

Dependence of knock-on collision electron emission on the orientation of fast diclusters in solids

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The cluster-orientation dependence of the emitted knock-on collision electron distributions when fast diclusters interact with condensed matter is investigated. The scattering by each centre of the dicluster is described by means of the phase shifts of a velocity dependent Yukawa potential describing the dynamic screening, and the multiple scattering effects are approximated within the second Born approximation. The applicability of this approximation as the charges and velocities of the diclusters are changed is also discussed, and numerical comparisons of our results with experiment are made.

1. Introduction

The distribution in space and time of perturbations of electron motion in solids caused by the passage of fast particles has been the subject of continued theoretical [1–8] and experimental interest [9–11]. Most of the experimental work in this field is related to measurements of the electric field strength and the wake potential, quantities that are obtained from certain averages of the induced electron density fluctuations; however, recent experimental research has been concerned with the distribution in space of valence electron density fluctuations induced by the passage of fast ions [12]: measurements of the knock-on collision electrons emitted under bombardment of fast dimolecular ions have been performed, since the electron density fluctuations induced by the leading ion around the trailing ion of the bombarding dicluster may appear experimentally in the dependence of the emitted knock-on electron yield on the orientation of the projectile.

It has been shown [13] that for an interatomic distance within the projectile of about 2 a.u. the electron density fluctuation of target valence electrons in the position of the trailing ion is most prominent when the trailing ion is in the conical region behind the leading ion with half-angle of opening $\theta \approx \sin^{-1}(\beta/v)$, which defines the envelopes of the collective wake, β being the

velocity of propagation of density disturbances in an electron gas [8]. This is in qualitative agreement with the experimental result obtained by Yamazaki and co-workers [12], who have found that the yield of knock-on electrons emitted at 0° with respect to the beam axis from carbon foils bombarded by 4.5 MeV N_2^+ ions decreases as the angle θ defining the orientation of the projectile increases (see fig. 1).

Nevertheless, it is not well known what the relationship between the yield of knock-on electrons and the electron density fluctuations of the target is; moreover, the cross sections of 0° knock-on electrons also depend on the orientation of the bombarding diclusters, even when there is no valence electron density fluctuation in the target. Consequently, in order to give an interpretation of such experiments it is necessary to study in detail the result of the multiple scattering involved in

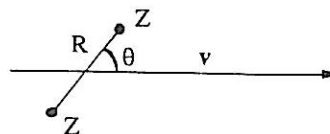


Fig. 1. Geometry of the bombarding dicluster, each ion having charge Z and velocity v . R is the distance between the pair of ions, and θ is the angle formed by the molecular axis of the dicluster with the beam axis.

the interaction of fast diclusters with matter leading to knock-on electron emission. This paper attempts to study theoretically the dependence of multiple scattering effects on the orientation of bombarding diclusters, by means of second order perturbation theory.

2. Second Born approximation

We consider a solid target and the process of valence electrons being scattered by the passage of fast dimolecular clusters, each ion having charge Z and velocity v , as shown in fig. 1; R is the distance between the pair of ions of the dicluster, and θ is the angle between the molecular axis of the projectile and the beam axis. Treating the ions as infinitely massive, we work in the projectile inertial frame. Unless otherwise stated, atomic units are used throughout.

The second Born approximation to the scattering amplitude of electrons in the potential $U(r)$ can be written as [14]

$$f_{B_2} = -\frac{V}{2\pi} \left[\langle \varphi_{k_f} | U | \varphi_{k_i} \rangle + 2 \langle \varphi_{k_f} | U G_0^{(+)} U | \varphi_{k_i} \rangle \right], \quad (1)$$

where $\varphi_{k_i}(r)$ and $\varphi_{k_f}(r)$ are the incident and scattered plane waves with momentum k_i and k_f , respectively, and $G_0^{(+)}(r, r')$ is the outgoing Green's function

$$G_0^{(+)}(r, r') = -(2\pi)^{-3} \lim_{\epsilon \rightarrow 0^+} \int \frac{e^{ik' \cdot (r-r')}}{k'^2 - k^2 - i\epsilon} dk'. \quad (2)$$

The scattering potential of the bombarding dicluster is

$$U(r) = U_1(r) + U_1(r+R), \quad (3)$$

where $U_1(r)$ and $U_1(r+R)$ represent the potentials created by the leading ion and the trailing ion of the dicluster, respectively. For high momentum transfers, the wake potential of fast ions may be approximated by a spherically symmetric form of the total potential that electrons in the medium feel, that is, a velocity dependent Yukawa potential

$$U_1(r) = -\frac{Z}{r} e^{-\alpha r}, \quad (4)$$

where

$$\alpha = \omega_p/v. \quad (5)$$

Here ω_p is the plasmon frequency and v is the velocity of the projectile.

Substituting eq. (4) into eq. (3), and then introducing eqs. (2) and (3) into eq. (1) leads, after some algebra, the following result:

$$f_{B_2}(k_i, k_f) = (1 + e^{i\Delta \cdot R}) f_{B_2}^0(k_i, k_f) + f'(k_i, k_f), \quad (6)$$

where Δ is the momentum transfer,

$$\Delta = k_i - k_f, \quad (7)$$

R represents the position vector of the leading ion with respect to the trailing ion, $f_{B_2}^0(k_i, k_f)$ is the second Born scattering amplitude of electrons in the potential of a single ion of the projectile [14] and $f'(k_i, k_f)$ represents the scattering amplitude related to first order multiple scattering effects:

$$f' = \frac{2Z^2}{\pi^2} \int \frac{dq}{q^2 - k^2 - i0^+} \times \frac{e^{-i(k_i - q) \cdot R} + e^{-i(q - k_f) \cdot R}}{(\alpha^2 + |k_i - q|^2)(\alpha^2 + |q - k_f|^2)}. \quad (8)$$

In the case of a single fast charged particle moving with velocity exceeding the Fermi velocity, $k/\alpha \gg 1$ for typical electron densities of the target, and the criterion for convergence of the Born series becomes

$$\frac{Z}{k} \ln \frac{k}{\alpha} \ll 1. \quad (9)$$

Thus we expect the Born approximation to be valid for large incident velocities and small charges. We have compared, taking k_i and k_f to be $-v$ and v , respectively, the first and second Born differential scattering cross section of electrons in the central potential created by a single ion, with the exact result deduced by squaring the modulus of the well known exact scattering amplitude of target valence electrons in the potential of each ion,

$$f^0(k_i, k_f) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \frac{e^{2i\delta_l} - 1}{2i} P_l(\cos \phi), \quad (10)$$

and we have found [15] that the second Born approximation offers no improvement over the first Born approximation, even at high velocities for which we would expect the Born series to converge rapidly. The reason for this failure of the second Born approximation has been pointed out by Joachain [16], noting that the second order differential scattering cross section does not account for all the corrections of order k^{-2} to the first order differential cross section. In eq. (10) the quantities δ_l represent the phase shifts accounting for the interaction with a single ion of the dicluster, which are computed solving numerically the radial Schrödinger equation, ϕ is the angle between k_i and k_f , and the quantities P_l are the Legendre polynomials.

Consequently, when scattering of electrons in the potential created by the dicluster is considered, instead of approximating the exact scattering amplitude by the second Born scattering amplitude of eq. (6), we approximate it by

$$f(k_i, k_f) = (1 + e^{i\Delta \cdot R}) f^0(k_i, k_f) + f'(k_i, k_f), \quad (11)$$

where we have introduced the exact scattering amplitude $f^0(k_i, k_f)$ of eq. (10) instead of the second Born scattering amplitude of electrons in the potential of a single ion; $f'(k_i, k_f)$ is given by eq. (8) and accounts for the first order multiple scattering effects. Therefore, in this approximation we calculate the differential scattering cross section of target valence electrons in the potential (3) of bombarding diclusters as

$$\frac{d\sigma}{d\Omega} = |(1 + e^{i\Delta \cdot R})f^0(k_i, k_f) + f'(k_i, k_f)|^2. \quad (12)$$

Figs. 2 and 3 exhibit plots of the differential scattering cross section (12) of electrons being initially at rest in the laboratory frame to be emitted at 0° with respect to the beam axis, as a function of θ , together with the differential scattering cross section obtained when the contribution f' to the scattering amplitude coming from multiple scattering effects is not included; the internuclear distance has been taken to be $R = 2.2$ a.u.. In fig. 2 the charge has been taken to be $Z = 1$ and different values of the velocity have been considered; in fig. 3 the velocity has been taken to be $v = 2.5$ a.u. and

different values of the charge have been considered. These figures show that, even when multiple scattering is neglected, the differential scattering cross section strongly depends on the orientation of diclusters and presents oscillations depending on the velocity and internuclear distance of the projectiles. These figures also show that as a result of including multiple scattering by means of the first order multiple scattering amplitude f' of eq. (8) the electron yield decreases as θ increases, especially for high values of Z where multiple scattering becomes more important.

3. Initial momentum distribution of target valence electrons

When bombarding diclusters penetrate condensed matter, the different contributions to the emission yield coming from all allowed initial states must be taken into account. In particular, the differential scattering cross section per target valence electron of knock-on electrons

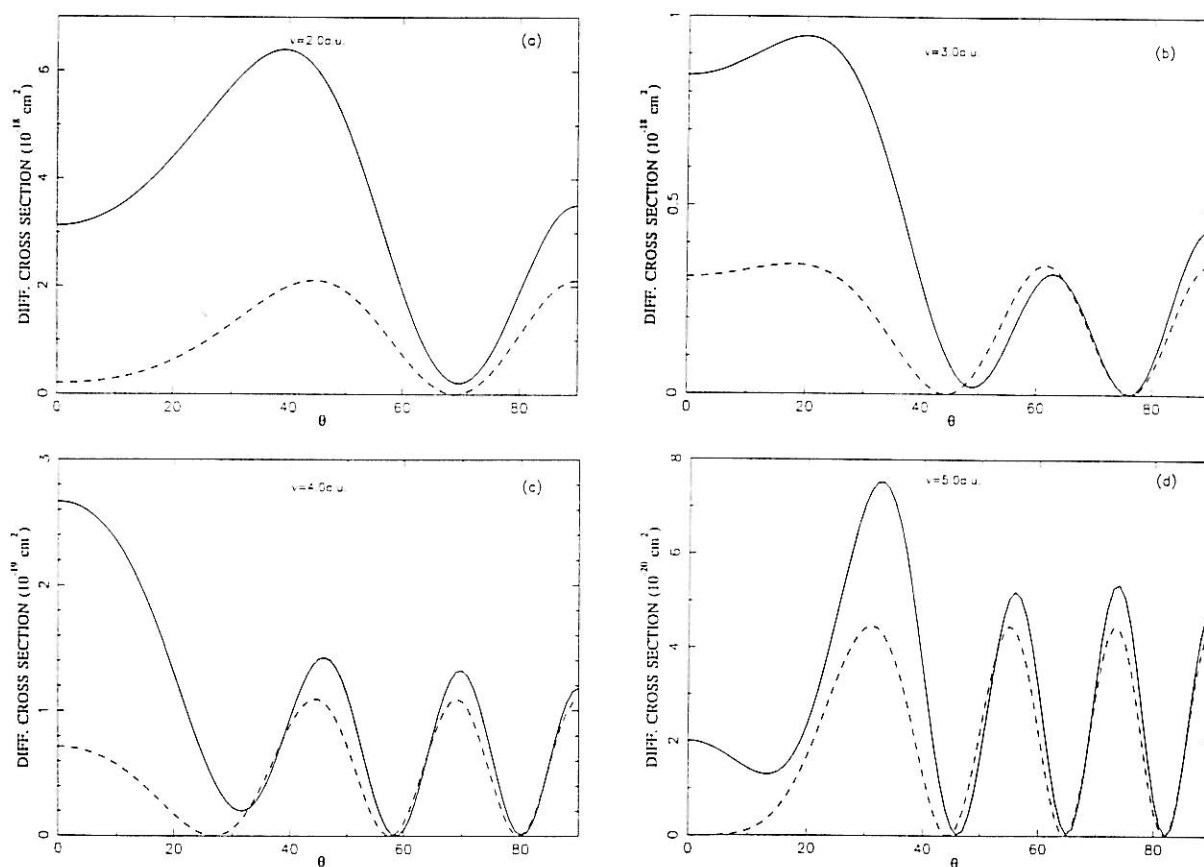


Fig. 2. Differential scattering cross sections deduced from eq. (12) (solid curves), as a function of the orientation of bombarding diclusters moving with velocity $v = 2.0$ a.u. (a), $v = 3.0$ a.u. (b), $v = 4.0$ a.u. (c) and $v = 5.0$ a.u. (d), together with the scattering cross sections obtained when the contribution f' to the scattering amplitude coming from multiple scattering effects is not included (dashed curves). k_i , k_f , Z and R are taken to be π , π , 1 and 2.2 a.u., respectively.

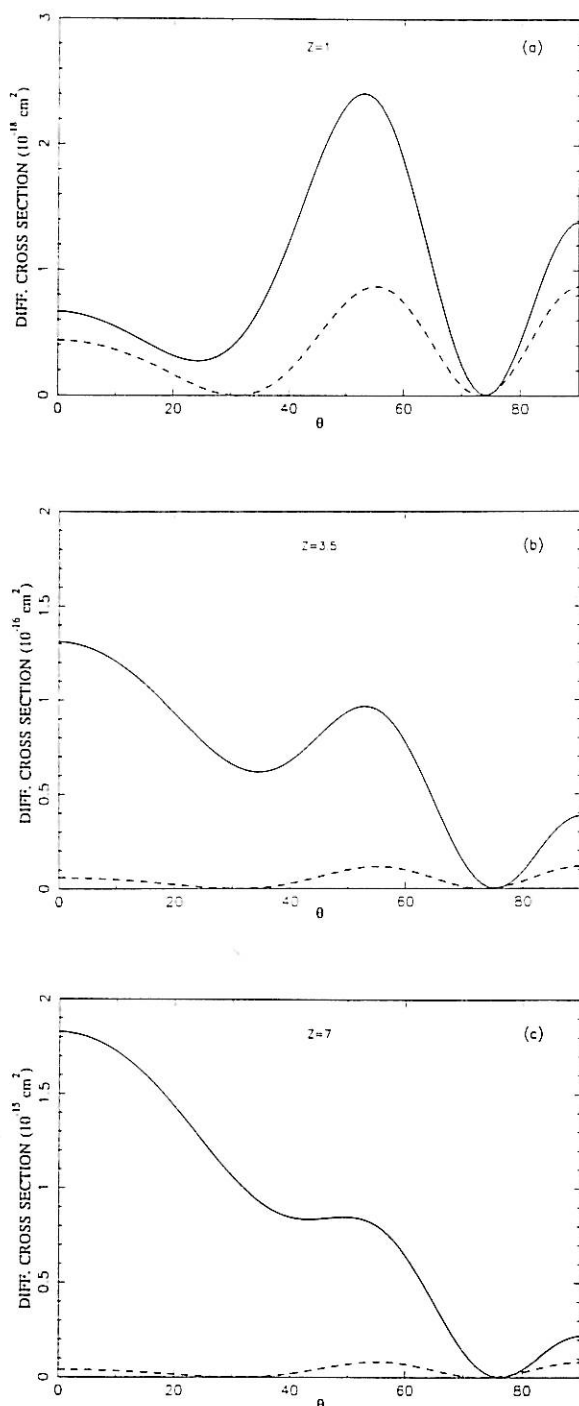


Fig. 3. Differential scattering cross sections deduced from eq. (12) (solid curves), as a function of the orientation of bombarding diclusters moving with velocity $v = 2.5$ a.u., together with the scattering cross sections obtained when the contribution f' to the scattering amplitude coming from multiple scattering effects is not included (dashed curves). k_i , k_f and R are taken to be $-v$, v and 2.2 , respectively, and different values of the charge are considered: $Z = 1$ (a), $Z = 3.5$ (b) and $Z = 7$ (c).

emitted at 0° in a velocity region of $\lambda_1 v \leq k_f \leq \lambda_2 v$ is found to be, choosing the z -axis along the direction of $-v$,

$$\frac{d\sigma}{d\Omega} = \frac{3}{4\pi k_F^3 v} \int_{k_{\min}}^{k_{\max}} dk k^3 \int_{\mu_{\min}}^1 d\mu \int_0^{2\pi} d\varphi |f(k, \mu, \varphi)|^2, \quad (13)$$

where

$$k_{\min} = \max(v - k_F, \lambda_1 v), \quad (14)$$

$$k_{\max} = \min(v + k_F, \lambda_2 v), \quad (15)$$

$$\mu_{\min} = \frac{k^2 + v^2 - k_F^2}{2kv} \quad (16)$$

and

$$f(k, \mu, \varphi) = \left\{ 1 + \exp \left[-ikR \left((1 + \mu) \cos \theta - \sqrt{1 - \mu^2} \cos \varphi \sin \theta \right) \right] \right\} f^0(k, \mu, \varphi) + f'(k, \mu, \varphi), \quad (17)$$

$f^0(k, \mu, \varphi)$ and $f'(k, \mu, \varphi)$ being the exact scattering amplitude of electrons in the potential of each ion and the scattering amplitude related to first order multiple scattering effects [15], respectively, and k , μ and φ being the spherical coordinates of the initial momentum k_i of target electrons.

Yamazaki and co-workers [12] have measured the yield of 0° knock-on electrons emitted from thin carbon foils in the velocity region of $1.95v \leq k_f \leq 2.15v$ under bombardment of 4.5 MeV dinitrogen molecular ions. Therefore, the velocity of bombarding diclusters is $v \approx 2.5$ a.u., and the charge and internuclear distance of the pair of ions are $Z = 1$ and $R \approx 2$ a.u., respectively, before entering the target; however, as they penetrate the target, some of the binding electrons are lost and the resulting fragment ions undergo a Coulomb explosion, so that the effective charge and internuclear distance both change during the experiment and depend on the velocity of diclusters and the thickness of the target.

Making use of the empirical formula proposed by Betz [17], the mean charge of the ions constituting 4.5 MeV dinitrogen projectiles can be assumed to be $Z \approx 3.5$. On the other hand, for very thin targets ($d < 100$ Å) the internuclear distance of the bombarding dinitrogen clusters can be assumed to be approximately equal to the interatomic distance of N_2 molecules; however, for thicker targets it increases very rapidly. Therefore, we have considered in our calculations different values of the internuclear distance of bombarding diclusters. In fig. 4 we plot, as a function of θ , the differential scattering cross section of target valence electrons to be emitted at 0° in the velocity region of $1.95v \leq k_f \leq 2.15v$ calculated from eq. (13), together with the result obtained not integrating over initial states and assuming that all initial states contribute as the initial state having

momentum zero in the laboratory frame, for $v = 2.5$ a.u., $Z = 3.5$ a.u. and two different values of the internuclear distance. Fig. 5 exhibits the experimental yield of 0° knock-on electrons emitted from a $2 \mu\text{g}/\text{cm}^2$ carbon foil ($d \approx 100 \text{ \AA}$) under 4.5 MeV N_2^+ bombardment measured by Yamazaki [12].

As a result of the contributions from all allowed initial states, the oscillations appearing in the dependence of 0° knock-on electron emission on the orientation of projectiles become less pronounced; this is due to the fact that the value of the angle θ making the emission probability maximum or minimum depends not only on the velocity and internuclear distance of the projectile but also on the momentum of the initial target valence electron, thus becoming different for the different contributions to the total yield. On the other hand, fig. 4 shows that the integrated differential scattering cross section is a decreasing function of θ , which is a consequence of multiple scattering effects, as also shown in figs. 2 and 3.

The experimental results qualitatively agree with the calculations shown in fig. 4: the yield of knock-on electrons emitted in the forward direction has been found to be a decreasing function of θ , and a small peak appears at $\theta \approx 60^\circ$, in agreement with our theoretical calculation obtained for $R = 2.2$ a.u.; the position of this peak should appear at larger values of θ as R increases, thus depending on the thickness of the target. Nevertheless, the experimental results are not fitted quantitatively by our calculations, since the experimentally observed enhancement of the yield produced by the longitudinally aligned projectiles is not as large as the one predicted by our theoretical results; the discrepancy between our theoretical results and the experimental curve may be a consequence of having included

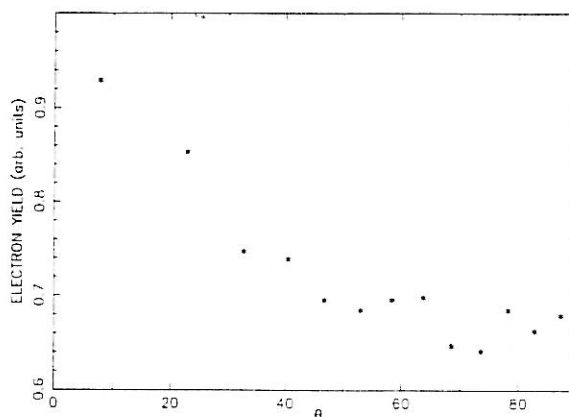


Fig. 5. The knock-on electron yield measured by Yamazaki [12] at 0° in the velocity region of $1.95v \leq k_f \leq 2.15v$, as a function of the orientation of 4.5 MeV N_2^+ diclusters passing through a $2 \mu\text{g}/\text{cm}^2$ carbon foil. The dotted line is to guide the eye.

in our calculations only the first order multiple scattering for projectiles with high effective charge.

4. Conclusions

It has been demonstrated that the dependence of electron emission on the orientation of bombarding diclusters presents oscillations depending on the velocity and interatomic distance of the projectiles, and that the electron yield increases as the bombarding diclusters get longitudinally aligned with respect to the beam direction, as a consequence of multiple scattering effects. The experimental results have been shown to be

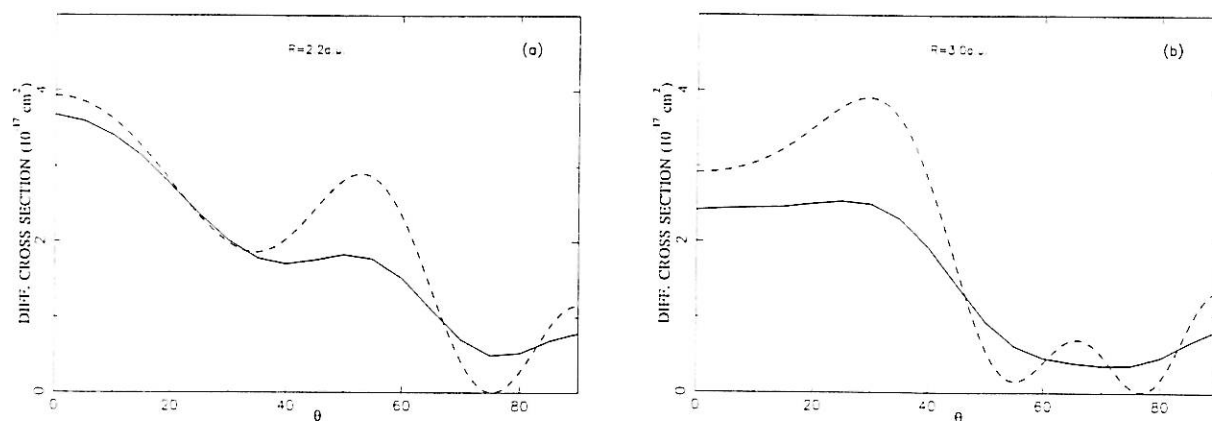


Fig. 4. Differential scattering cross section of target valence electrons to be emitted at 0° in the velocity region of $1.95v \leq k_f \leq 2.15v$ calculated from eq. (13), together with the result obtained not integrating over initial states and assuming that all initial states contribute as the initial state with velocity zero in the laboratory frame (dashed curves). v , Z and r_s are taken to be 2.5 a.u., 3.5 and 1.53 a.u., respectively, and two different values of the internuclear distance are considered: $R = 2.2$ a.u. (a) and $R = 3.0$ a.u. (b).

very sensitive to these multiple scattering effects and also to the effective charge of the projectiles, so that new experiments performed for different charges and velocities would be very useful in order to investigate the applicability of linear theories and capture and loss theories, and also to detect the effect of electron density fluctuations.

Acknowledgements

This research has been sponsored by Eusko Jaurlaritza and by the Office of Health and Environmental Research, U.S. Department of Energy, under contract DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

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