Metastable He*Atom–3ML Ag/Cu (111) Surface Interaction by Using Wave Packet Propagation Method

Falah Hassan[1], **Suha Hadi**[2]

[1, 2]Thi-Qar University, College of Science, Physics Department

Abstract: ***This research deals with the static metastable He*atom when interacts with C(111) surface and with this surface modification when Ag (i.e. noble metal) deposit on it as a thin film with3mono layers(3ML). This study gives the charge transversprocess with Resonance Ionization (RI) theoretically by solve the time dependent Schrodinger equation (wave packet propagation method) with new surface potential , and show the dependence of charge transvers on the time interaction ,particle- surface distance as well as the 3ML effects on this process. The results Shows that the density of state and the survival probability for pure Cu(111) metal and for Ag/Cu(111) and also show the wave function spreading on the surface. The results have good agreement with experimental results.***

Keywords: Auger neutralization, Wave packet propagation, Survival probability, Surface potential.

1. Introduction

The electronic structure of metal gives the physical and chemical properties[1].Due to their extreme surface sensitivity, the Shockley states of (111) noble metal surfaces can be used to study the modifications of atomic and electronic properties of epitaxial ultra thin films and self-organized nanostructures. The thickness of the film plays the important role of many parameters such as energy band, effective mass, spin- orbit splitting, and by the way effects on the Resonance charge transfer RCH, Auger neutralization (AN) and resonance Ionization (RI) process, when ion interacts with the metals system. For thin films the spectroscopic properties investigated by angle-resolved-photoemission-spectroscopy (ARPES) and scanning tunneling spectroscopy (STS) of Shockley states are very sensitive to the atomic structure and thickness of the film. the thickness dependence of the surface state energy can be used in STM to study this system[3]. There are many theoretical methods treat the charge transfer process when ion closes to the surface (like the tip of many devices that give the surface picture) such as Anderson-Newns Hamiltonian, rate equation method and Wave packet propagation method[4].The band of the pure surface will be shift when thin film of noble metal covers it, and so the electron of the negative ion suffer from another different state we can show it from the wave function of this ion [5]. 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 surfaces(desorption, fragmentation of adsorbates, chemical reactions, quenching of meta stable species, etc.) [6–9]. The potential of the surface effects on the Auger neutralization process, theoretically since it is one of the term of the time dependent Schrodinger equation and some researches take it as jellium or pseudo potential[5]. This potential will be change when epitaxial thin film of many layer on it and so we give new one dimensional potential model describes this system.

2. Theoretical Model

The time dependent electron wave function $\Psi(\mathbf{r},t)$ is a solution of the time dependent Schrodinger equation with the Hamiltonian H. The initial electron wave function $\Psi(\mathbf{r},0)$ is taken equal to Ae^{-Br} (Hydrogeen like atom)[10]. The surface potential have four region formula.

a)-$Z < Z_\circ - \pi / G$,
$V_{e-sur\,(z)} = -V_\circ + V_G \cos[G(Z - Z_\circ)]$,(1)

(b)-$Z_\circ - \pi/G < Z < Z_\circ$,
$V_{e-sur}(z) = -V_\circ - 0.5V_G\{1 - \cos[G(Z - Z_\circ)]\}$,(2)

(c)-$Z>Z_\circ$, $V_{e\text{-surf}}(z)$ is given by
$V_{film}(z) = [a_1 x + a_2 \sin(\sin a_3 x^{a_4})] - V_\circ$ (3)
Where $a_1=0.2$, $a_2=2$, $a_3=.7$, $a_4=1.8$.

(d)- $Z>Z_\circ +2L$ where L=number of Ag layers
$V_{e-sur}(z) = [1 - \exp(-\lambda z)]/4z, z > 0$ (4)
$V_{e-sur}(z) = -V_\circ / [1 + A\exp(Bz)] \cdot z < 0$

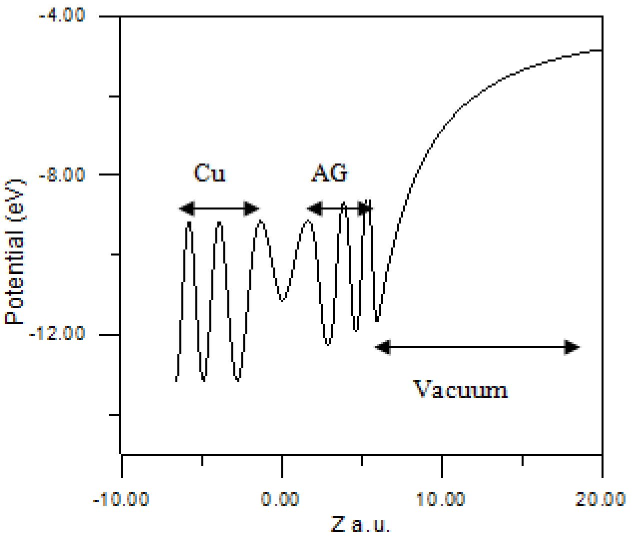


Figure 1

one dimension pseudo potential model used in the time dependent Schrodinger equation (current study).

Let:
$f(r,t)=\sqrt{\rho}\ \psi(r,t)$

in the time dependent Schrodinger equation and that givs:

$$i\frac{df(r,t)}{dt}=\widetilde{H}f(r,t) \qquad (5)$$

$$\widetilde{H}=T_z+T_\rho+V_{e-He}(r)+V_{e-sur}(z) \qquad (6)$$

Where

$$T_z=-\frac{1}{2}\frac{d^2}{dz^2} \qquad (7a)$$

And

$$T_\rho=-\frac{1}{2\sqrt{\rho}}\frac{d}{d\rho}\left(\rho\frac{d}{d\rho}\right)\frac{1}{\sqrt{\rho}} \qquad (7b)$$

We can get the wave function sfter any time by using the time operator $U(\Delta t)$ i.e.

$$f(r,t+\Delta t)=U(\Delta t)f(r,t) \qquad (8a)$$

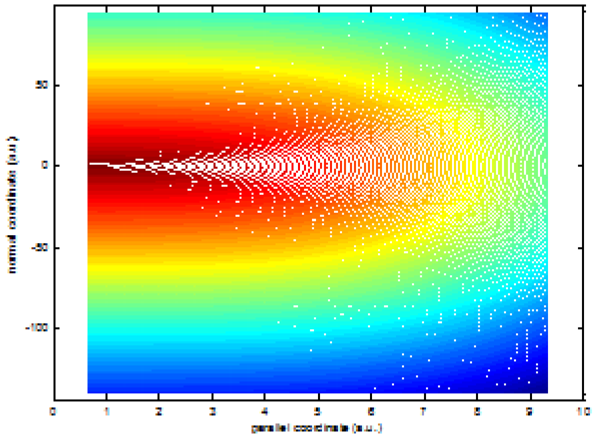
Where

$$U(\Delta t)=exp\left(-i\widetilde{H}\Delta\Delta t\right) \qquad (8b)$$

By splitting the Hoperator we get:

$$U(\Delta t)=\exp\left(-i\widetilde{H}_1\frac{\Delta t}{2}\right)\exp\left(-i\widetilde{H}_2\Delta t\right)\times\exp\left(-i\widetilde{H}_1\frac{\Delta t}{2}\right)+0(\Delta t^3) \quad (9)$$

$$\widetilde{H}_1=T_z+V_{e-He}(r)+V_{e-sur}(z) \qquad (10)$$



$$\widetilde{H}_2=T_\rho$$

The exponential operators in Eq. (9) are calculated using the unitary and unconditionally stable Cayley scheme [11,12]

$$\text{Exp}(-i\widetilde{H}\Delta t)=\frac{1-i(\Delta t/2)\widetilde{H}}{1+i(\Delta t/2)\widetilde{H}}+0(\Delta t^3) \qquad (11)$$

The operators are discretised using a three-point differentiation scheme:

$$\left(\widetilde{H}_1 f\right)_{i,j}=\frac{-1}{2(\Delta z)^2}\left[f_{i,j+1}+f_{i,j-1}-2f_{i,j}\right]+\left[\left[V_{e-He}\left(r_{i,j}\right)+V_{e-sur}\left(z_j\right)\right]\right]f_{i,j} \quad (12)$$

$$\widetilde{H}_2=T_\rho$$

$$T_\rho=-\frac{1}{2\sqrt{\rho}}\frac{d}{d\rho}\left(\rho\frac{d}{d\rho}\right)\frac{1}{\sqrt{\rho}}$$

$$\widetilde{H}_2 f=-\frac{1}{2\sqrt{\rho}}\frac{d}{d\rho}\left(\rho\frac{d}{d\rho}\left(\frac{f}{\sqrt{\rho}}\right)\right)$$

$$\widetilde{H}_2 f=-\frac{1}{8x_i^2(\Delta x)^2}\left[\frac{x_i+\frac{\Delta x}{2}}{x_i+\Delta x}f_{i+1,j}+\frac{x_i-\frac{\Delta x}{2}}{x_i-\Delta x}f_{i-1,j}-2f_{i,j}\right]. \quad (13)$$

the electronic wave-packet autocorrelation function or the survival probability is define as

$$A(\langle t)=\psi_a(r)|\psi(r,t)\rangle \qquad (14)$$

And its laplace transform

$$g(w)=\frac{1}{\pi}\int_0^\infty dte^{iwt}A(t)$$

$$=\frac{1}{\pi}\int_0^\infty dte^{iwt}\langle\psi_a(r)|\psi(r,t)\rangle \qquad (15)$$

The real part of g(w) gives n(w), the projected density of states DOS. n(w) presents a Lorentzian peak at the neutralization position.

3. Results and Discussion

Figure 1. presents the wave packet distribution of the He* atom at five different times, 0, 40, 500, 1500, 2000 a.u. and the ion at fixed distance (7 a.u.). The logarithm of the modulus of the electron wave packets is plotted as a function of the parallel coordinates (x) and the normal of the coordinates (z).One can see when the time equal zero (no interaction) the contour of the wave function is smoothly and symmetry but at time 40 (short time interaction) the wave packet has slightly changed and expand parallel to the surface because the electron has no time to go far in the metal. Also when the time interaction becomes long the electron represent itself as pumping of the wave packet in the different positions in the normal direction as we can see from the figure 2(c) .

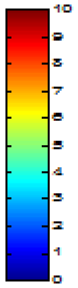
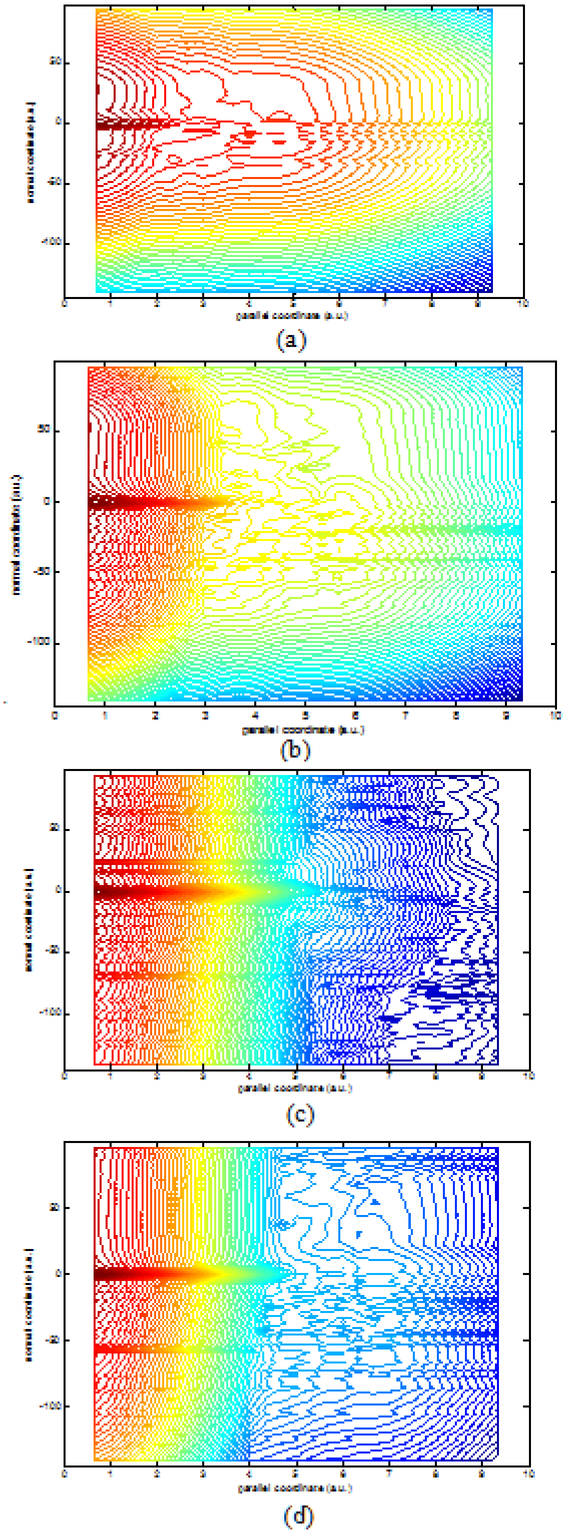


Figure 2

Logarithm of the modulus of the initial electron wave packet in the static WPP calculation as the function of the z and x electron coordinates, respectively, normal and parallel to the Cu/Ag (3ML) system with ion surface distance =7 a.u. and the origin of coordinates is at the ion center.



(a)

(b)

(c)

(d)

Figure 3

Logarithm of the modulus of the initial electron wave packet in the static WPP calculation as the function of the z and x electron coordinates, respectively, normal and parallel to the Cu/Ag system with ion surface distance =7 a.u. after a propagation time: (a= 40 , b=500 c=1500 d=2000) a.u.

Figure .4. shows the projected density of state at the distance z=2, 5,7 a.u. , one can see the shape of the density of states like the Lorentzian or quasi lorentezian peak and from it one can get the width of the level as well as the energy position. This figure presents the proportional between the width of the density of state and the separation of the ion – surface also the proportional between the position energy and this separation as in many researches [9-13],but this feature is different from another by the slightly changing , long time interaction and very big matrix to get the effect of both surfaces (Cu,Ag) especially in the short distances.

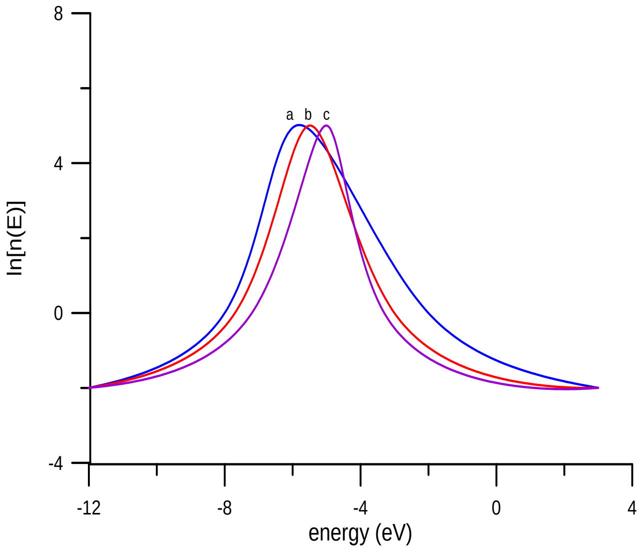


Figure 4

Density of states for the case of an He*atom interacting with Cu/Ag potential surface (research potential) .The ion surface distance equal to (a= 2 b=5 c=7)a.u.

Figure.5. represents the survival probability of the ion, for the potential that use in this study this probability gives the indicator of the interaction and one can see that the interaction depend on the ion surface distance , also one can divide the curve in to two part ,the first part is linearly at short time interaction and the second part is oscillatory curve at the end of the time interaction.

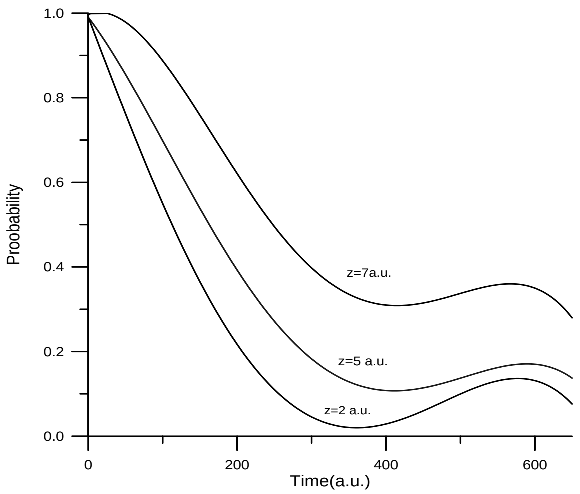


Figure 5

Survival probability as a function of time for an He*atomat three distances of from the Ag/Cu(111) surface

4. Conclusion

We presented the results of a study of the He^*atom - Ag/Cu(111) surface by using the wave packet propagation method to study the resonance charge transfer process. It has revealed a very strong effect of this surface system on this process. With short time interaction the decay of the He^*atom and its interaction with the band gap of this surface is very slightly because this ion has no long time to interact with image state or with surface state, for long time interaction the charge goes far in the normal of the surface. The behavior of the projected density of states shows that the peaks of the lorentzian shape becomes narrow and drift to the right of the energy . The another test for ion surface interaction is the survival probability which decay from 1(on interaction)to the 0.1 (approximately) very strong interaction. Twhe wave packet propagation method is very sensitive for the initial wave function and surface potential and it is the best method to sho clearly that the charge transfer coupling for He^*atom - Cu/Ag is very strong in the short distance and long interaction time. From the probability one can note that 3Ml of Ag represents as shielding charge transfer process between ion and clean Cu surface

References

[1] Y.Zheng,y.Jiao,M.Jaronice,S.Z.Qiao, Angeuu. Che. Int. Ed. 2014, 53.
[2] D.Malterre, B. Kierren, Y. Fagot- Revurat, S. Pons, A.Tejeda,C.Didiot,H.Cercercellier,Bendounan,NewJ.Phys.9,391,2007.
[3] T.Andreev, I.Barke, H.Horel, Phys. Rev,
[4] A.Nourtier, Phys.(France) 50,311.1989.
[5] A.G.Borisov,A.K.Kazansky,J. P. Gauy-acq, Phys. Rev B, Vol 59,N 16,1999.
[6] G.J.Schulz, Rev. Mod.Phys.45,1973,423.
[7] L.Sanche, J. Phys.B 23, 1990,1597.
[8] R.E.Palmer and P.J.Rous,Rev.Mod. Phys. 64,1992,383.
[9] T.S.Jones,M.R.Ashton,M.O.Dingand, N ,V,Richardson,Chem.Phys.Lett.161,1989,467.
[10] -A.A.Sh,Thesis ,University of Basrah, College of Science,Basrah,Iraq,2014.
[11] J.R.Taylar,Scattering Theory:The Qu Antum Theory of NonrelativistisCollisions,Kriege -r,Malabar,FL,1983.
[12] W.H.Press,S.A.Tenkolsky,W.T.Vette - rling,B.P.Flannery,Numerical Recipes in Fortran,
[13] Cambridge University Press,Cambridge,1982.