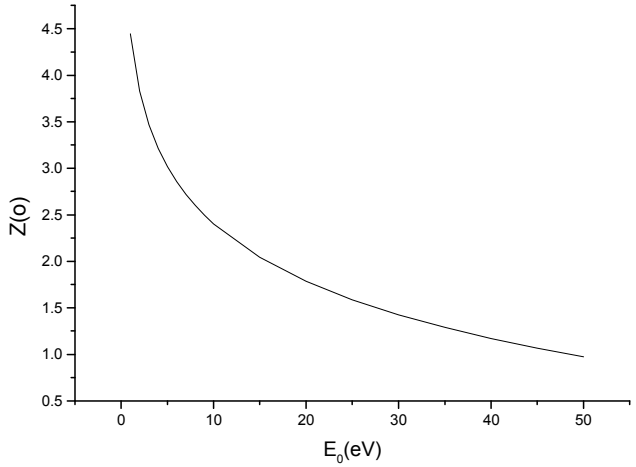

Fig (2). *Classical path for scattered atom in region closest neighbor as function for its initial energy.*

Behaviour of path of scattered ion Z(t) at region nearest neighbour (nearest distance between scattered atom and adatom on the surface)decrease when increase the initial energy for scattered atom, this results agree energy equation $E(t) = E_0 - w(z)$,see (fig(2)).

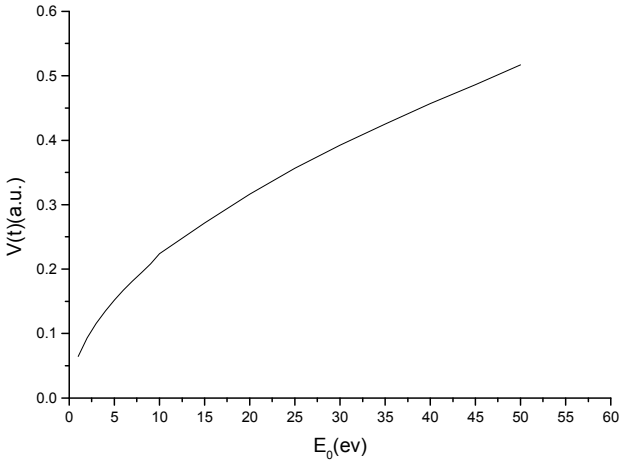

Fig (3). *Reaction between orbitals of scattered atom and adatom as function for initial energy for scattered atom.*

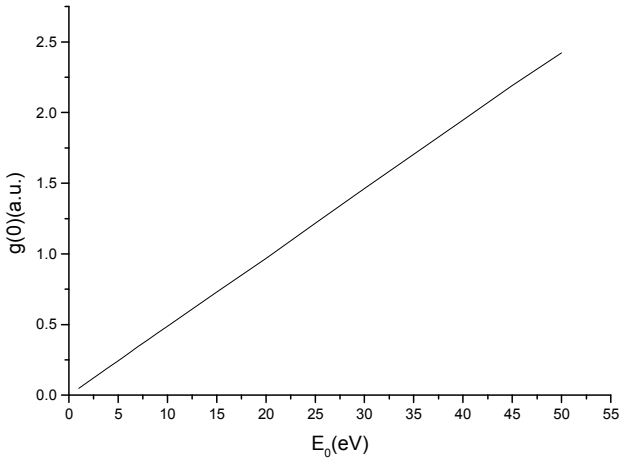

Fig (4). *External force for scattered atom which affect on adatom as function for initial energy for scattered atom.*

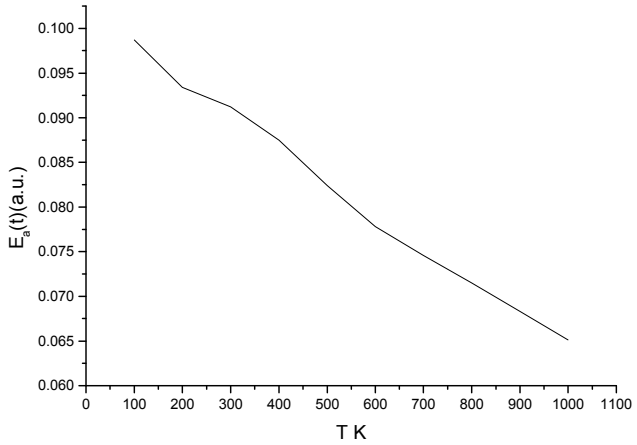

Fig (5). *Relationship between locations of atomic level for scattered atom and temperature of system.*

Fig (3), (4) show that the interactions g(t) and V(t) as a functions of initial energy and these interactions depend on initial energy for scattered atom.

In this paper, we have been studied the relationship between location of atomic level for scattered atom and the system temperature, and value of φ becomes $\varphi=\varphi-1.7\times10^{-4}T$ where T represent system temperature and $\varphi=4.75$ (work function for energy band of surface).we have been found the value of $E_a(t)$ becomes near to Fermi level when increasing system temperature, see fig(5).

Table (1). *Occupation number for scattered atom, adatom, number of phonons and hopping integral as function for force coupling between scattered atom and adatom.*

$v_0(eV)$	V(t)(a.u.)	$\|C_a(t)\|^2$	$\|Cd\|^+$ (0)	$\|a\|^+$ (0)
0.5	0.0333	0.979642	0.00783	46.35
1	0.0543	0.921698	0.02732	46.34
1.5	0.1086	0.835671	0.05019	46.30
2	0.1629	0.733156	0.06982	46.23
2.5	0.2172	0.623651	0.08455	46.14
3	0.3258	0.534210	0.09433	46.04
3.5	0.3801	0.433412	0.09468	45.93
4	0.4342	0.351995	0.09569	45.81
4.5	0.4344	0.291122	0.09598	45.68
5	0.4887	0.235511	0.09723	45.44

The table (1) showed increasing the coupling force between scattered atom and adatom cause increasing V(t) (hopping integral between orbitals scattered atom and adatom on the surface). The table (1) determined the behaviour occupation number values on the atomic level for the scattered atom and adatom at nearest neighbour for surface and number of phonons on the harmonic oscillator.

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