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Atom (Ion)- Surface Scattering Process: Configurations Interaction Method

Shakir.I.Easa and Falah.H.Hanaon
Physics Department, Colledge of Education, Basrah University, Basrah, Iraq
E-Mail: Shebes72@yahoo.com
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Abstract

The shape effect of the surface density of state on the charge transfer in atom(ion)-surface scattering process is investigated in detail by formulating the configurations interaction (CI) method. The method is applied to the formation of exited silicon ion Si^{+*} from the scattering of Si^{2+} from Si surface as we used as well the method to clarify the nonlinear behaviors of the H^{+} survival probability as a function of the scattering angle during its specular scattering from graphite (HOPG) surface.
Keywords: Surface Physics, Atom-surface scattering, Charge transfere

1.Introduction

When an atom or molecule be close to a solid surface, its electronic state interacts with those of the solid, leading to the possibility of charge transfer between the atom (molecule) and the solid. This charge transfer process plays a very important role in a variety of different situations. In particular, it often occurs as an intermediate step in reactions at surface (desorption, fragmentation of adsorbates, chemical reactions, etc.). The one-electron transfer between energetically degenerate electronic levels of the atom and the solid is called the resonant charge transfer (RCT) process [1-6], which is an effective one. The specific mechanisms are relevant to ion-surface interactions that made us use the ion scattering as a probe of surface electronic properties.

Experimentally, if an ion is sent against the surface it can neutralize by detaching from the surface one electron. This process of the ion neutralization during scattering from surface [7] has been the subject of much experimental [8] and theoretical [9-15] interests. Since the neutralizing electron originates in the valance band of the solid; the process is closely related to the solid-state nature of the target. In this case, one can consider the effect of the surface density of states on the electron transfer process. And it turns out that the whole process can be considered as a probe for the surface density of states structure.

Charge exchange between a metal surface and an atom, or ion, has been observed in many ion-and atom-surface scattering experiments [16-21]. For example, if the incoming particles are He^+ (or H), then the scattered beam may contain He and He^+ (or H^-, H^+ and H). The distributions of the scattered particles among the various charged states are strongly dependent on the velocity of the incoming particles and the nature of the surface. Therefore, experiments of this kind are important in many techniques of surface analysis, such as ion-beam scattering spectroscopy (ISS), neutral-beam scattering spectroscopy (NSS) and secondary ion mass spectroscopy (SIMS) [22-24].

This paper gives the shape effect of the surface density of state on the charge transfer process. The model used here is dynamic Anderson-Newns model [25], this model is applied to two different cases:

The first is to describe the oscillating character of the energy spectrum of excited secondary Si ions under electron exchange with the surface.

The second case is to study H^+ ion scattering from C (graphite) surface to make matching between experimental and theoretical results for the survival probability as a function of the final ion velocity. Figures (1) and (2) explain the band density of states for Si bulk and graphite respectively.

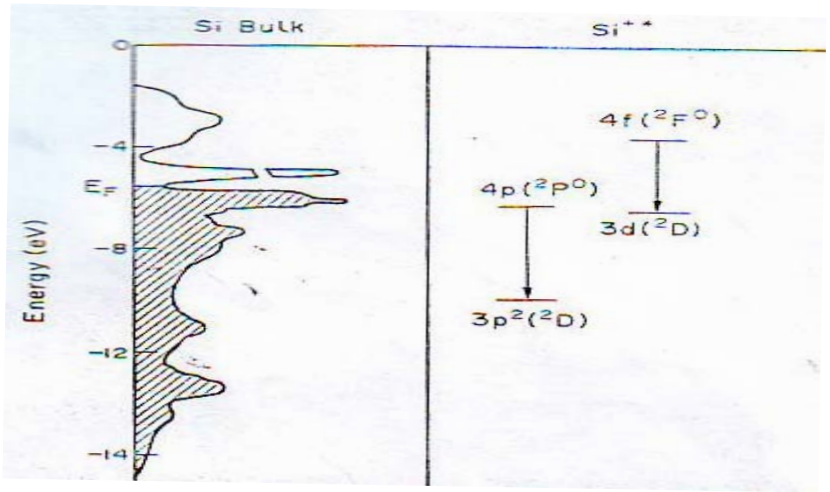

Figure (1): Energy structure of Si single crystal and the arrangement of Si^+ ion energy Level [26].

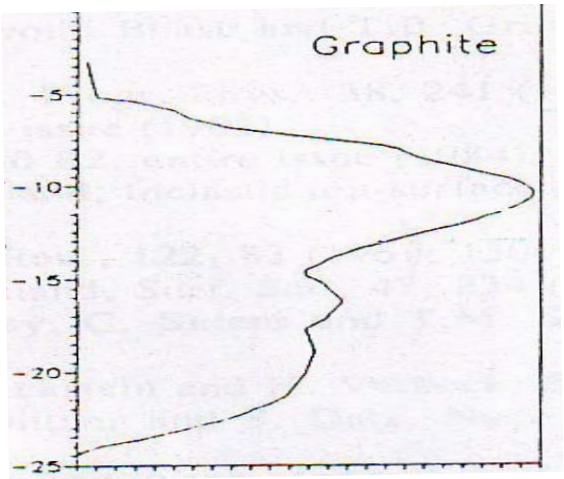

Figure 2: The band density of states for graphite [27]

2. Theoretical Model

The interaction between a solid surface and an atomic (ionic) particle is described by means of the dynamic Anderson-Newns Hamiltonian for the surface-atom (ion) system as[25],

$$H = H_o + H_I(t) \qquad (1)$$

With,

$$H_o = E_A a_A^+ a_A + \sum_k E_k a_k^+ a_k \qquad (2)$$

Where, a_A^+ is an electron creation operator into the discrete state $|A\rangle$ of energy E_A of the atom, and a_k is the annihilation operator from the state $|k\rangle$ of energy E_k of the valence band of the solid. And,

$$H_I(t) = \sum_k [V_{kA}(t) a_A^+ a_k + H.C.] \quad (3)$$

which represents the time-dependent interaction between the state $|A\rangle$ and $|k\rangle$ through the approximation matrix element V_{Ak} and the interaction potential V_o. Above, H. C. denotes the Hermition conjugate.

Let $|\phi_o\rangle$ and $a_k^+ a_A \ |\phi_o\rangle$ denote two electronic configuration states of the atom (ion)-surface system (for a given position of the atom (ion) in front of the surface and also assuming the Born-Oppeheimer separation). These configuration states will be defines by:

$|\phi_o\rangle$: In this configuration all one-particle solid states $|k\rangle$ up to Fermi states are occupied and atomic (ionic) state $|A\rangle$ is empty.

$a_k^+ a_A \ |\phi_o\rangle$: In this configuration the atomic (ionic) state $|A\rangle$ is doubly empty.

Due to the interaction between the two configurations one electron bound within the solid surface "jumps" to the ion and remains there bound after the ion is scattered and becomes infinitely separated from the solid. We have,

$$\left.\begin{aligned} \langle\phi_o | H a_k^A a_A | \phi_o\rangle &= V_{Ak}(t) \\ \langle\phi_o | H | \phi_o\rangle &= E_o \\ \langle\phi_o | a_A a_k^+ H a_k^+ a_A | \phi_o\rangle &= E_o + E_A - E_k \end{aligned}\right\} \qquad (4)$$

The electron wave function $\Psi(r,t)$ obeys the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi(r,t)}{\partial t} = \hat{H}\, \Psi(r,t) \qquad (5)$$

the system wave function $\Psi(r,t)$, we write as a linear combination of the overmentioned two states,

$$\Psi(r,t) = C_0(t) e^{-\frac{i}{\hbar}E_o t} |\phi_o\rangle + \sum_k C_k(t) e^{-\frac{i}{\hbar}(E_o + E_A - E_k)t} a_k^+ a_A |\phi_o\rangle \qquad (6)$$

In the given case $|C_0(t)|^2$ is the probability for the electron to be on the ion level.

$\sum_k |C_k(t)|^2$ is the probability for the electron to be in the surface-state zone.

The substitution of eqs.(1) and (6) in eq. (5) produce the following set of equations for the coefficients,

$$\dot{C}_k(t) = -\frac{i}{\hbar} V_{ak}(t) e^{\frac{i}{\hbar}(E_k - E_A)t} C_o(t) \quad (7)$$

$$\dot{C}_0(t) = -\frac{i}{\hbar} \sum_k V_{ka}(t) e^{-\frac{i}{\hbar}(E_k - E_A)t} C_k(t) \quad (8)$$

The above equations are obtained after the substituting for $\Psi(r,t)$ in the Schrödinger equation and multiplying the resulted equation by either $\langle\phi_o|$ or $\langle\phi_o | a_A a_k^+$ then integrating the result over all the space (using the orthonormality of the wave functions). Now assuming

$$V_{kA}(t) = \upsilon_k V(t) \qquad (9)$$
$$C_k(t) = \upsilon_k C(E,t)$$

where the quantity υ_k enters in the definition of the surface density of states $\rho_s(E)$ as,

$$\rho_s(E) = \sum_k |\upsilon_k|^2 \delta(E - E_k) \qquad (10)$$

Accordingly, eqs. (7) and (8) become

$$\dot{C}_k(E,t) = -\frac{i}{\hbar} V(t) e^{-\frac{i}{\hbar}(E-E_A)t} C_o(t) \quad (11)$$

$$\dot{C}_0(t) = -\frac{i}{\hbar} \int \rho_s(E) V(t) e^{-\frac{i}{\hbar}(E-E_A)t} C(E,t) dE \quad (12)$$

The coupling interaction as a function of time is chosen to be of the form,

$$V(t) = V_o e^{-\gamma_\perp |t|} \quad , \gamma = \sqrt{2|E_A|}/\hbar \quad (13)$$

The distance of the ion to the surface is written as $R = \upsilon_\perp t$ where $\upsilon_\perp$ is the ion velocity component normal to the surface. The choice of $\upsilon_\perp$ rather than of υ has been made because the interaction is not of binary character. In the following, we discuss some physical situation related to the shape of the surface density of state $\rho_s(E)$ will be presented such as:

Assuming that initially (at t=-∞) the system is in the configuration defined by $|\phi_o\rangle$. Then, $C_o(-\infty) = 1$; $C(E,-\infty) = 0$. We are interested in the case, after the ion is scattered from the surface, where the ion survived, i.e. we are looking for the quantity $p = |C_o(+\infty)|^2$. Then the set of eqs. (11) and (12) are solved (starting with eq. (11)) to give (13)

$$\dot{C}_k(t) = -\frac{i}{\hbar^2} \int \rho_s(E) V(t) e^{\frac{i}{\hbar}(E - E_a)t} dE \int_{-\infty}^{t} V(t') e^{-\frac{i}{\hbar}(E - E_a)t'} C_o(t') dt' \qquad (14)$$

$$\dot{C}_o(t) = -\frac{i}{\hbar^2} V(t) \int_{-\infty}^{t} V(t') C_k(t') dt' \int \rho_s(E) e^{-\frac{i}{\hbar}(E - E_a)(t-t')}$$

We discrete the band to a certain number of partials parts say n extended from lower part E_{ml} to upper part E_{mu} and each has surface density of state ρ_{sn} with a corresponding weight W_n such that,

$$\int_{E_{ml}}^{E_{mu}} \rho_{sm}(E) E_{mu} dE = 1 \text{ and } \sum_{m=1} W_m \int_{E_{ml}}^{E_{mu}} \rho_{sm}(E) dE = \sum_m W_m = 1 \qquad (15)$$

Then eq. (19) reads as,

$$\dot{C}_o(t) = -\frac{i}{\hbar^2} V(t) \int_{-\infty}^{t} V(t') C_o(t') dt' \sum_{m=1}^{n} W_m \int_{E_{ml}}^{E_{mu}} \rho_{sm}(E) e^{-\frac{i}{\hbar}(E - E_a)(t-t')} dE \qquad (16)$$

Eq. (16) helps us to discuss the situation when the energy band has a narrowed part say no 1 centered at α1 and widened part say No 2. This situation allows us to write eq. (16) as,

$$\dot{C}_o(t) = -\frac{W_1}{\hbar^2} V(t) \int_{-\infty}^{t} V(t') e^{\frac{i}{\hbar}(\alpha_1 - E_a)(t-t')} C_o(t') dt' - \frac{\pi W_2}{4\beta} V^2(t) C_o(t) \qquad (17)$$

The above clearly shows that the effect of the band part 2 is to give a certain life time to the electron in the level E_a (since it is broadened to a value with half-width equals to

$\Delta(t) = \frac{\pi W_2}{4\beta} V^2(t)$). Hence, it leaves the situation with a modified two-level problem (α_1 and $E_a - i\Delta(t)$).

Note that since $W_1 + W_2 = 1$ then, W_1 increases the interaction between the two levels hence increases the number of the oscillations in $|C_o(t)|^2$, also increasing W_2 which is in the definition of $\Delta(t)$ increases the decay in $|C_o(t)|^2$. In figure (1) we try three situations, these are,

$W_1 = 0.25$ $W_2 = 0.75$

$W_1 = 0.5 = W_2$

$W_1 = 0.75$ $W_2 = 0.25$

in order to clarify our points other values of the parameters are shown in the curve

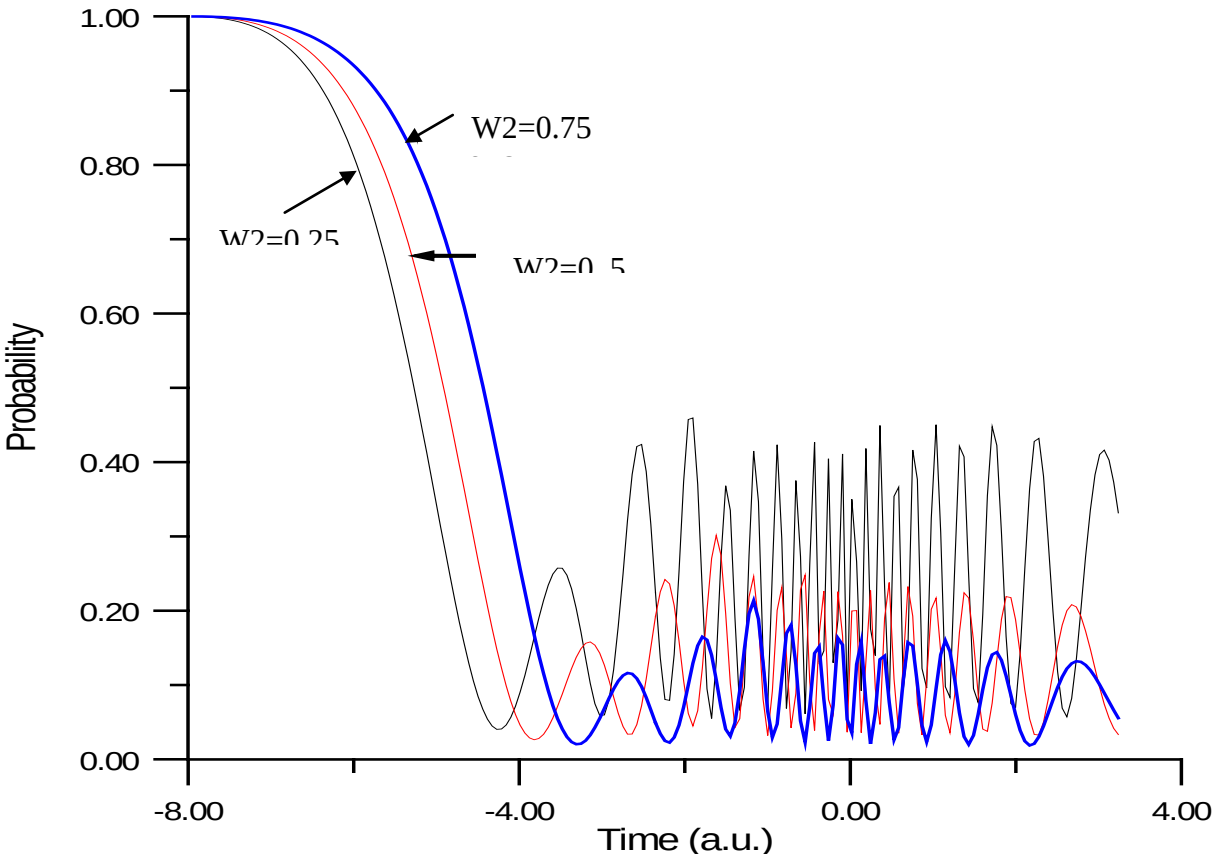

Figure (3): the survival probability at three values of W1 (W2=1.0-W1)

3. Applications and Results

3.1: The formation of exited secondary Si ions

The oscillating character of the energy spectrum of ions, scattered from the surface of a solid, can be explained in terms of the quasi-resonant charge exchange between an ion and a surface atom [28]. The probability of Si^{+*} formation has been calculated for the following process:

$Si^{2+} + \bar{e} \rightarrow Si^{+*}$.

From this probability we get the transition velocity (the probability differentiation with the ion surface distance) as a function to the ion surface distance. This factor (transition velocity) is an indicator for zone-to-ion and ion –to-zone transitions, depend on

the positive and negative value, respectively and the intensity by multipling it with term proportional to the incident ion energy E as E^{-2}.

This case is aimed at theoretical analysis of the electron charge exchange processes resulting in production of excited secondary ion, and the oscillation is the indicator to the electron exchange with the zone surface. The reduction in oscillation amplitude is used to identify and measure surface features [29].

We can see from figure (1) the quasi-resonance between the peak of filled electron state (E=5.9 eV) that locates in front of excited level (E=6.3 eV) and this narrowest of the peak of the surface density of states permits us to use the level – level interaction (i.e. 4p – level interaction). In the other hand this approximation is not correct for 4f level that locate in front the vacant zone so the surface density of states is replaced by the triangle and rectangle shapes as can as possible.

From figure (4) one can see the oscillations in the survival probability for the kinetic energy of the secondary ion 200 eV.

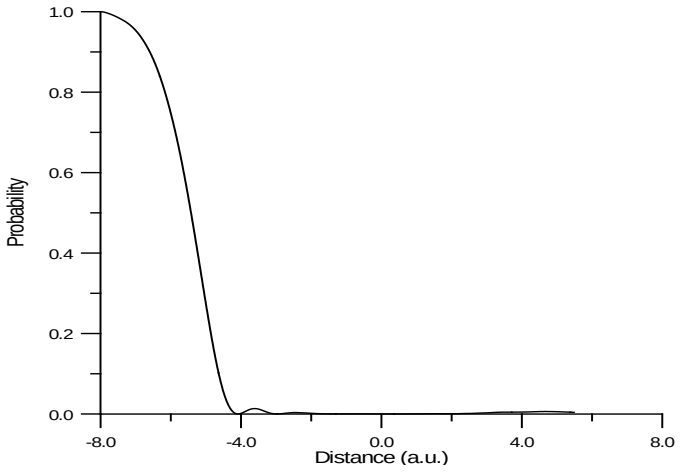

Figure (4): Survival probability vs distance (E=200 eV)

Figure (5) represents the survival probability for the kinetic energy of the secondary ion 560 eV, note that the oscillations are very clear and the space is large more than in the previous case (E=200eV).

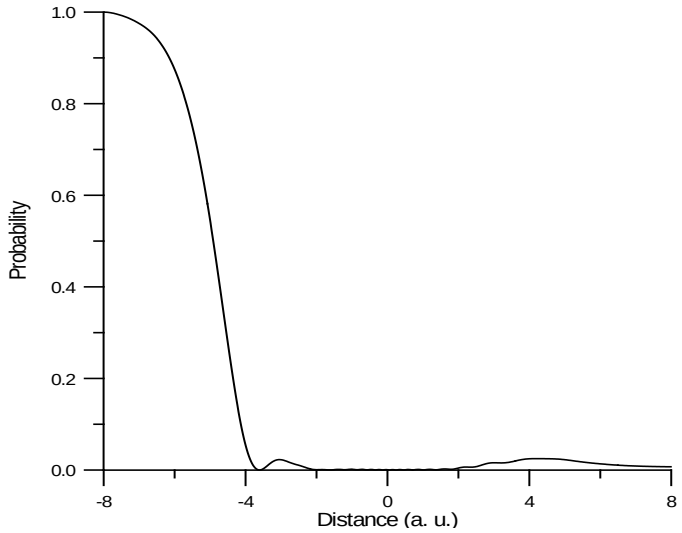

Figure (5): Survival probability vs distance (E=560 eV)

The ion production probability in figure (6) is the most important result from which we can get the intensity of the secondary ions (figure (7)), in this approximation we have good agreement with the experimental results [28]. The peaks of the oscillation in the experimental results are not equal in magnitude (i. e. are not in the same level), and that what we get.

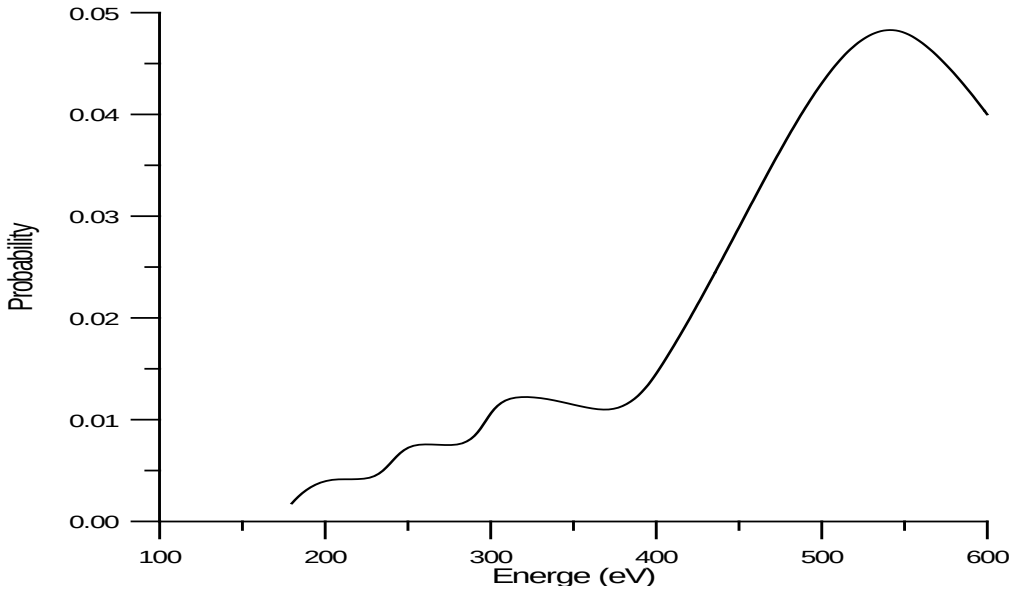

Figure (6): Energy spectrum of secondary Si^{+*} ions

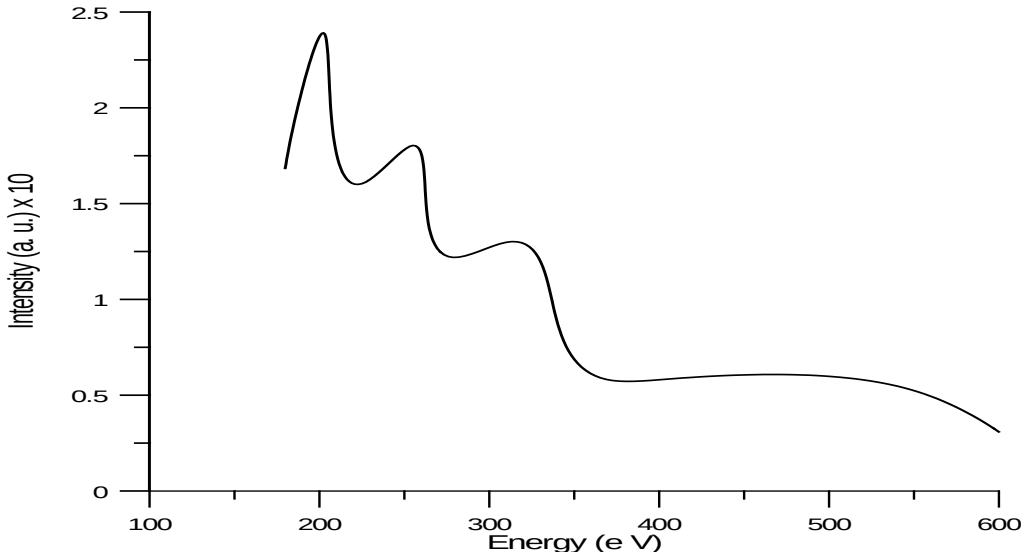

Figure (7): intensity of secondary Si^{+*} ions (multiplying figure (6) by E^{-2})

The comparison between theoretical and experimental shows that our result has good agreement with the experimental result [28].

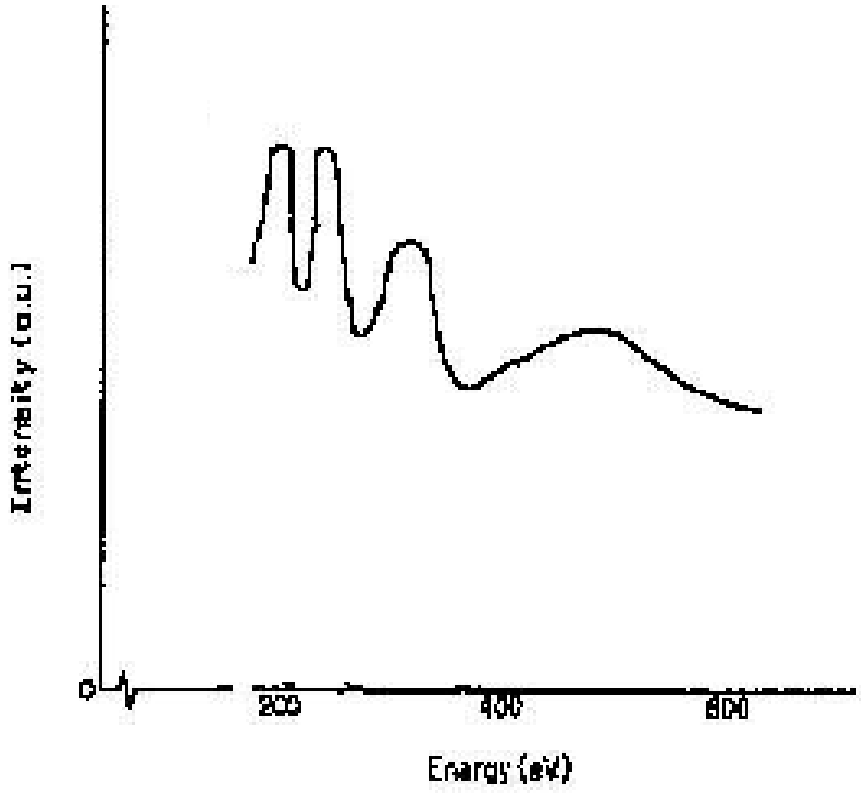

Figure (8): Intensity of Si^{+*} ions (Experimental) [28].

3.2: H^+ - Graphite Interaction

This application is important to make sure from the theoretical results when one compared with the experimental for survival probability results.

Figure (8) and (9) present survival probability (p) as a function of velocity after H^+ ion scattering (Vf)with incident energy of 1 keV and 2 keV respectively. We choice V_0=.75 for 1keV energy and V_0=.85 for 2keV energy to get more accuracy.

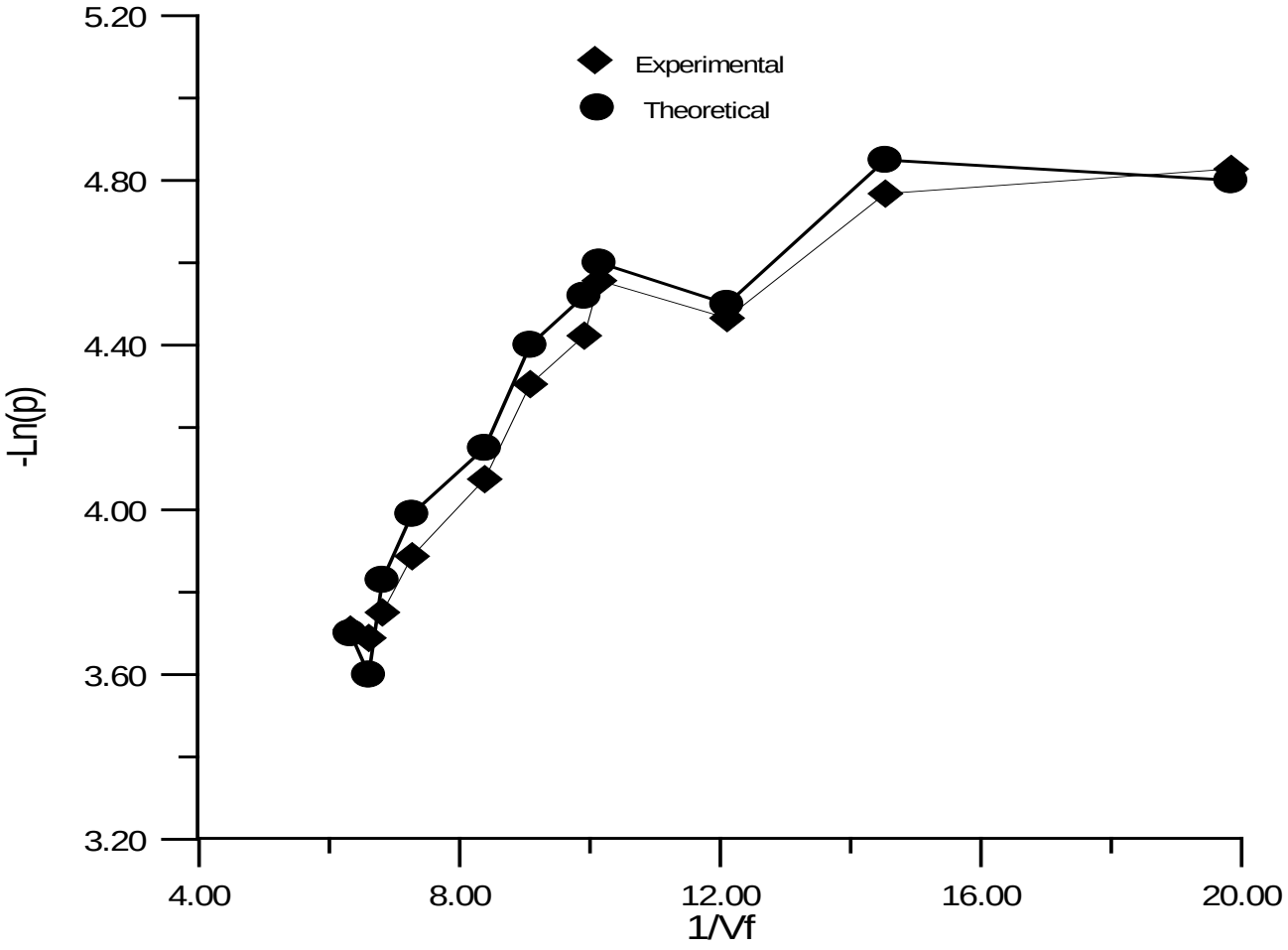

Figure (8): The experimental [29] and theoretical ion fraction as a function of the final ion velocity with initial incident ion energy of 1 keV

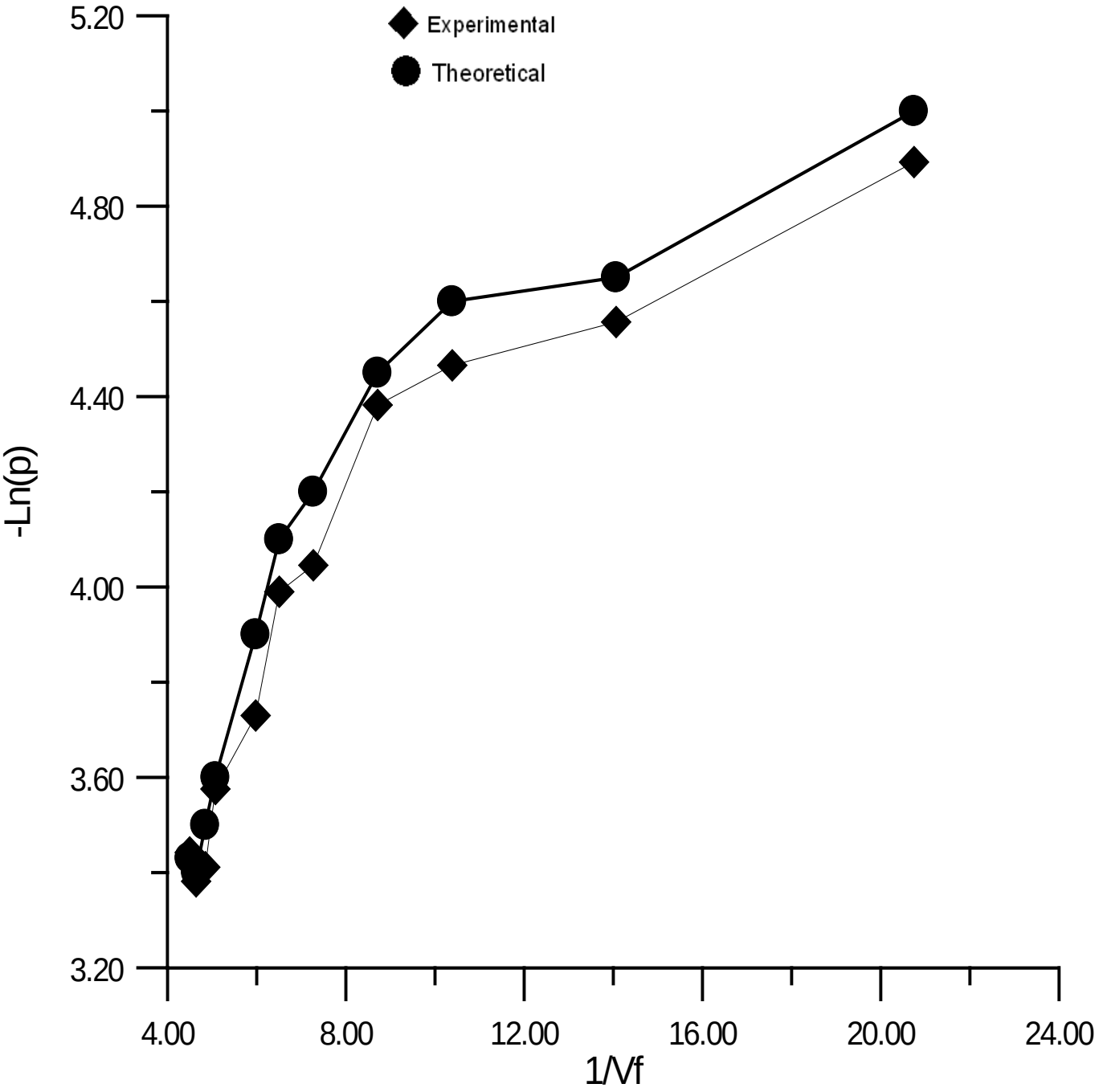

Figure (9): The experimental [29] and theoretical ion fraction as a function of the final ion velocity with initial incident ion energy of 2 keV

4. Conclusions

We present results of our study for the charge transfer process using Anderson-Newns Hamiltonian. The different approximations show the influence of the zone width and the relative position of the level and the zone on the oscillation amplitude and the survival probability (i.e. the intensity). The oscillating character of the energy spectrum can arise under interaction with the zone as V_{ak} increases then the characteristic time τ of electron diffusion be small. In the

case of the wide zone ($\Delta E > V_o$) no oscillations occur.

We explained the oscillating character of the energy spectra observed for two exited Si^{+*} state, this oscillation can be occur when charge exchange process between projectile and surface is exist our results have good agreement with experiment.

We use this model to get the survival probability of H^+ on C , also our results have good agreement with experimental results one when we change V_0 for different incident energies.

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عملية استطارة ذرة (أيون) – سطح: طريقة تفاعل الترتيبات

شاكر ابراهيم عيسى و فلاح حسن حنون

قسم الفيزياء– كلية التربية– جامعة البصرة

قسم الفيزياء كلية العلوم– جامعة ذي قار

الملخص:

تأثير هيئة كثافة الحالات للسطح على عملية انتقال الشحنة تم التحقق منها بالتفصيل بواسطة صياغة طريقة تفاعل الترتيبات (CI) . الطريقة طبقت لعملية انتاج سليكون متهيج Si^{+*} من استطارة سطح Si^{2+} من سطح Si وكذلك استخدمت الطريقة لتوضيح التصرف اللاخطي لأحتمالية بقاء أيون H^{+} كدالة لزاوية الأستطارة خلال الأستطارة المرآوية من سطح الكرافيت.