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Study to the Main Effects on the Auger de-excitation Transition

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Abstract

An Eigen-state expansion method is applied to the transition of the Auger de-excitation charge transfer (AD) process in the interaction between clean Cu,Al and Na surfaces and excited incident gases H and He .We use this method to describe the effective surfaces electronic structure. It's shown that the AD efficiency is deeply influenced by the presence of the energy band for the surfaces and the potential energy stored within the excited incident atom, thus for long interaction time we use a slowly atom's about 1KeV to scatter from metals surfaces where the electron couldn't probe the metal band structure and Z_a the surface - projectile distance. Also we drive a new formula for AD interaction Matrix element.

Keywords: Auger De-excitation (AD), Scattering, Ion Surface interaction.

Introduction

Charge exchange phenomena of ions (atoms) in front of a metal surface are of considerable interest in fundamental research as well as in technological applications. The basic processes for electron transfer in the scattering of thermal and hyperthermal beams were established some decades ago[1-3] and comprise resonant one- electron tunneling and two-electron Auger processes .when a slowly moving projectile incident on a metal surface of sufficiently small work function Φ the possible processes for Auger charge transition are shown in fig.(1)[4]. Neutralization of scattered ions is well-known to be an important effect which enhances the surface sensitivity of the technique but leads to low scattered ion yields. The main mechanism of charge exchange with the target material (usually metallic) has been generally agreed to be Auger neutralization

(AN) fig.1 (b), involving direct transfer of a surface valance electron into He^+ ion core hold ground state. With the excess energy being given, as kinetic energy, to other valence electron of the surface. An alternative process of charge exchange is resonance neutralization (RN) fig.1 (a) in which a metal surface valance electron tunnels across into an unoccupied state of the ion at essentially the same binding energy in a one-electron process. This mechanism is believed to be important, for example, in charge exchange with incident alkali metal ions whose ground state empty levels lie energetically close to the Fermi level [5-7].

Some important resurgence of interest in the theory of surface charge exchange processes , the one-electron resonant mechanism, demonstrate a special case of "quasi-resonant" charge exchange with a deeper lying occupied state of the solid as in fig.1(d)[8,9].

Auger De-excitation Background

The Auger de-excitation process[10] is shown in fig.1(c). Where, an excited atom is de-excited with simultaneous ejection of an electron from the system. The ejected electron that originated from the metal is shown clearly in fig. (2) (direct capture). Whereas, the other one in which the ejected electron originated from the atom is shown in the same figure (indirect capture).In either case, one of the two electrons must originate in a specific level, namely, the atomic excited level. The excited electron may appear outside the solid if it poses a sufficient momentum component (normal to the surface) to surmount the surface potential barrier [11, 12].

As clear from fig. (2) Auger de excitation, it is two-electron process, but in fact, it is quasi one-electron in character .This property causes Auger de-excitation to have fundamentally different energetic character resulting in a quite different kinetic energy distribution of the excited electron from that of the auger neutralization.

The potential energy stored within the excited atom and the work function of the metal surface are the driving parameters for the electronic transitions which are studied by detecting and measuring both the yield and kinetic energy distribution of the emitted electrons during these processes which are Auger character .

$X^*(e_1) + n\,e_m \longrightarrow X(e_1) + (n-1)\,e_m + e_2$ direct capture

$X^*(e_1) + n\,e_m \longrightarrow X(e_2) + (n-1)\,e_m + e_1$ indirect capture

X^* incident excited atoms; $n\,e_m$ denoted n electrons in the metal surface, e_1, e_2 free electrons[13] .

Theoretical model

We use Eigen-state expansion method to describe the scattering of excited atom from the metal surface, where the Auger level described by the wave function φ_q with kinetic energy ε_q outside the metal. For incident excited atom ε_m , ε_a are excitation and ground energies near the metal respectively, also ε_o , ε_f are the energies of vacuum, Fermi levels above the bottom of the conduction band in the metal respectively , Φ is the metal work function .

The kinetic energy for the emitted electron is given as:

$$\varepsilon_q = \varepsilon_a(z_a) - \varepsilon_m(z_a) - \varepsilon_j$$

The maximum ε_q is when $\varepsilon_j = \Phi$ and the minimum is when $\varepsilon_j = \varepsilon_o$.

Starting from the broadening coefficient for the final level $b_{qa}(t)$ taken from Ref [14]:

$$b_{qa}(t) = -\sum_j b_{jm}(t_0) M_j(\varepsilon_j, z_a) e^{iE_j(t-t_0)} \left[E_j - \sum_{j'} \frac{\left|M_{j'}(\varepsilon_j, z_a)\right|^2}{E_j - E_{j'}} \right]^{-1} \quad \text{........ (1)}$$

$$E_j = \varepsilon_j + \varepsilon_m(z_a) - \varepsilon_a(z_a) - \varepsilon_q$$

For the case that the projectile is fixed (i.e. incident velocity equals zero) then:

$$\text{................(2)} \quad \left|b_{qa}(z_a)\right|^2 = \pi \sum_j \left|M_j(\varepsilon_j, z_a)\right|^2 f(\varepsilon_j, T) B(\varepsilon_j, z_a)$$

Where $B(\varepsilon_j, z_a)$ represent the energy broadening function for AD spectrum, and it's defined as:

$$\text{............. (3)} \qquad B(\varepsilon_j, z_a) = \frac{1}{\pi} \left\{ \left[E_j - \Lambda(\varepsilon_j, z_a)\right]^2 + \left[\Delta(\varepsilon_j, z_a)\right]^2 \right\}^{-1}$$

Where,

.... (4) $$\Delta(\varepsilon_j, z_a) = \gamma_d \pi \rho_s(\varepsilon_j) \left| M_j(\varepsilon_j, z_a) \right|^2$$

γ_d is normalization constant, $\rho_s(\varepsilon_j)$ is the surface density of state, $2\Delta(\varepsilon)$ is Auger de-excitation transition rate , $M_j(\varepsilon_j, z_a)$ represents the matrix element for AD transition

.... (5) $$\Lambda(\varepsilon_j, z_a) = P\frac{1}{\pi}\int \frac{\Delta(\varepsilon_j, z_a)}{\varepsilon_j - \varepsilon_{j'}}$$

The effective density of state for the metal surface is given by:

.... (6) $$\rho_{eff}(\varepsilon_j) = \sum_q \rho_a(\varepsilon_j, \varepsilon_q, z_a)$$

Where

.... (7) $$\rho_a(\varepsilon_j, Z_a) = \frac{1}{\pi}\frac{\Delta(\varepsilon_j, Z_a)}{\left[\varepsilon_j + \varepsilon_m - \varepsilon_a - \varepsilon_q - \Lambda(\varepsilon_j, Z_a)\right]^2 + \left[\Delta(\varepsilon_j, Z_a)\right]^2}$$

Matrix element

For the above equation we drive a new formula to find AD matrix element where M' is the matrix element for indirect capture, M'' for the direct capture.
The general form for matrix element is [3]:

.... (8) $$M = \langle \psi_f(t) | V(1,2) | \psi_i(t) \rangle$$

$\psi_i(t)$, $\psi_f(t)$ represent initial, final wave function for AD interaction respectively *V(1,2)* represents colomb interaction potential between the two electrons.

Substituting in eq (8) we get:

.... (9-a)
$$M' = \langle \phi_a(1)\phi_q(2) | V(1,2) | \phi_j(1)\phi_m(2) \rangle$$
.... (9-b)
$$M'' = \langle \phi_a(1)\phi_q(2) | V(1,2) | \phi_j(2)\phi_m(1) \rangle$$

Where $\phi_{j,}\phi_{m,}\phi_a$ represent the wave functions for the electron in metal, excited and ground levels for the incident atom respectively.

$M_a = M' + M''$ For singlet case

$M_b = M' - M''$ For triplet case

By sitting

$$\phi_j(r) = \frac{1}{\sqrt{L^2}} \sum_{\bar{g}} A_g^j e^{i(\overline{k_{//}} + \bar{g}).\bar{r}_{//}} u_{\overline{k_{//}} + \bar{g}}(z)$$ .... (10)

L is the normalize area, g is the reciprocal lattice A^j_g is factor depends on the surface density of state . So we interest with g=0.

$$u_{\bar{k}_{//}+\bar{g}}(z) = e^{-q_j Z} \quad \text{.................... (11)}$$

This is the solution for Schrödinger equation for one demotion.

$$\text{........................ (12)} \quad f_a(\bar{r}) = \sqrt{\frac{b_a^3}{p}}\, e^{-b_a r}$$

$$\text{........................... (13)} \quad f_m(\bar{r}) = \sqrt{\frac{b_m^3}{p}}(1 - b_m r) e^{-b_m r}$$

$b_{a(m)}$ (Effective core charge)

$$\text{................. (14)} \quad f_q = L^{-3/2} e^{iq.\bar{r}}$$

$$\text{............. (15)} \quad q = \sqrt{\frac{2m}{h^2}(e_q - e_0)}$$

By substituing the above wave functions in equations (9-a) & (9-b) and simplify we get the final form for the matrix element as:

$$M' = (2p)^2\sqrt{\frac{b_a^3 b_m^3}{p^2}}\left\{-\frac{e^{-q_j Z_a}}{b_a(q_j+b_a)^2}\left[\frac{1}{b_a}+\frac{2}{q_j+b_a}\right]-\frac{e^{-q_j Z_a}}{b_a(q_j-b_a)}\left[\frac{1}{b_a(q_j-b_a)}-\frac{2}{(q_j-b_a)^2}\right.\right.$$

$$\left.\left.+e^{(q_j-b_a)(Z_a-g)}\left\langle (Z_a-g)^2+(Z_a-g)\left[\frac{1}{b_a}-\frac{2}{(q_j-b_a)}\right]-\frac{1}{b_a(q_j-b_a)}+\frac{2}{(q_j-b_a)^2}\right\rangle\right]\right\}$$

$$\int_{-\infty}^{Z_a-g} w'\,dw'\int_0^{\infty} r'\,dr'\,\frac{e^{-b_m\sqrt{r'^2+w'^2}}}{(r'^2+w'^2)^{3/2}} \quad \text{.........(16)}$$

$$M' = (2p)^2\sqrt{\frac{b_a^3 b_m^3}{p^2}}\,\frac{e^{-q_j g}}{q_j}\left\{-\frac{6}{b^4}+24\frac{b_m}{b^5}+\frac{e^{-b(Z_a-g)}}{b^2}\left[(Z_a-g)^2+\frac{3}{b}(Z_a-g)+\frac{1}{b^2}-\frac{2}{b^3}\right]\right.$$

$$\text{....... (17)}\left.+\frac{b_m}{b^2}e^{-b(Z_a-g)}\left[(Z_a-g)^3+\frac{5}{b}(Z_a-g)^2+\frac{12}{b^2}(Z_a-g)+\frac{12}{b^3}\right]\right\}$$

Where

$$b = b_m + b_a$$

Results and Discussion

We apply the theoretical model on real systems such as He/Cu , He/Al , He/Na ,(as shown in Fig.3) to investigate the effects of the energy band on the AD transition , then we campier the results of He/Cu , H/Cu ,(as shown in Fig.4) to investigate also the effects of the stored potential energy in the incident projectile.

We show in fig.5 that the direct capture transition is the most effective in (AD) process, where this transition describes the effective density of state ρ_{eff} for the metal surface as shown in fig. 6 , where ρ_{eff} is effected by the elliptic shape for ρ_s that used. Fig.7 shows that the transition rate Δ increases as the metal energy band width increases (See table.1 also).Fig.9 shows that Δ_{pik} decries exponentially as z_a increase, and that's means that AD interaction increase as the projectile becomes closer to the surface.

Fig.8 also shows that Λ increase as the surface energy band width increases. From Fig.10 we see that Δ for He/Cu system is larger than H/Cu system because the excited energy for He atom is larger than H atom which means that as the stored potential energy in the excited incident atom increases then AD transition decreases.

Acknowledgment

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Table (1): The transition rate Δ increase as the metal energy band width

	ε_0	ε_F	$\varepsilon_F - \varepsilon_0$	ε_a	ε_m	$\varepsilon_a - \varepsilon_m$
Al	-15.91	-4.26	11.65	-	-	-
Cu	-11.61	-4.65	6.96	-	-	-
Na	-8.2	-2.75	5.45	-	-	-
He	-	-	-	-24.6	-4.75	19.85
H	-	-	-	-13.56	-3.4	10.16

* All energies in eV

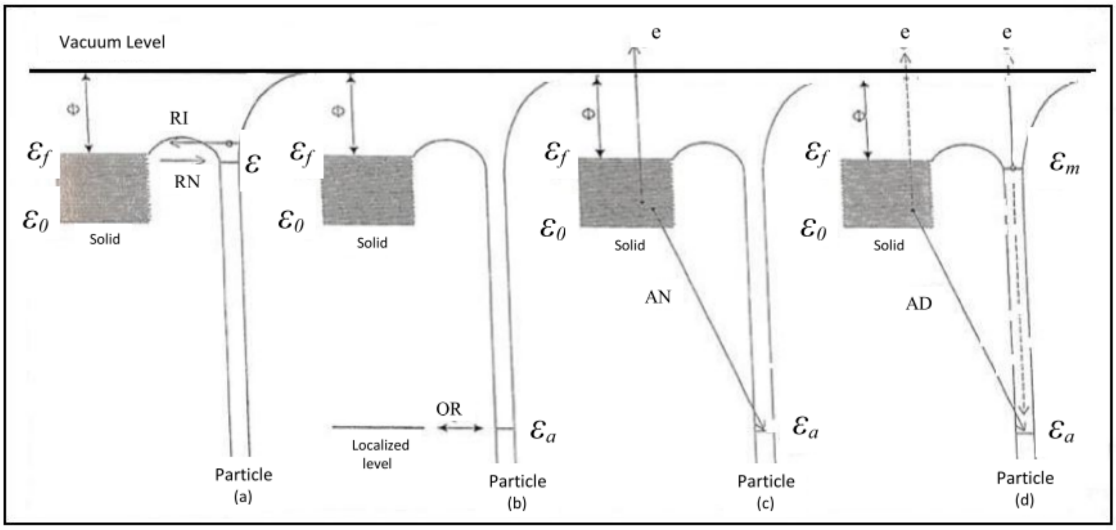

Fig.(1):Types of Auger charge transition

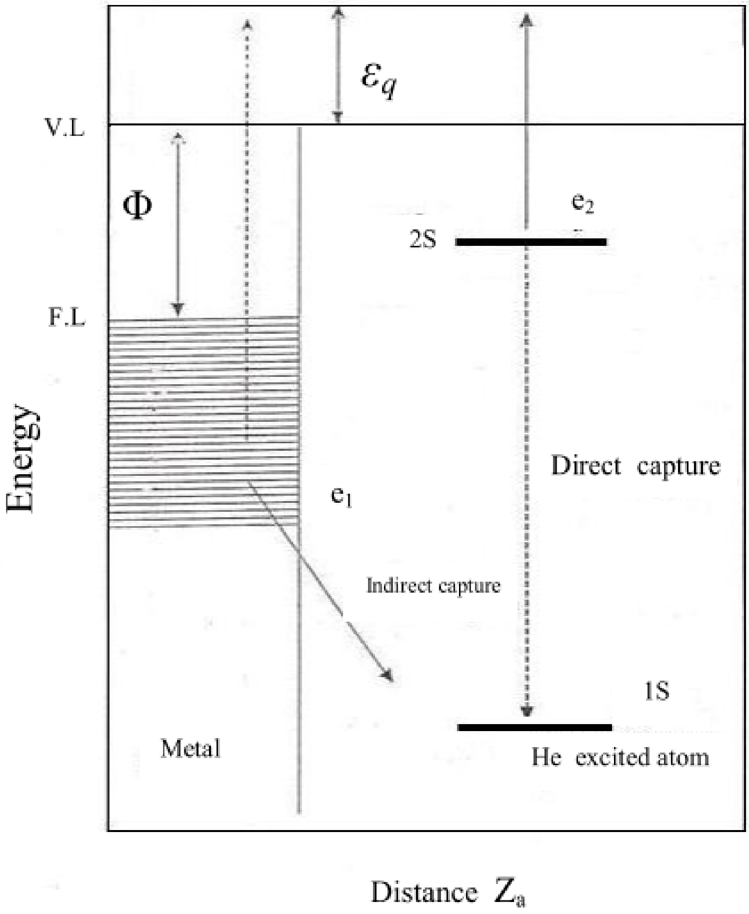

Fig.(2): The ejected electron that originated from the metal

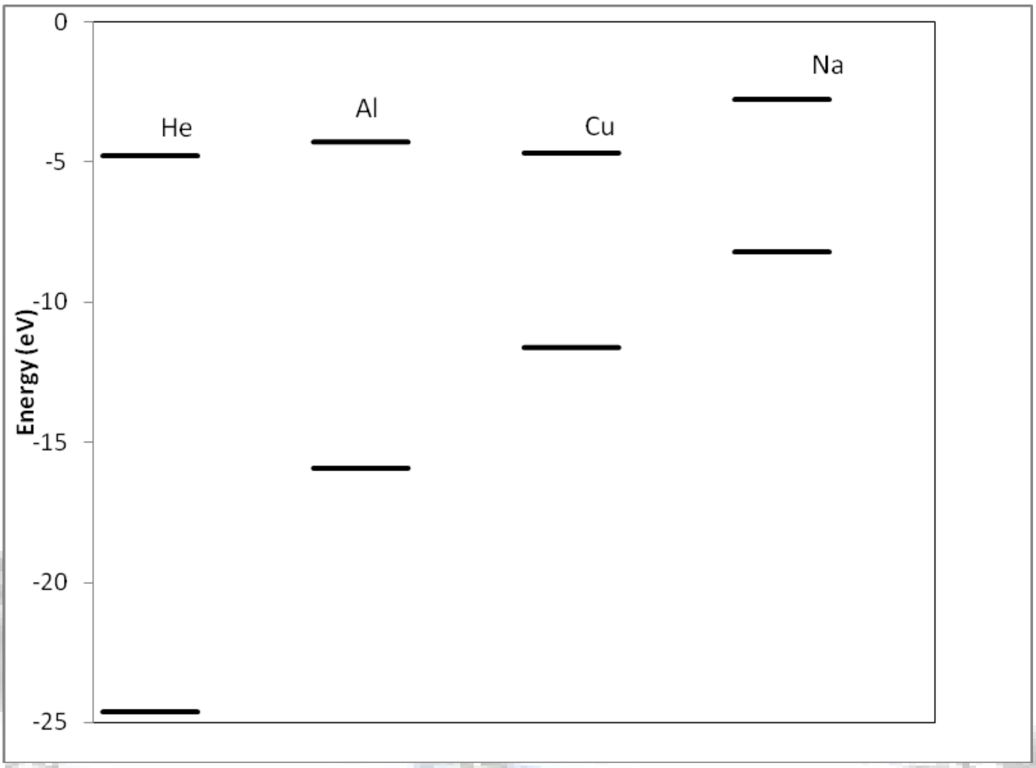

Fig.3: The theoretical model on real systems such as He/Cu , He/Al , He/Na , to investigate the effects of the energy band on the AD transition

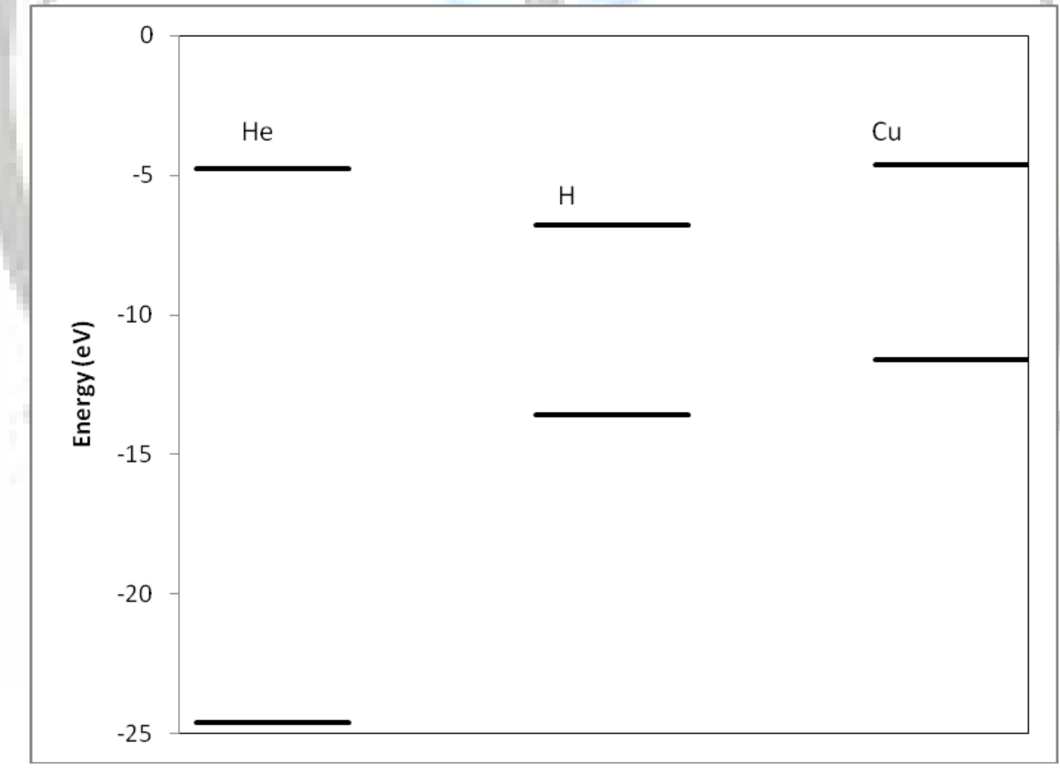

Fig.(4): The effects of the stored potential energy in the incident projectile

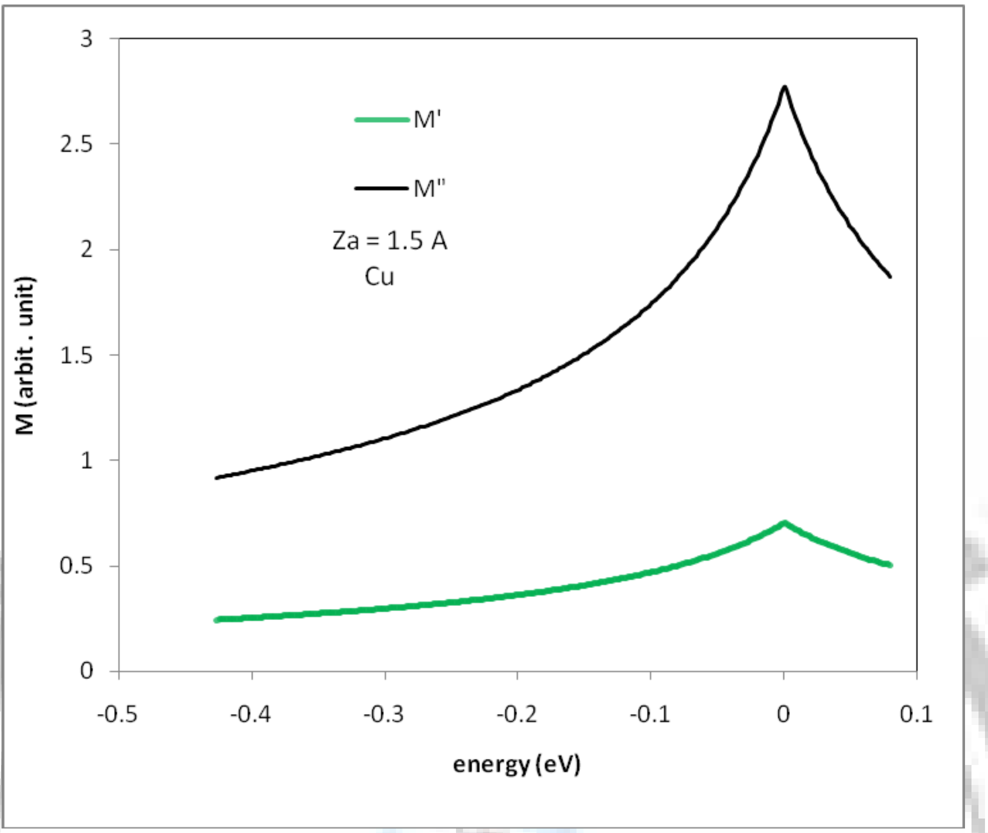

Fig.(5): The direct capture transition is the most effective in (AD) process

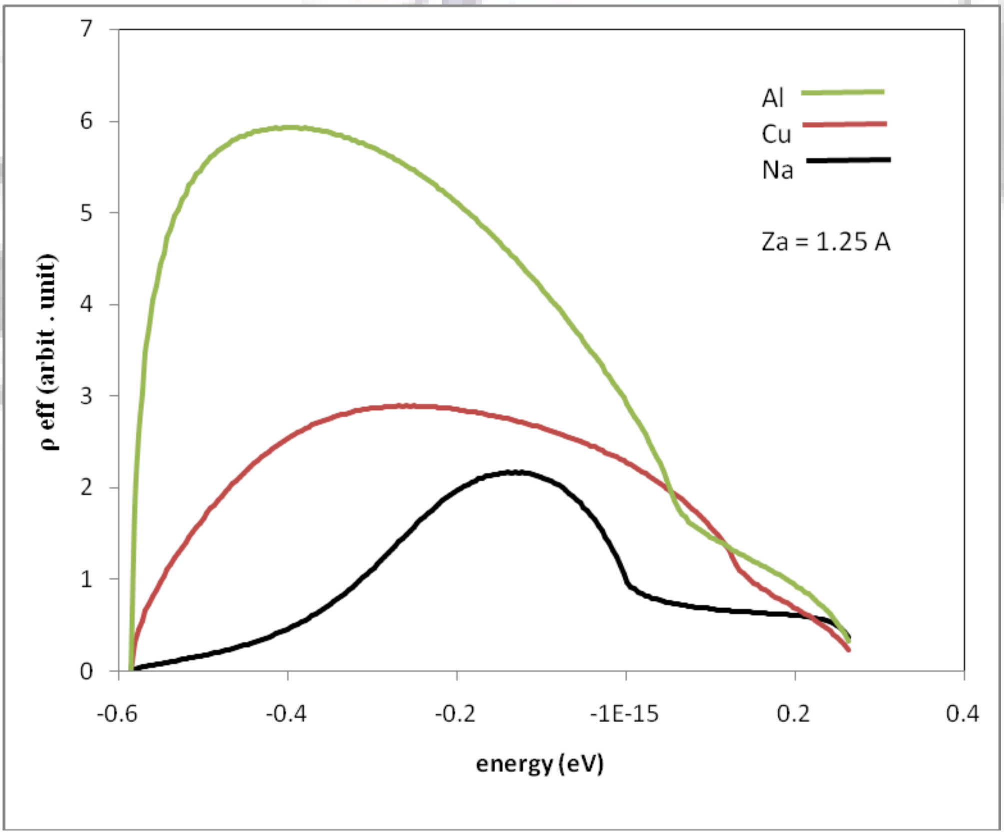

Fig.(6): The transition describe the effective density of state ρ_{eff} for the metal surface

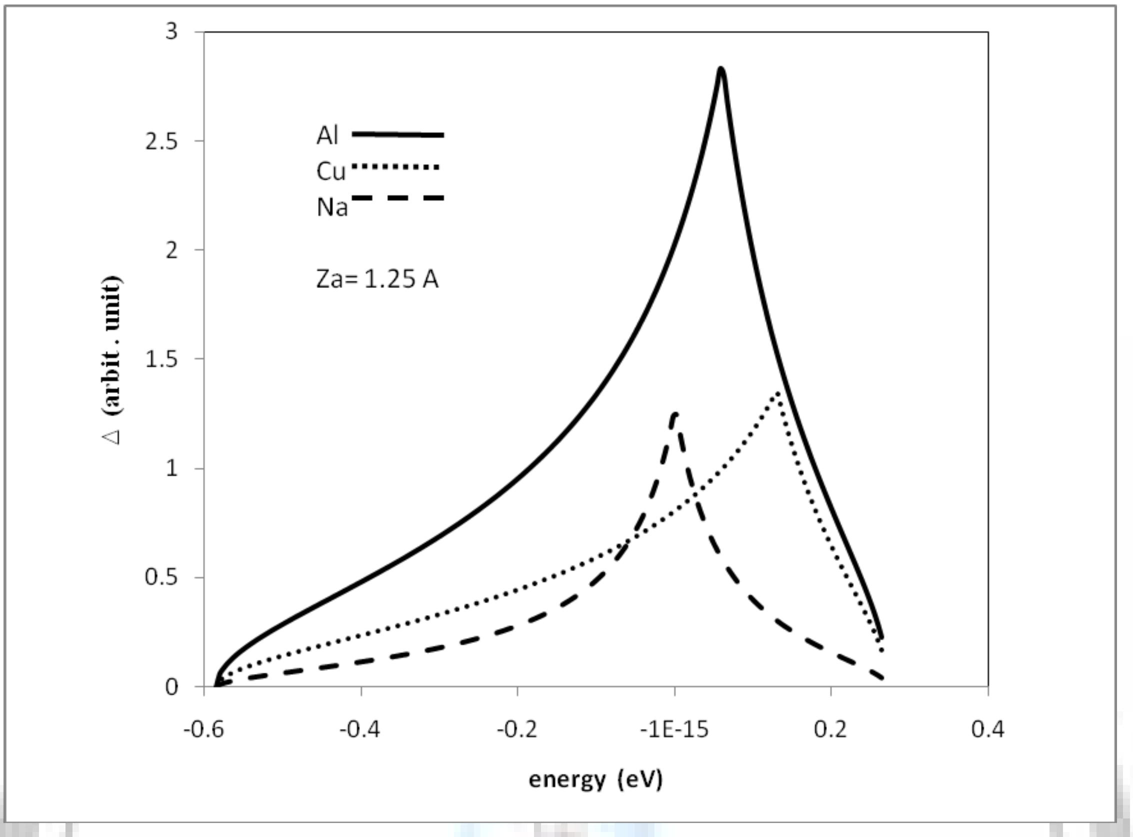

Fig.(7): The transition rate Δ increase as the metal energy band width increase

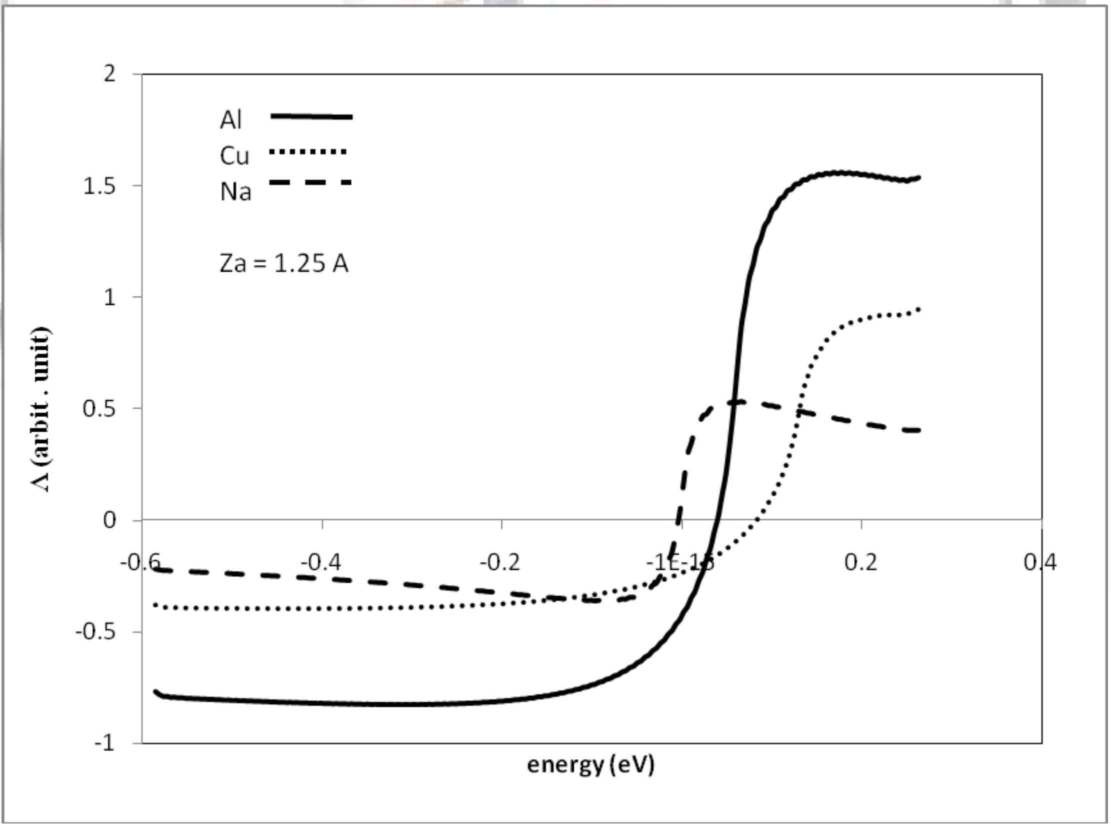

Fig.(8): The Λ increase as the surface energy band width increase

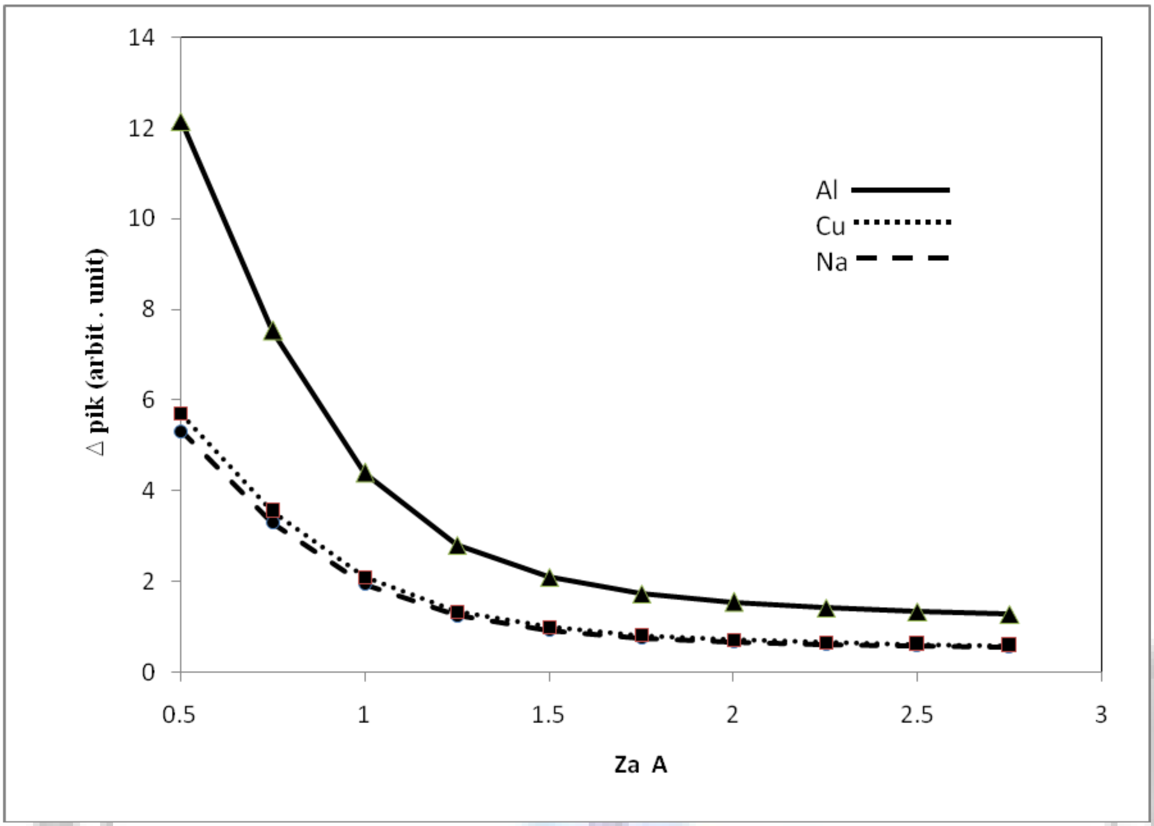

Fig.(9): Tthe Δ_{pik} decries exponentially as z_a increase

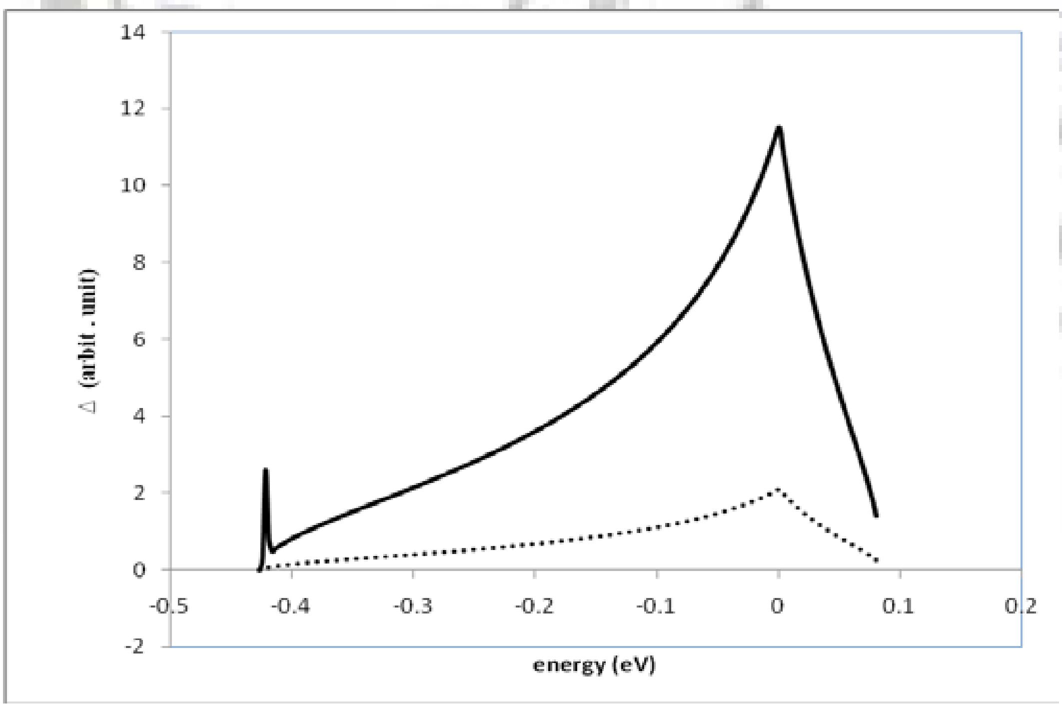

Fig.(10): Comparison between Δ for He/Cu and H/Cu systems

دراسة التأثيرات الاساسية في انتقال اوجيه غير المثار

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قسم الفيزياء ،كلية العلوم ، جامعة ذي قار

استلم البحث في 20 ايلول 2011، قبل البحث في : 7كانون الاول 2011

الخلاصة

استخدم في هذه الدراسة طريقة مفكوك الحالة الذاتية لعملية انتقال اوجبه للشحنة بين سطوح Na, Cu, Al وغازي H, He استخدمنا هذه الطريقة لوصف تاثيرات التركيب الالكتروني للسطوح في عملية انتقال الشحنة . وقد تبين ان كفاية عملية الانتقال تتاثير كثيرا بحزم الطاقة للسطوح وان طاقة الجهد تخزن داخل الذرات المتهيجة الساقطة وعلية ففي زمن تفاعل كبير اي ذرات بطاقة 1KeV للاستطارة من السطح المعدني وجد ان الالكترون لايتحسس تركيب الحزمة للمعدن ويعتمد على المسافة Z_a بين القذائف والسطوح . كما قمنا باشتقاق صيغة جديدة لعناصر المصفوفة لتفاعل اوجيه غير المتهيج.

الكلمات المفتاحية : اوجيه اللامثار ، استطارة، تفاعل ايون سطح.