

Multiple scattering effects on electron emission by fast diclusters in solids

J.M. Pitarke

Fisika Teorikoa Saila, Zientzi Fakultatea, Euskal Herriko Unibertsitatea, 644 Posta Kutxatila, 48080 Bilbo, Basque Country, Spain

P.M. Echenique

Materialen Fisika Saila, Kimika Fakultatea, Euskal Herriko Unibertsitatea, 1072 Posta Kutxatila, 20080 Donostia, Basque Country, Spain

Multiple scattering effects on the cluster-orientation dependence of the knock-on collision electrons emitted when fast diclusters penetrate condensed matter are studied using methods developed in the theory of low energy electron diffraction (LEED). The dynamic screening of the Coulomb potential is described by means of a Yukawa potential with an electron-density and velocity dependent screening parameter.

1. Introduction

Recent experimental research has been concerned with the scattering of electrons by fast dimolecular ions penetrating matter [1]: the yield of knock-on collision electrons emitted under bombardment of fast dimolecular ions has been measured as a function of the orientation of the bombarding projectiles, since this dependence could give experimental evidence of the electron density fluctuation [2–4] induced by the leading ion around the trailing ion of the bombarding dicluster.

In order to interpret such experiments for the fluctuation detection, it would be necessary to use a nonlinear theory which accounts at the same time for the induced electron density fluctuations and the nonlinear effects associated with the multiple scattering between bombarding diclusters and target valence electrons; however, no detailed nonlinear theory exists at present. In this paper some preliminary theoretical work involving the multiple scattering between incident diclusters and target valence electrons is presented, combining scattering theory with methods developed in the theory of low energy electron diffraction (LEED).

2. Quantum analysis

We consider a solid target and the process of valence electrons being scattered by the passage of fast dimolecular ions, 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.

If the potential created by each ion constituting the incident dicluster were the Coulomb bare potential, the Schrödinger equation could be expressed in prolate spheroidal coordinates, and the spheroidal phase shifts and scattering amplitudes could be computed [5–11], though it would be a cumbersome task. However, the Coulomb potential of the ions is screened by the polarization of the medium, and the scattering between bombarding diclusters and target valence electrons is not exactly solvable. Thus with the aim of calculating the scattering amplitudes of this interaction process and its dependence on the orientation of the molecular axis of the projectiles, first of all we consider the scattering of target valence electrons from two independent ions, and then we assume that each ion is out of the range of the potential created by the other ion and use methods developed in the theory of low energy electron diffraction to account for multiple scattering effects.

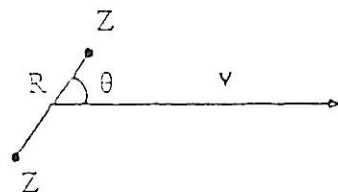


Fig. 1. Geometry of the bombarding dicluster, each ion having charge Z and velocity v . R is the distance between the pair of ions, and θ is the angle formed by the molecular axis of the dicluster with the beam axis.

If scattering were sufficiently weak for multiple scattering to be neglected, the incident electronic wave on each ion would be a plane wave, which can be expanded about the j th ion of the dicluster as

$$\varphi_{k_i}(r) = \frac{1}{\sqrt{V}} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} A_{lm,j}^0 j_l(k|r-r_j|) Y_{lm}(s_j), \quad (1)$$

where

$$A_{lm,j}^0 = e^{ik_i \cdot r_j} 4\pi i^l Y_{lm}^*(k_i/k). \quad (2)$$

In these expressions k_i is the momentum of the incident electron with respect to the projectile, k represents the momentum modulus of the incident electron, which keeps constant when scattering is elastic, s_j is given by

$$s_j = \frac{r-r_j}{|r-r_j|}, \quad (3)$$

j_l represents the spherical Bessel function of the first kind and l th order, and Y_{lm} are the spherical harmonics. Hence, out of the range of the potential created by the moving ions the scattered wave functions would be given by

$$\Psi_{k_i}^{(s)}(r) = \frac{1}{\sqrt{V}} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} A_{lm,j}^0 \frac{e^{2i\delta_l} - 1}{2} h_l^{(1)}(k|r-r_j|) \times Y_{lm}(s_j), \quad (4)$$

where the quantities δ_l are the phase shifts displaying the influence of the interaction with each ion; then the differential scattering cross section of target valence electrons upon interaction of bombarding diclusters would be given by

$$\frac{d\sigma}{d\Omega} = |(1 + e^{i\Delta \cdot R}) f^0(k_i, k_f)|^2, \quad (5)$$

R being the position vector of the leading ion of the projectile with respect to the trailing ion, k_f and Δ being the momentum of the scattered electron and the momentum transfer, respectively, and $f^0(k_i, k_f)$ being the scattering amplitude of target electrons in the potential of each ion.

Nevertheless, in cases where scattering is strong enough there are other contributions to the scattering cross section, since the electronic flux scattered by one ion can scatter the other ion again, so that the incident electronic wave on each ion is no longer an unscattered plane wave. Indeed, the total incident electronic wave on the j th ion can be written as [12–14]

$$\Psi_{k_i}(r) = \frac{1}{\sqrt{V}} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} A_{lm,j} j_l(k|r-r_j|) Y_{lm}(s_j), \quad (6)$$

where $A_{lm,j}$ is the total amplitude. Thus, out of the range of the potential the scattered wave function can be found as

$$\Psi_{k_i}^{(s)}(r) = \frac{1}{\sqrt{V}} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} A_{lm,j} \frac{e^{2i\delta_l} - 1}{2} h_l^{(1)}(k|r-r_j|) \times Y_{lm}(s_j). \quad (7)$$

Consequently, as the total incident wave on each ion is the superposition of the unscattered wave and the scattered wave resulting from a multiple scattering process, one finds for the total incident wave on the j th ion

$$\begin{aligned} \Psi_{k_i}(r) &= \frac{1}{\sqrt{V}} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} A_{lm,j}^0 j_l(k|r-r_j|) \\ &\times Y_{lm}(s_j) \\ &+ \frac{1}{\sqrt{V}} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} A_{lm,k} \frac{e^{2i\delta_l} - 1}{2} h_l^{(1)}(k|r-r_k|) \\ &\times Y_{lm}^*(k_i/k) Y_{lm}(s_k), \end{aligned} \quad (8)$$

where r_j and r_k represent the position vectors of ions j and k , with $j \neq k$. Moreover, there are convenient formulas to transfer spherical waves about the k th site to spherical waves about the j th site [15]:

$$h_l^{(1)}(k|r-r_k|) Y_{lm}(s_k) = \sum_{l'm'} G_{lm,l'm'}(r_j-r_k) j_{l'}(k|r-r_j|) Y_{l'm'}(s_j), \quad (9)$$

where

$$\begin{aligned} G_{lm,l'm'}(r_j-r_k) &= \sum_{l''m''} 4\pi i^{l'-l''-l'''} (-1)^{m'+m''} h_{l'}^{(1)}(k|r_j-r_k|) \\ &\times Y_{l''-m''}(s_{jk}) B^l(l''m'', l'-m') \end{aligned} \quad (10)$$

and

$$s_{jk} = \frac{r_j-r_k}{|r_j-r_k|}; \quad (11)$$

$B^l(l''m'', l'-m')$ represents the integral of the product of three spherical harmonics, i.e.

$$\begin{aligned} B^l(l''m'', l'-m') &= \int Y_{lm}(\Omega) Y_{l''m''}(\Omega) \\ &\times Y_{l'-m'}(\Omega) d\Omega. \end{aligned} \quad (12)$$

Therefore, substituting eq. (9) into expression (8) and comparing with eq. (6) one finds

$$A_{lm,j} = A_{lm,j}^0 + \sum_{l'm'} A_{l'm',k} X_{l'm',lm}(r_j-r_k), \quad (13)$$

where

$$\begin{aligned} X_{l'm',lm}(r_j-r_k) &= \sum_{l''m''} C^{l'}(l''m'', lm) h_{l'}^{(1)}(k|r_j-r_k|) \\ &\times \frac{e^{2i\delta_l} - 1}{2} \end{aligned} \quad (14)$$

and

$$\begin{aligned} C^{l'}(l''m'', lm) &= 4\pi (-1)^{(l'-l''-l)} (-1)^{m''+m} \\ &\times Y_{l''-m''}(s_{jk}) B^{l'}(l''m'', l-m). \end{aligned} \quad (15)$$

Thus the total wave amplitudes incident on each ion of the dicluster can be obtained in the following way:

$$(A_1, A_2) = (A_1^0, A_2^0) \begin{pmatrix} \mathbb{1} & -X(R) \\ -X(-R) & \mathbb{1} \end{pmatrix}^{-1}, \quad (16)$$

where A_1 , A_2 , A_1 and A_2 are line matrices of dimension $l \times (l_{\max} + 1)^2$, and $X(R)$ and $X(-R)$ are square matrices of dimension $(l_{\max} + 1)^2 \times (l_{\max} + 1)^2$; $l_{\max}$ is the maximum value of l considered in expansions (6) and (7). The differential scattering cross section of target valence electrons is found to be

$$\frac{d\sigma}{d\Omega} = |f_1(k_i, k_f) + e^{-ik_f \cdot R} f_2(k_i, k_f)|^2, \quad (17)$$

where

$$f_j(k_i, k_f) = \frac{1}{k} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} A_{lmj} \frac{e^{2i\delta_l} - 1}{2} i^{-(l+1)} Y_{lm}(k_f/k), \quad (18)$$

A_{lmj} , being given by eq. (16), $j=1$ representing the trailing ion, and $j=2$ the leading ion.

For high momentum transfers, the wake potential of fast ions may be approximated by a velocity dependent Yukawa potential of the form

$$U_1(r) = -\frac{Z}{r} e^{-\alpha r}, \quad (19)$$

where

$$\alpha = \omega_p/v, \quad (20)$$

ω_p being the plasmon frequency.

The differential scattering cross section of electrons having zero velocity in the laboratory frame to be emitted at 0° with respect to the beam axis and calcu-

lated from eq. (17) is plotted in fig. 2, as a function of orientation of the projectiles, for $Z=1$, $v=1.5$ a.u. and $R=2.2$ a.u., together with the differential scattering cross section of eq. (5) which neglects multiple scattering; in these calculations the phase shifts of the velocity dependent Yukawa potential of eq. (19) have been computed numerically, and in expansion (18) for the scattering amplitude $l_{\max}$ has been taken to be 7.

The results presented in fig. 2 are consistent with the results obtained in the second Born approximation [16]: in addition to the oscillations also appearing when multiple scattering is neglected, as a result of multiple scattering effects the intensity of scattered electrons is enhanced for the longitudinal orientation of the bombarding diclusters. However, the results presented here are preliminary ones, since for the charges and velocities of interest it is necessary to take greater values of the angular momentum in the expansion (18), thus turning the numerical approach into a very long and tedious calculation; on the other hand, the scattered wave function can be expressed as eq. (7) only for positions out of the range of the potential, so that this approximation cannot be made unless

$$v/\omega_p < R. \quad (21)$$

3. Conclusions

It has been shown that methods developed in the theory of low energy electron diffraction (LEED) may become a useful tool in calculating the multiple scattering for low velocities of the projectiles ($v < 2.0$ a.u.); in future work we shall investigate the nonlinearity appearing for high values of Z , considering larger values of the angular momentum, and we shall calculate the differential cross section integrated over all allowed initial states. For higher values of the velocity, second or even third order perturbation theory may be applied.

The available experimental data have been obtained for rather large effective charges and intermediate velocities ($v = 2.5$ a.u.); on the other hand, measurements of the knock-on electron yield emitted upon bombardment of fast diclusters seem to be very sensitive to multiple scattering effects and to the mean charge state of the bombarding ions, 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 study the effect of electron density fluctuations.

Acknowledgement

This research has been sponsored by Eusko Jauriaritza.

II. CLUSTERS

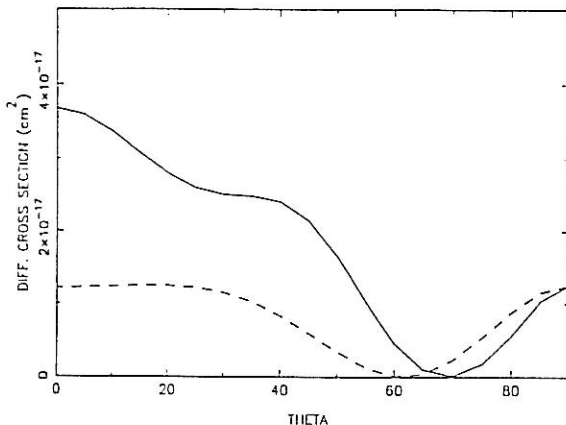


Fig. 2. Differential scattering cross section of electrons having velocity zero in the laboratory system to be emitted at 0° with respect to the beam axis ($k_i = -v$ and $k_f = v$) calculated from eq. (17) (solid curve), vs angle θ , for $Z=1$, $v=1.5$ a.u., $R=2.2$ a.u. and $l_{\max}=7$. For comparison, the differential scattering cross section of eq. (5) is also given (dashed curve).

References

- [1] Y. Yamazaki, Proc. NATO Meeting on the Interaction of Charged Particles with Solids and Surfaces, Alacant, Spain, 1990.
- [2] J. Neufeld and R.H. Ritchie, Phys. Rev. 98 (1955) 1632; 99 (1955) 1125.
- [3] R.H. Ritchie, W. Brandt and P.M. Echenique, Phys. Rev. B14 (1976) 4808.
- [4] P.M. Echenique, R.H. Ritchie and W. Brandt, Phys. Rev. B20 (1979) 2567;
See also P.M. Echenique, F. Flores and R.H. Ritchie, Dynamic Screening of Ions in Condensed Matter, Solid State Physics, vol. 43, eds. H. Ehrenreich and D. Turbull (Academic Press, New York, 1990).
- [5] M.C. Li, J. Math. Phys. 12 (1971) 936.
- [6] M.C. Li, J. Math. Phys. 13 (1972) 1381.
- [7] D.I. Abramov and L.V. Komarov, Theor. Mat. Fiz. 13 (1972) 209.
- [8] M.C. Li, 14 (1973) 1358.
- [9] M.C. Li, J. Math. Phys. 15 (1974) 570.
- [10] L.I. Ponomarev and L.N. Somov, J. Comp. Phys. 20 (1976) 183.
- [11] N.F. Mott and H.S.W. Massey, The Theory of Atomic Collisions (Oxford University Press, 1965).
- [12] J.B. Pendry, J. Phys. C5 (1972) 2567.
- [13] J.B. Pendry, Low Energy Electron Diffraction (Academic Press, London, 1974).
- [14] M.A. Van Hove and S.Y. Tong, Surface Crystallography by LEED (Springer, Berlin, Heidelberg, New York, 1979).
- [15] Ref. [13], p. 272.
- [16] J.M. Pitarke, P.M. Echenique and R.H. Ritchie, Nucl. Instr. and Meth. B, to be published.