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Effect of projected band gap in the F^-- Cu system on the resonant charge transfer

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Abstract:

In this paper we study the effect of projected band gap on the resonant charge transfer when we use the grazing F^- projectile on the Cu surface with jellium potential. A wave-packet propagation method is used in the treatment of the resonant charge transfer process (RCT).Our study describe the long interaction time (low collision velocities)and we find the RCT efficiency is drastically reduced by the presence of the band gap. The important parameters are studied such that energy and width as a function to the distance between the surface and the projectile as well as the projected density of state at two different distance near (1 a.u.) and far from the surface (6 a.u.).

Introduction:

This study gives the important physical phenomena which happen in the solid state, it is the resonant charge transfer process (RCT) [1]. When the projectile close to the surface the surface may be take an electron from it and the electron suffers from which state go to his own. This is what we called the resonance and so the probability of the wave function gives us the information weather electron escape from the projectile or not [2]. The wave packet propagation method (WPP) is used to discuss both the free electron (jellium) description of the metal target and the model description of the metal (hkl) electronic structure [3]

Mathematical Model:

The free electron model is identical to the one used in [4]. The electron interacts with the surface via potential of the form given by Jennings et al [5]. It is only a function of Z, the electron - surface distance, measured from the surface image reference plane Z0 and (Z > 0 is the vacuum side) [4]:

$$\left.\begin{aligned} V_{e\text{-}surf}(Z) &= -[1-\exp(-\lambda Z)]/4\ Z, && Z>0 \\ V_{e\text{-}surf}(Z) &= -V_0/[1+A\exp(B\ Z)], && Z<0 \end{aligned}\right\} \quad (1)$$

Here, λ , A and B are constant referred to the type of surface .

The above definition puts the origin for the Z coordinates on the image reference plane. This origin is for all the distance from the surface and the potential energy is measured with respect to vacuum level. Below, we present the jellium metal model

Wave packet propagation method (WPP)

The wave packet propagation method (WPP) consists in studying the time evolution of an electron wave packet in the compound potential defined previously.

The time – dependent electron wave function is a $\psi(r,t)$ solution of the time dependent Schrödinger equation with the Hamiltonian H. The initial electron wave function is taken to be equal to $\psi_a(r)$, the eigenfunction of $\psi(r,0)$ the potential of projectile state, i.e., the free projectile wave function. Within the chosen model, the system is invariant by rotation around OZ, the axis normal to the surface and going through the projectile center. Therefore a cylindrical coordinates is used (z is the electron coordinates along the symmetry axis, ρ is the normal distance to the axis, and ϕ the azimuth angle). It has been found that the convergence of the time propagation scheme is improved by the following change of the function:

$$f(r,t)=\sqrt{\rho}\,\psi(r,t) \quad (2)$$

Substitution of Eq. (2) into the time dependent Schrödinger equation in a.u. yields

$$i\frac{df(r,t)}{dt}=\tilde{H}f(r,t) \quad (3)$$

with,

$$\tilde{H}=T_z+T_\rho+V_{e-core}(r)+V_{e-surf}(z) \quad (4)$$

where,

$$T_z = -\frac{1}{2}\frac{d^2}{dz^2} \quad (5)$$

and,

$$T_\rho = -\frac{1}{2\sqrt{\rho}}\frac{d}{d\rho}(\rho\frac{d}{d\rho})\frac{1}{\sqrt{\rho}} \quad (6)$$

And, Ve-core defines the interaction potential for the outer electron with the atomic core, Ve-surf defines the interaction potential for the outer electron with the surface.

The time propagation of the electron wave function is obtained via the evolution operator $U(\Delta t)$:

$$f(r,t+\Delta t) = U(\Delta t)\, f(r,t) \quad (7)$$

where,

$$U(\Delta t) = \exp(-i\tilde{H}\Delta t) \quad (8)$$

The Hamiltonian $\tilde{H}$ is independent of time in the static case. For the evolution operator, we use the split operator approximation and unitary stable Cayley scheme [6] so that

$$\exp(-i\tilde{H}\Delta t) = \frac{1-i(\Delta t/2)\tilde{H}}{1+i(\Delta t/2)\tilde{H}} + O(\Delta t^3) \quad (9)$$

The origin of the coordinates is placed at the projectile center; the zj mesh points, are equally spaced with a step Δz equal to 0.2 a0, where a0 is the Boher radius. For the ρ coordinate, it's first performing the change of variable $\rho = x^2$ and use equally spaced points x_i with a step Δx equal to 0.02 a01/2.

By using finite difference method [7], we have from eq(4):

$\tilde{H} = \tilde{H}_1 + \tilde{H}_2$ where, $\tilde{H}_1 = T_z + V_{e-core}(r) + V_{e-surf}(z)$ and $\tilde{H}_2 = T_\rho$ then,

$$(\tilde{H}_1 f)_{i,j} = \frac{-1}{2(\Delta z)^2}[f_{i,j+1} + f_{i,j-1} - 2f_{i,j}] + [V_{e-core}(r_{i,j}) + V_{e-surf}(z_j)]f_{i,j} \quad (10a)$$

$$(\tilde{H}_2 f)_{i,j} = \frac{-1}{8x_i^2(\Delta x)^2}[\frac{x_i+\Delta x/2}{x_i+\Delta x} f_{i+1,j} + \frac{x_i-\Delta x/2}{x_i-\Delta x} f_{i-1,j} - 2f_{i,j}] \quad (10b)$$

During the propagation of the electron wave packet it goes into the metal and spreads over the entire grid. In the static problem, one studies the electron dynamics for a fixed projectile–surface distance with the initial electron wave function equal to ψa(r). The wave- packet propagation scheme then provides ψ(r,t),

from which we define the survival amplitude in the free projectile bound state or equivalently the electronic wave- packet autocorrelation function [8]

$$A(t) = \langle \psi_a(r) | \psi(r,t) \rangle \tag{11}$$

and its Laplace transform

$$g(\omega) = \frac{1}{\pi} \int_0^\infty dt e^{i\omega t} A(t) = \frac{1}{\pi} \int_0^\infty dt e^{i\omega t} \langle \psi_a(r) | \psi(r,t) \rangle \tag{12}$$

The real part of g(ω) gives n(ω), the projected density of states (DOS). n(ω) poses a Lorentzian peak at the resonance position, i.e., at the energy of the quasibound state of projectile which it can be used to extract the resonance characteristics, i.e., the level energy position (E) and its width (Γ).

In order to avoid long propagation times, we directly analyze the autocorrelation function as a superposition of a few exponential terms, the parameters of which are determined by a fit procedure [4]:

$$A(t) = \sum_{j=1}^{L} a_j \exp\{-i(E_j - i\frac{\Gamma_j}{2})t\} \tag{13}$$

Here L is the number of opens band gap located between -5.9 and -0.8 eV. In the present case, the number of structures in the projected density of states is rather limited, so that an excellent convergence of the fit can be reached and checked with L=3 (for L > 3 is also checked but it does give nothing).

By using eqs.(12) and (13) one get after carrying out the investigation,

$$g(\omega) = \frac{1}{\pi} \sum_{j=1}^{3} \frac{a_j \Gamma_j / 2}{(\omega - E_j)^2 + (\Gamma_j / 2)^2} + i \frac{1}{\pi} \sum_{j=1}^{3} \frac{a_j (\omega - E_j)}{(\omega - E_j)^2 + (\Gamma_j / 2)^2}$$

where, the projectile density of state $n(\omega)$ is given by the real part of $g(\omega)$ as [9],

$$n(\omega) = \frac{1}{\pi} \sum_{j=1}^{3} \frac{a_j \Gamma_j / 2}{(\omega - E_j)^2 + (\Gamma_j / 2)^2}$$

Applications and Results:

We carry out a theoretical investigation of F- projectiles impinging on Cu. The parameter values of equation (1) are as follows:-

λ is equal to 1.5 (a0)-1 , V0 is equal to 12.61 eV, . the λ parameter in eq. (1) have been adjusted so that the surface state and the first image state energies in the model are -5.33 eV and -0.82 eV, respectively which reproduce the characteristics of the Cu surface [8]. The full potential as a function of Z is presented in Figure (1).

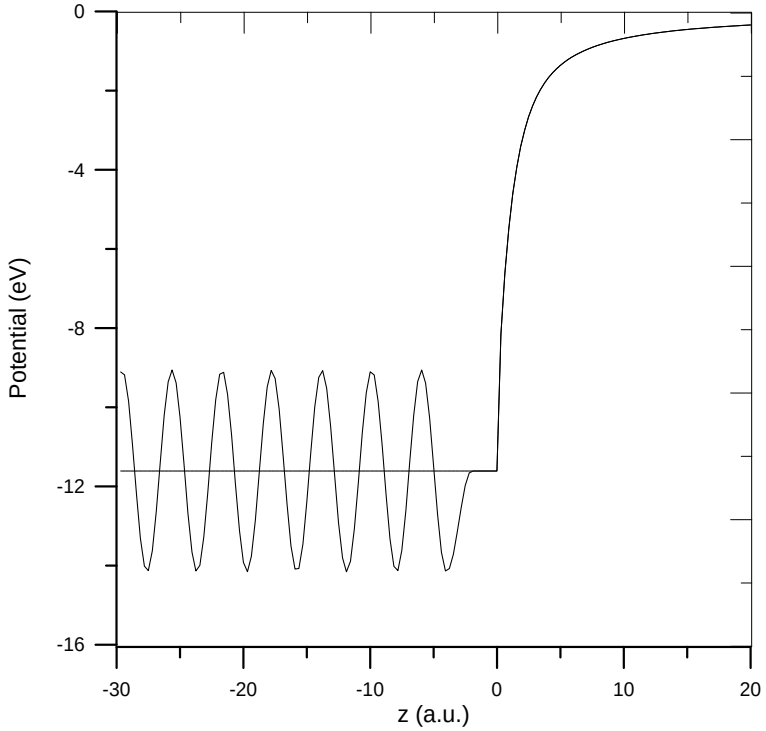


Figure (1): Model potential used to represent the electron – model Cu(111)interaction and the electron Cu jellium interaction, as a function of Z, the electron coordinate normal to the surface, Z=0 corresponds to the position of the image plane.

Figure (2) gives us three regions that can effect on RCT these three regions are obtained from ploting the following equation $E = \frac{k^2}{2} + E_i$ where, Ei denotes different part of the band, as an example $E = \frac{k^2}{2} - 5.33$. They are,

(i) The first image state at -0.82 eV which is in proximity to the F- level (-0.75 eV) at large ion distance.

(ii) The surface state at -5.33 eV at intermediate ion distance.

(iii) The top of the valance band at Eb =-5.93 eV at too small ion distance.

The projected L-band gap exists between Et=-0.70 eV and Eb=-5.93 eV, the surface state at Es=-5.33 eV while the first image state at EI=-0.82 eV lies barely in the band gap while higher ones are degenerate with the conduction band

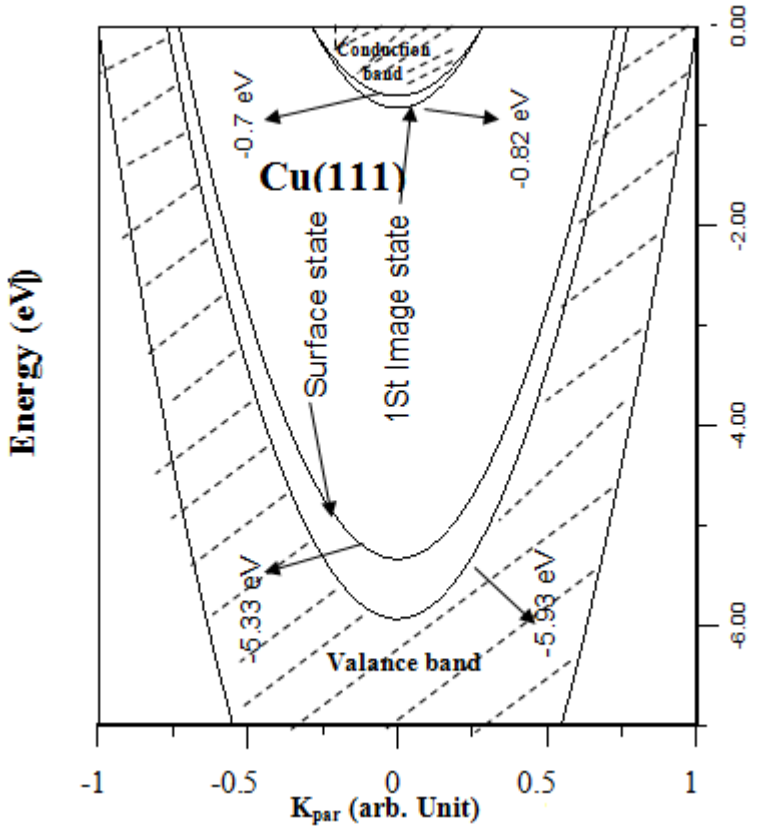
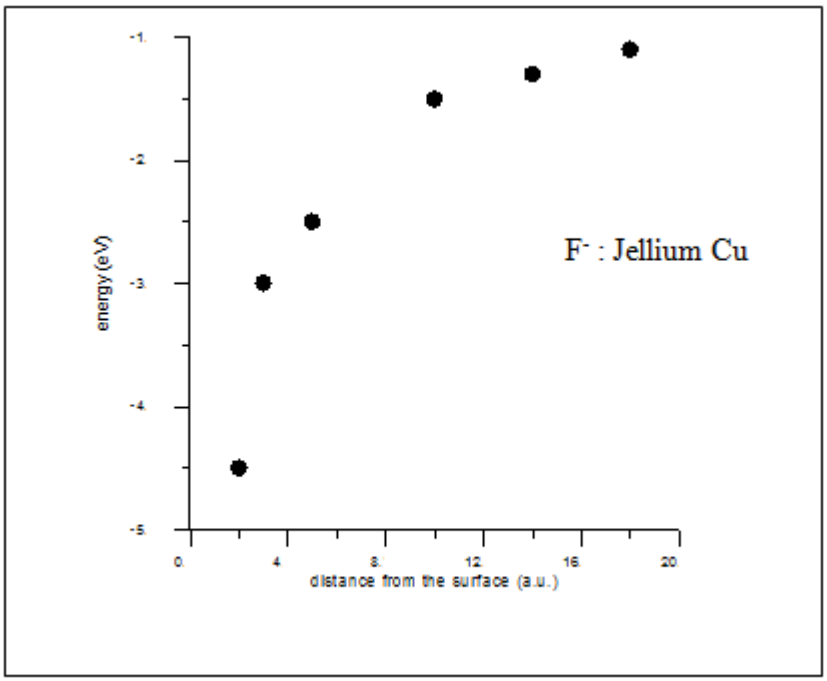
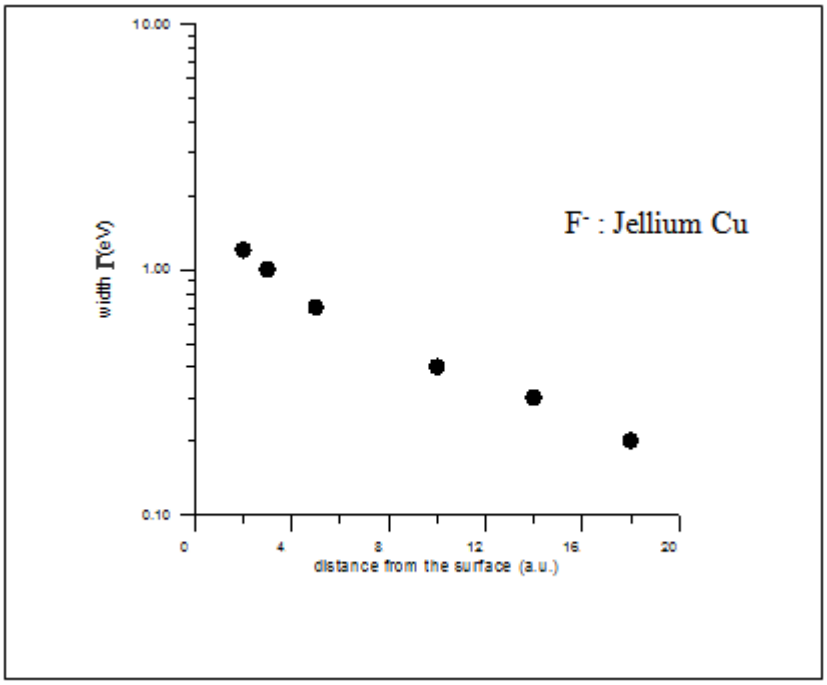


Figure (2): Schematic picture of the Cu(111) electronic structure as a function of the electron momentum parallel to the surface.



a



b

Figure (3): Energy position (a) and width (b) of the F- level in front of a Cu jellium surface, as a function of the ion-surface distance, measured from the image plane

The projected density of state:

Figure (4) and (5) present the projected density of states $n(\omega)$ in the jellium Cu case for an ion – surface distance Z equal to 6 a.u.and 1 a.u , respectively. On the logarithmic scale, the ion level appears as a sharp quasi-Lorentzian peak sitting on the top of a flat background ρ_0 i.e. $\rho(\omega) = \rho_0 + \frac{\Gamma/2}{(\omega - E)^2 + (\Gamma/2)^2}$. The position and width of the peak gives the energy and width of the quasistationary state.

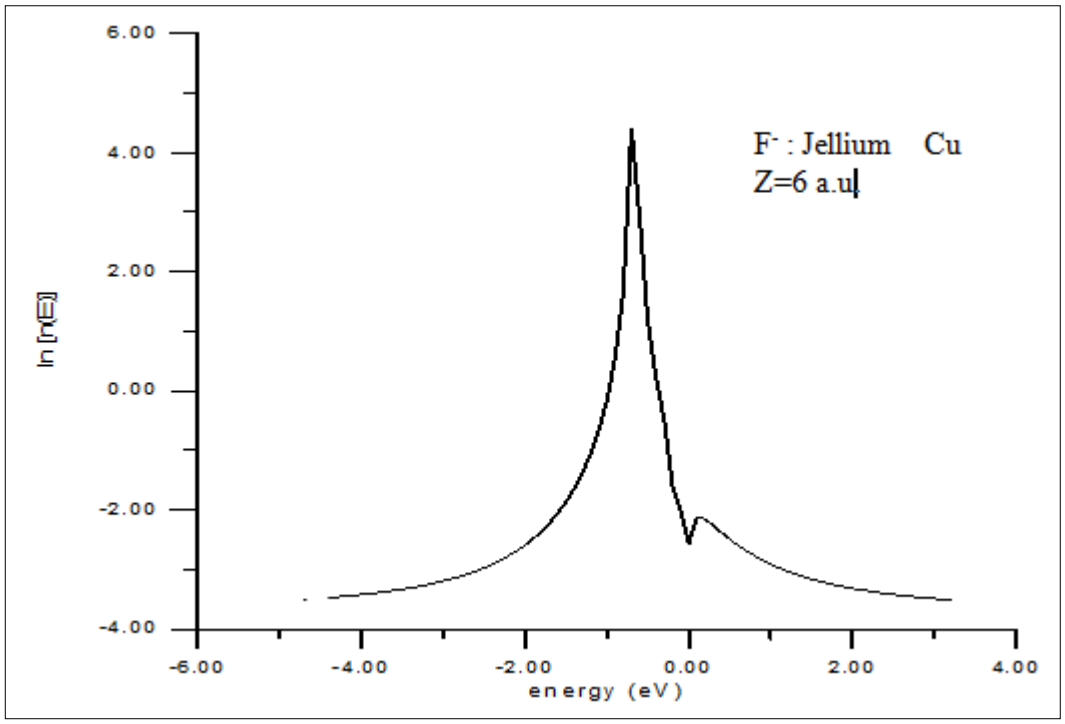


Figure (4): Logarithm of the projected density of state for the case of F^- ion interacting with a jellium Cu surface.

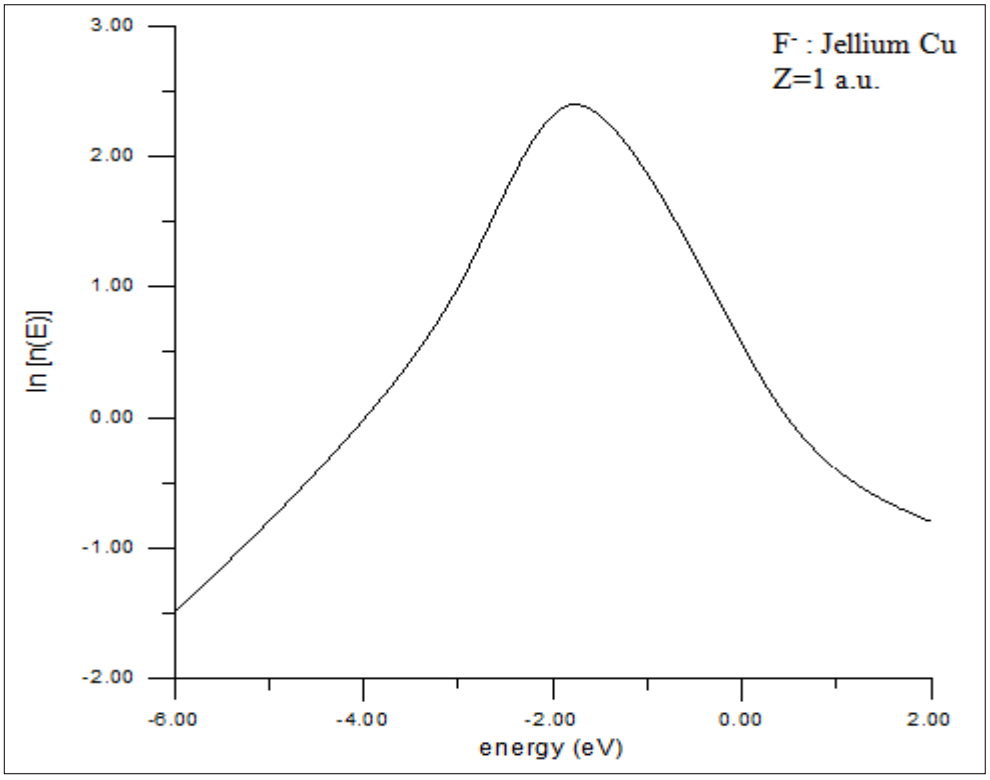


Figure (5): Logarithm of the projected density of state for the case of a F^- ion interacting with a jellium Cu surface.

Conclusion:

The wave packet propagation method is a good method for describing the behavior of the F- projectile on Cu surface with jellium potential. Because our results like the results of many negative ion interaction with this surface and from the curve that describe the density of state, we can find out the resonant sites from the peaks. The sharpness of beak is refers to the electron was interact with single state and so is happen in the far point but in the near point the electron interacts with many states so that the density of state was flat and wider .

References:

[1] A. G. Borisov and V. A. Esaulov, J. Phys. Condens, 12, 177 (2000).

[2] J. T. Kindt, J. C. Tully, M. Head-Gordon, and M. A. Gomez, J. Chem.Phys. 109, 3629 (1998).

[3] G. D. Billing, J. Chem. Phys. 112, 335 (2000).

[4]A. G. Borisov, D. Teillet . Billy, and J. P. Gauyacq, Phys. Rev. Lett., 68. 2842 (1992).

[5] P. J. Jennings, P. O. Jones, and M. Weinert, Phys.Rev., B37, 6113 (1988).

[6] W.H. Press, S.A. Tenkolsky, W.T. Vetterling, and B.P. Flannery, Numerical Recipes in Fortran (Cambridge University press, Cambridge, 1982).

[7] M. C. Desjonqueres and D. Spanjaard, Concepts in surface physics,Springer Series in Surface Science, 40 (Springer-Verlag, Berlin.1993).

[8] Y. Yang and J. A. Yarmoff, Phys. Rev. Lett. 89, 196102 (2002).

[9] M. M. Jassim, M.Sc. Thesis, University of Basrah, Iraq, (1998).

تاثير فجوة الحزمة المسقطة في نظام F^- - Cu على عملية انتقال الشحنة الرنيني

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الخلاصة:

درس في هذا البحث تاثير فجوة الحزمة المسقطةعلى عملية انتقال الشحنة الرنيني وذلك باستخدام قذائف F^- تسقط على سطح Cu بزوايا صغيرة معه .استخدمنا طريقة انتقال حزمة الموجة لوصف التفاعل الحاصل بين القذيفة والسطح عند ازمان طويلة اي عند التصادمات الضعيفة ولاحظنا ان عملية انتقال الشحنة تتاثر بالفجوة عن طريق دراسة طاقة الرنين وعرض حزمة كثافة الطاقة كدالة للمسافة وكذلك دراسة تاثير المسافة بين القذيفة والسطح عند مسافتين احدهما قريب (1 a.u.) والاخر بعيد (6 a.u.).