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Effect of surface temperature on the neutral probabilities of alkali-ions scattered at Al (111) surface

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Abstract

The non perturbative coupled-angular-mode (CAM) method is applied to the treatment of the parallel velocity-assisted charge-transfer process in grazing scattering of alkali-metal ions at Al(111) surface. The neutralization of Li^{+} , Na^{+} , K^{+} , and Rb^{+} projectiles is studied at different degrees of the temperatures .

Keywards : Alkali-ions , CAM , grazing scattering , parallel velocity, surface temperature.

Introduction

Charge exchange phenomena between atom (ion) and solid surface have been studied extensively [1-6]. Many experimental studies on charge exchange between atom(ion) and metal surfaces have been performed by scattering fast atoms or ions off clean surface under grazing angle of incident [7-11]. Grazing scattering conditions are characterized by a small velocity component normal to the surface (V_t). Allowing an almost elastic scattering from the topmost layer of the surface atoms. On the other hand, the velocity component parallel to surface (V_{ll}) is large. So, in these studies, the electron exchange depends essentially on the quantity of the parallel velocity V_{ll} of the projectile. Can should be taken with respect to the fact that electron states of the atomic particle and the surface are defined into different reference frames moving one with respect to the other. Clearly, translational factors arising from transformation from frame to the other [12-13] affect electronic transitions between the atomic particle and the surface. A pronounced effect of the collision velocity on the charge states of the scattered particles was observed experimentally for the neutralization of alkali_metal ions as well as for the formation of H^{-} ion in grazing scattering from metal surface [7-8].The results of these studies have been explained via kinematically affected resonant exchange processes [7,19-20]. Perturbative treatments including translational factors associated with V_{ll} were able to reproduce gross features of the experimental results [7,12] .

The nonperturbative methods were applied to obtain the properties of atomic particles in front of metal surface [13-16]. These methods provided quantitative tools to study charge-transfer processes.

In the present work, the influence of V_{ll} on electron exchange process is considered in case of grazing scattering of neutralization alkali ions at Al(111) surface using CAM method.We use the Al(111) target as a proto type of the free electron metal well described within the "jellium" approximation [17].The probabilities of the ion neutralization are calculated as a function of Z "the distance between ion and the surface" .We study the effect of the surface Temperature (T) on these probabilities.These results show a pronounced dependence of the ion neutralization on the surface temperature.

The kinematics effect of temperature bridges the energy gap between the affinity level of the projectile and the occupied states of the metal surface, so it has the same effect of parallel velocity V_{ll}.

Method :

The non perturbative coupled-angular-mode (CAM) method is applied to the treatment of parallel velocity-assisted charge-transfer process in grazing scattering of alkali-metal ions at Al(111) surface . The method considers the electron scattering in the compound potential **V** created by the ion-core and the metal surface .Quasistationary atomic states appear as scattering resonance .

The energies and widths of the atomic states coupled to the Metal surface are associated with the energies and widths of the those resonances .The effective potential V consists of three terms [21] :

$$V=V_{e\_core}+V_{es}+\Delta V_{es} \qquad (1)$$

V_{e_core} is electron interaction with the ion core . It described by a pseudo potential given Bardslay[22]. V_{es} is the electron interaction with the surface [24-25] ; ΔV_{es} is the modification of the electron-surface interaction due to the presence of the ion.

Since the temperature affected the work function (Ø) and the Fermi energy (E_F) of the surface results in the increase of the neutralization probabilities as (T) increases.

The wave function of the electron scattered by the compound potential V in eq. (1) is expanded over spherical harmonics Y_{lm} centered on the proton :

$$Y=\sum_l \frac{1}{r} F_l(r) Y_{lm} \qquad (2)$$

Where m is the projection of the electron angular momentum on the atomic axis perpendicular to the surface. Since the system is invariant by rotation around this axis, m is a good quantum number .

$F_l(r)$ are the radial parts of the electron wave function. They are solutions of the coupled equations:

$$-\frac{1}{2}\frac{d^2}{dr^2}F_l+\sum_l < lm|V|l`m > F_l = EF_l \quad (3)$$

At small r distance , the F_l behave like coulomb waves at the energy ($E - < lm|V_{es}+\Delta V_s\,|\,lm >$). From the solution of eq.(3) obtained by a Fox_ Goodwin_Numerrov integrator [25], one gets the scattering S matrix and the time delay matrix Q[26]:

$$Q=\frac{ih}{2} S \frac{dS^+}{dE} \qquad (4)$$

Some of the eigen values of the time delay matrix present a resonant behavior with the energy which indicates the presence of a tomic levels.

For grazing scattering the collision velocity component perpendicular to the surface (V_t) is small (some x 10^{-3} a.u) . Then we deduce from CAM method that the evolution of the population of the projectile state can be described by the rate equation [29]:

$$\frac{dp_a}{dt} = g^c\ \Gamma_c(z)(1-p_a) - g^l\ \Gamma_l(z)p_a \qquad (5)$$

Where g^c , g^l are spin statistics factors (in the present case, g^c is equal to 2 and g^l is equal to 1).On the other hand ,the velocity component parallel to the surface is large, so that one has to take into account the Galilain transformation from the projectile to the surface frames.Within the rate equation approach, the evolution of the projectile population along the trajectory is described by electron capture and loss rates (Γ_c and Γ_l). The rates depend on the projectile-surface distance (z), E_a (z) and Γ(z) of the ion level in front of the surface. V_{ll} effects are incorporated via the shifted Fermi sphere model . The capture and loss rates can derived in a spherical coordinate:

$$\Gamma_c(z)=\Gamma(z)\int_0^{\pi/2} \sin\theta d\theta \int_0^{2\pi} d\emptyset |\sigma(\theta,\emptyset,z)|^2 f(E_F-\frac{(k_f+v_{ll})}{2}) \qquad (6)$$

$$\Gamma_l(z)=\Gamma(z)\int_0^{\pi/2} \sin\theta d\theta \int_0^{2\pi} d\emptyset |\sigma(\theta,\emptyset,z)|^2 (1-f(E_F-\frac{(k_f+v_{ll})}{2})) \qquad (7)$$

Then the occupation probability is:

$$p_a(t) = p_a\, e^{\int_{t_o}^{t}[\Gamma_l(t')+2\Gamma_c(t')dt']} + \int_{t_o}^{t} 2\Gamma_c(t)\left[e^{-\int_{t'}^{t}[\Gamma_l(t'')+2\Gamma_{c(t'')}]} dt''\right] dt' \qquad (8)$$

We use W (the work function) which includes the temperature effect .
In the system energy E [28] :

$$E = E_F + W - |E_a| \qquad (9)$$

Where

$$W = \emptyset - (1.6x10^{-4}T) \qquad (10)$$

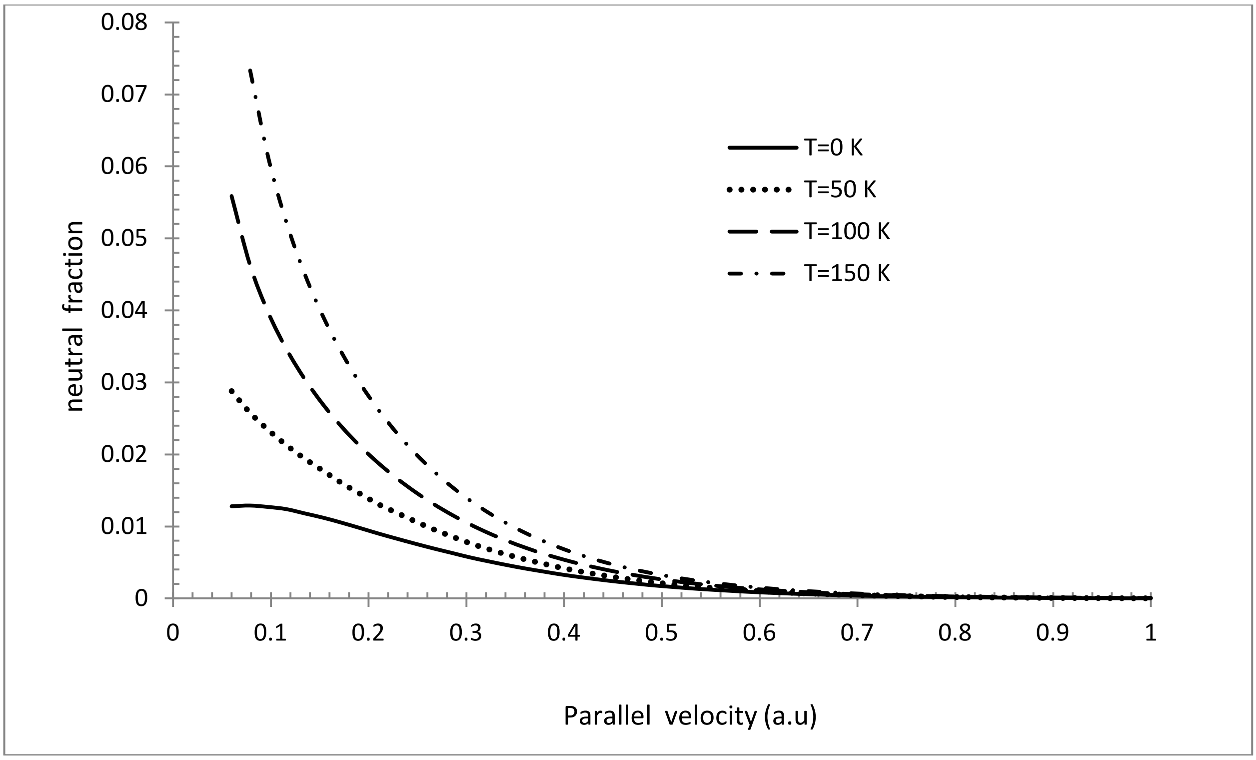
Where Ø is the work function at (T=0) , E_F is Fermi energy, and E_a is the ionization energy

Results and discussion

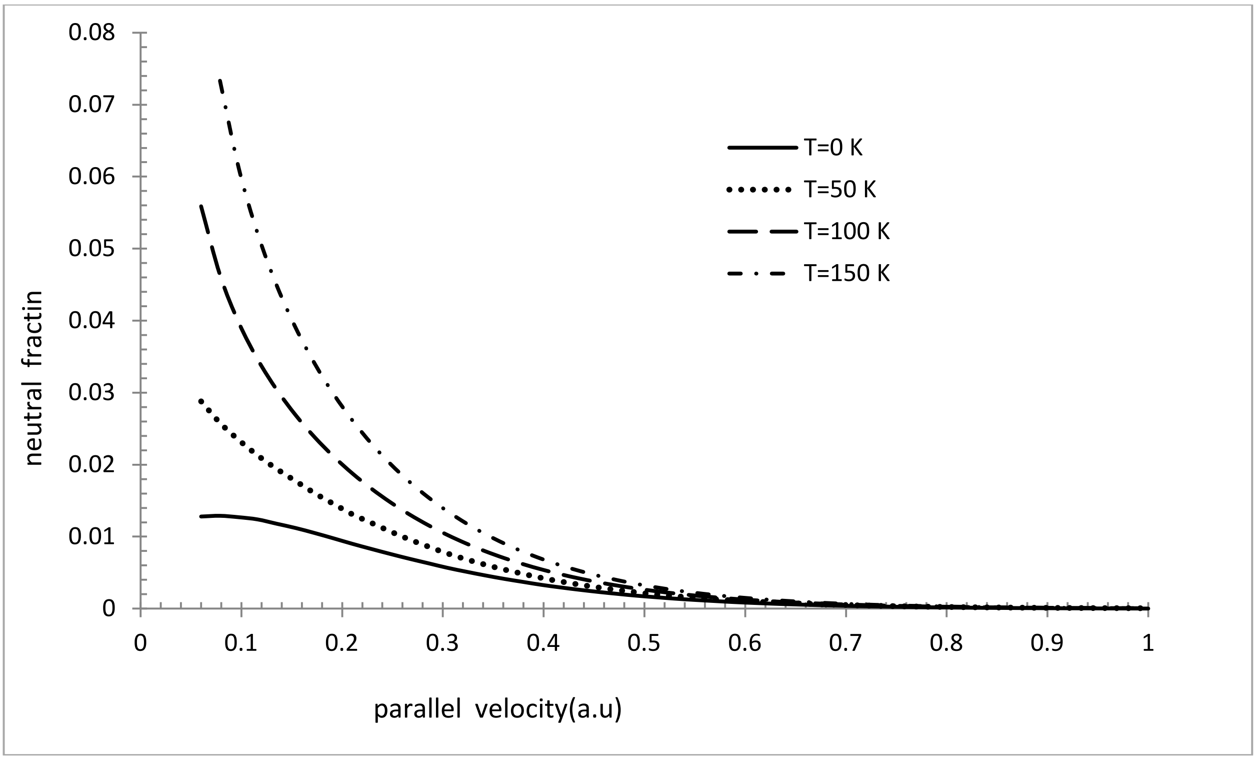
The major effect of increasing the surface temperature (T) is the reduction of the work function (equation (9)) due to the positive shift to the surface Fermi-level energy. So additional charge might be transferred from the surface to the ion, this introduces a strong temperature dependence of the neutral fraction.

In order to introduce this effect on the neutral fraction of Li^+, Na^+ , K^+ and Rb^+ ions at Al(111) surface , we plot P_a as a function of (V_{ll}) in figs. (1-4) at a fixed normal distance (z=3 a.u) and for different surface temperature (0 ,50 ,100 ,150 K). It is found from these figs. That the neutral fraction (P_a) will be changed due to this increasing.

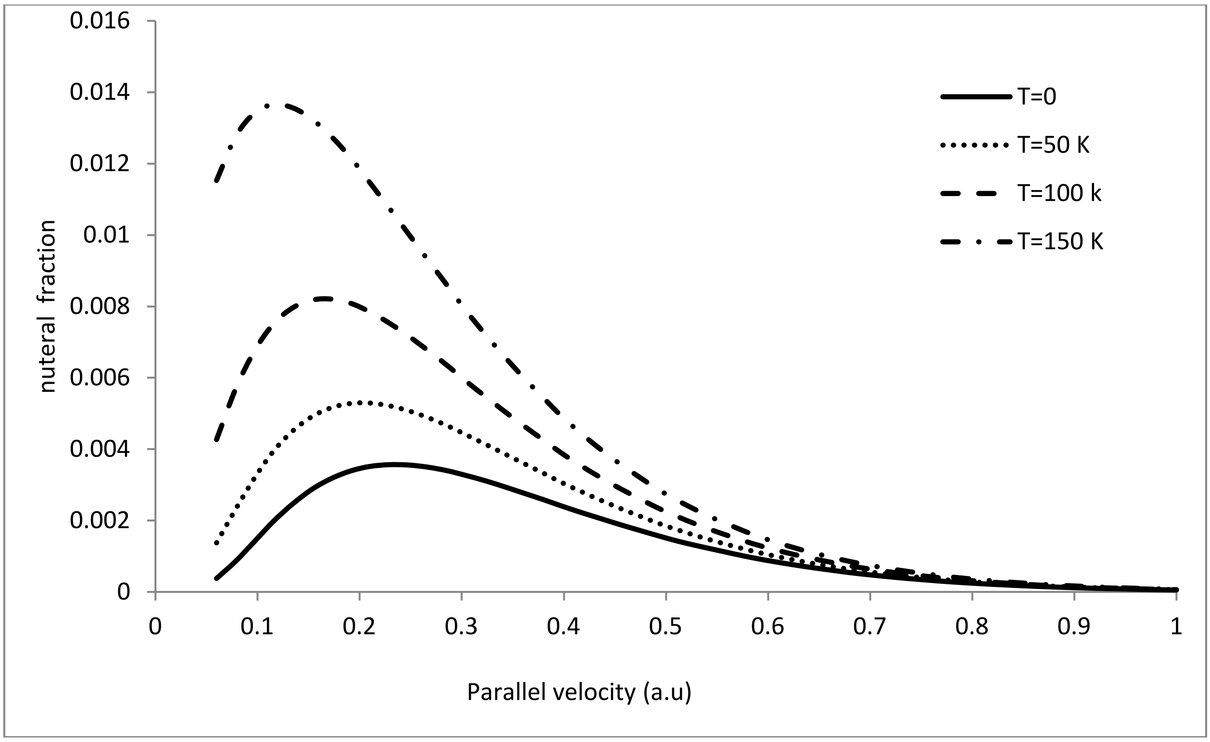
Three different behaviors are shown together with the clean surface (T=0 K) in these figs. and an increasing in (P_a) shows with increasing the surface Temperature especially in the range of velocities ($V_{ll} = 0.1 - 0.4$ a.u) .Therefore, one can conclude that the increasing in the neutral fraction (p_a) for positive ions can be controlled by varying the surface temperature.



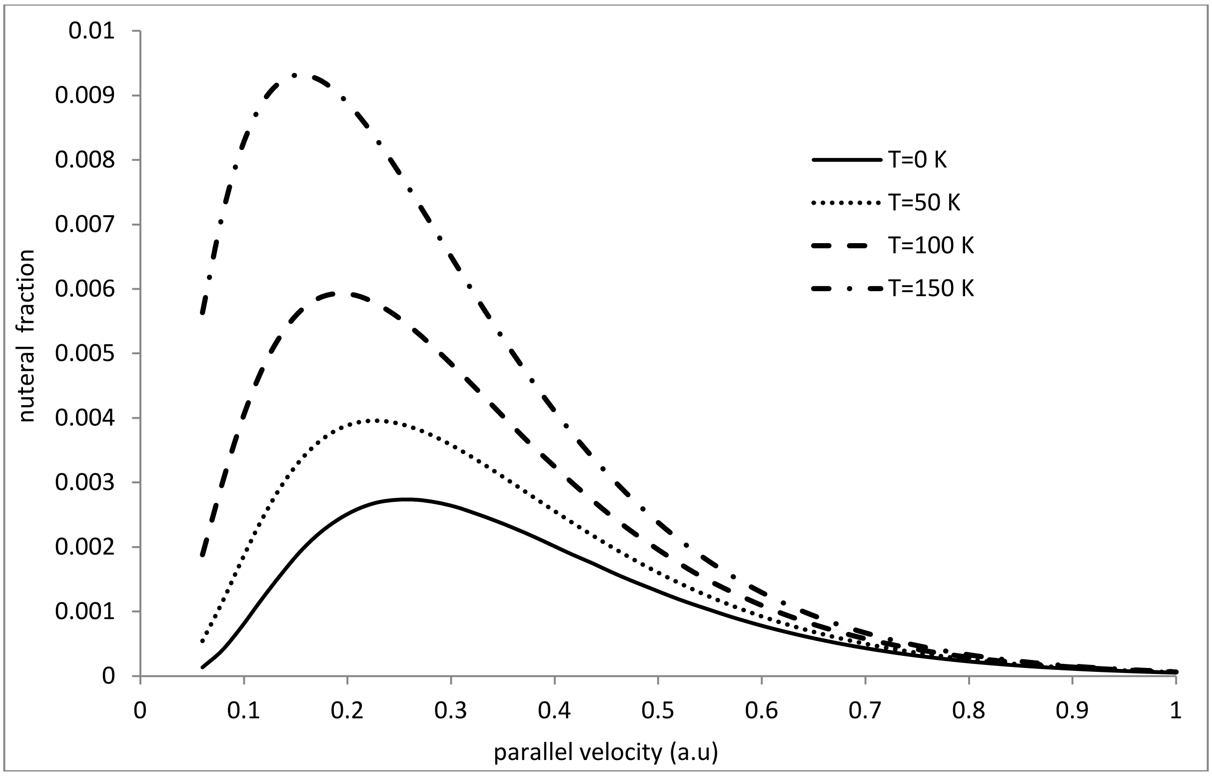
Figure(1): Neutral fraction Li^{+} ions at Al(111) surface as a function of the velocity component parallel to the surface for different surface temperature.



Figure(2): Neutral fraction Na^{+} ions at Al(111) surface as a function of the velocity component parallel to the surface for different surface temperature.



Figure(3): Neutral fraction K^{+} ions at Al(111) surface as a function of the velocity component parallel to the surface for different surface temperature



Figure(4): Neutral fraction Rb^{+} ions at Al(111) surface as a function of the velocity component parallel to the surface for different surface temperature.

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تاثير حرارة السطح على احتمالية تعادل الايونات القلوية المستطارة عند سطح Al(111)

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الخلاصة

تم اعتماد طريقة نمط ازدواج الزخم الزاوي غير المضطربة (CAM) في معالجة عملية انتقال الشحنة للايونات القلوية المستطارة ,استطارة مس (Grazing scattering) من سطحAl(111) ,حيث أدخل تأثير حرارة السطح على احتمالية تعادل هذه الايونات. والايونات التي تضمنها البحث هي ايون Li^+ , Na^+ , K^+ بالاضافة الى ايون Rb^+ في درجات حرارة مختلفة للسطح .