Universal Expression for Blocking Cone Size in Low Energy Ion Scattering Based on MD Simulations

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Abstract. Calculations of blocking cone sizes for low energy ion scattering have been performed. By fitting calculated points in the space of the parameters of the interacting atomic species, a universal formula for calculating the blocking cone size for arbitrary energies and interacting species has been derived.The blocking cones in this low energy range are appreciably asymmetric with respect to the interatomic axis. At small interatomic distances and low projectile energies, the difference in the upper and lower halves of the blocking cone can be as large as 15 %. The results of MD simulations using the Ziegler–Biersack–Littmark (ZBL) potential are in good agreement with experimental blocking cone sizes

1 Model Used

We address the problem of calculating the size of a blocking cone, i. e. a shadow region formed behind a particle (atom) placed in the flux of incoming particles scattered by another atom. Blocking cones can be observed in ion scattering experiments [**?**].

Consider a system of two atoms separated by a distance d (Fig. **??**). When a beam of keV ions with parallel trajectories interacts with atom 1 (scattering atom), the latter acts as a source of scattered particles with a near isotropic angular distribution. The position of the source is displaced a very small

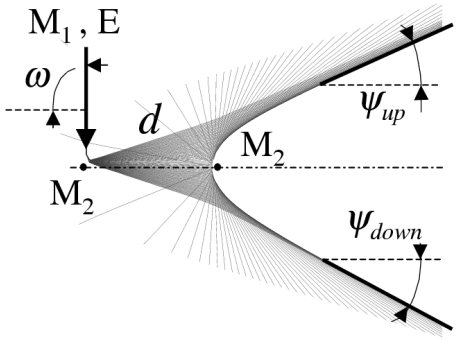

Fig. 1. System of two atoms with interatomic distance d. The parallel beam of particles of energy E and mass M_1 is incident on two atoms of mass M_2. There are two critical scattering angles ψ_{up} and ψ_{down} on both sides of the interatomic axis. The critical blocking angle ψ_c is defined as $\psi_c = \frac{1}{2}(\psi_{up} + \psi_{down})$

distance $\rho \sim 0.1\,\mathring{A}$ from atom 1. Some of these trajectories are deflected by the repulsive potential of atom 2 (blocking atom). This results in a hyperboloid-like "blocking cone" with apex on atom 1 and centered approximately on the interatomic axis. It is necessary to determine the critical blocking angle ψ_c when atom 2 begins to block the scattered trajectories from atom 1.

As an example, the simulated dependence of the exit angle for 10 keV He^+ impinging on two Pt atoms separated by $5\,\mathring{A}$ as a function of the projectile impact parameter p with the first Pt atom is shown in Fig. **??** (solid dots). The critical blocking angles above and below the interatomic axis are ψ_{up} and ψ_{down}, with corresponding p_{up} and p_{down}. The dashed line corresponds to the calculation for a system with the second atom removed. The inset shows the differential scattering cross-section $\sigma_{d\Omega} = p\,(d\psi/dp\ sin\psi)$ versus the exit angle with respect to the interatomic axis for the two-atom (solid line) and one-atom (dashed line) targets. The area under each curve is preserved and corresponds to the flux of particles scattered into the -20^0 to $+20^0$ angle range. The purpose of the MD simulation is to find the two minimum in-plane projectile exit angles ψ_{up} and ψ_{down} on both sides of the interatomic axis whose sum $\psi_{up} + \psi_{down}$ yields the size of the blocking cone.

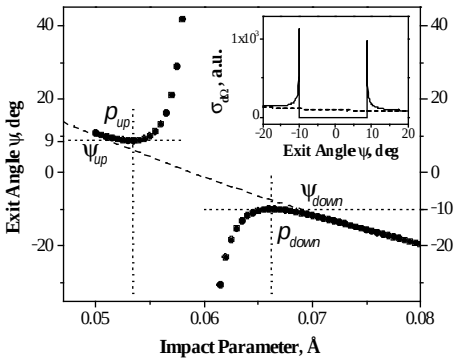

Fig. 2. (dots) Dependence of the exit angle for 10 keV He^+ impinging on two Pt atoms separated by $5\,\mathring{A}$ on the impact parameter p with the first Pt atom. The critical blocking angles above and below the interatomic axis ψ_{up} and ψ_{down} and the corresponding projectile impact parameters p with the first atom p_{up} and p_{down} are indicated. (dashed line) Calculation for a system with the second atom removed. (inset) The differential scattering cross-section versus exit angle for two-atom (solid line) and one-atom (dashed line) targets

2 MD simulations

A molecular dynamics (MD) trajectory simulation code for calculation of the critical takeoff angle has been created. It finds the trajectory of the particle (projectile) in a field created by two target atoms, assuming the Ziegler–Biersack–Littmark (ZBL) interaction potential [?] and neglecting the interaction between the target particles.

In order to follow the trajectories of the particles, the Newtonian equations of motion are numerically solved using a fourth-order Runge–Kutta method [?]. The included parameters affecting the size of the blocking cone are: mass ratios and atomic numbers of projectile and target atoms, interatomic distance d, primary energy of projectile E, and "incident angle" ω, defined as the angle between the incident beam and interatomic axis in the direction from the first to the second atom. The angles of incidence are large enough (from 70^0 to 120^0) to allow projection of scattered particles both above and below the second atom. In-plane quasi-single scattering trajectories that described the two halves (upper and lower) of a blocking cone were calculated. The trajectory of the projectile which, after being scattered with all possible impact parameters from atom 1 towards atom 2, would have the minimal exit angle, contributes to the envelope of the blocking cone. In order to find such a trajectory for each side of the blocking cone, the projectile was directed at atom 1 with p corresponding to the two values of the single scattering angle θ_1. For example, for the upper side, the first value of θ_1 chosen was slightly greater than the projectile incidence angle ω in order to direct the projectile almost head-on at the second atom. This corresponds to the large value of the total scattering angle due to atom 2. The second value of θ_1 was chosen large enough to ensure a large total scattering angle mostly due to atom 1 and almost no interaction with atom 2. The smallest value of the total scattering angle corresponding to the upper half-size of the blocking cone lies somewhere between these two limiting values. This minimum value was found using the golden section minimum search algorithm for a one-variable function [?].

3 Universal Fitting Formula

The procedure for obtaining a universal formula for the blocking cone size will now be described. The critical blocking angles are determined as $\psi_c = \frac{1}{2}(\psi_{up} + \psi_{down})$, where $\psi_{down} = k\psi_{up}$, with $k \geq 1$. In a first approximation, $k \approx 1$ so that $\psi_{down} \approx \psi_{up}$, and $\psi_c \approx \psi_{up}$. As a result, the calculated values of ψ_{up} can be fitted with a second-order surface $z = z(x, y)$ with $x = lnd$, $y = lnE$, and $z = ln(\psi_{up})$, where E is the projectile energy in keV and d is the distance between the target atoms in $\mathring{A}$. The blocking cone sizes found for various parameters $(M_1, M_2, Z_1, Z_2,\ \omega)$ are fitted with a formula $\psi_{up} = Dd^{-n}E^{-m}$ where D, n, and m are functions of the five parameters $(M_1, M_2, Z_1, Z_2,\ \omega)$.

Table 1. Numerical values of parameters in (??), (??) found from fitting MD calculations of the blocking cone size (ψ_{up}).

	0	1	2	3	4	5
f_i	1.34 ±0.04	0.13 ±0.03	-0.074 ±0.003	-0.060 ±0.004	0.0096 ±0.0009	-0.0404 ±0.0009
h_i	0.90 ±0.01	-0.24 ±0.01	0.0255 ±0.0006	0.0084 ±0.0008	0.047 ±0.0002	-0.0010 ±0.0001
g_i	0.174 ±0.001	-0.133 ±0.003	0.0093 ±0.0002	0.0043 ±0.0001	0.0167 ±0.0004	0.00253 ±0.00003
e_i	0.36 ±0.01	-0.078 ±0.007	0.0053 ±0.0005	0.0140 ±0.0009	-0.069 ±0.003	0.0032 ±0.0002

Not all of these parameters are independent, as follows from the properties of the equations of motion and form of the potential function, and therefore, the set (M_1, M_2) can be reduced to the ratio M_1/M_2, and the set (Z_1, Z_2) to combinations of $ln(Z_1 Z_2)$ and $({Z_1}^{0.23} + {Z_2}^{0.23})$. As a result, we can write:

$$\begin{aligned} ln(D) &= f(\frac{M_1}{M_2},\ ln(Z_1 Z_2),\ ln(\omega)) \ , \\ n &= n(\frac{M_1}{M_2},\ {Z_1}^{0.23} + {Z_2}^{0.23},\ ln(\omega)) \ , \\ m &= m(\frac{M_1}{M_2},\ ln(Z_1 Z_2),\ ln(\omega)) \ . \end{aligned} \tag{1}$$

After fitting $ln(\psi_{up}) = z$ with a second-order surface in x and y ($z = F_0 + F_1 x + F_2 x^2 + F_3 xy + F_4 y + F_5 y^2$) for a fixed set of $(M_1/M_2; Z_1, Z_2,\ \omega)$, six values of F_i in $(M_1, M_2, Z_1, Z_2,\ \omega)$ space are obtained. It was possible to fit the calculated points for 120 projectile-target combinations by a hyperplane in $(M_1/M_2, ln(Z_1\ Z_2),\ ln(\omega))$ space for four of the coefficients (F_0, F_3, F_4, F_5) of decomposition of $ln(\psi_{up})$ in x and y and in $(M_1/M_2, {Z_1}^{0.23} + {Z_2}^{0.23},\ ln(\omega))$ space for the other two (F_1 and F_2). The range of target interatomic distances used in the calculations was d = 2–13 Å, the energy range was E = 3–20 keV, the ω range was 70^0–125^0, the M_1/M_2 range was 0–0.33, and the product $Z_1 Z_2$ varied between 40 and 1600. The final fitting expression for finding ψ_{up} is

$$\psi_{up} = exp(F_0 + F_1 x + F_2 x^2 + F_3 xy + F_4 y + F_5 y^2) \ , \tag{2}$$

where

$$F_i = f_i + h_i \frac{M_1}{M_2} + g_i ln(Z_1 Z_2) + e_i ln(\omega) \tag{3}$$

for i = 0, 3–5, and

$$F_i = f_i + h_i \frac{M_1}{M_2} + g_i ({Z_1}^{0.23} + {Z_2}^{0.23}) + e_i ln(\omega) \tag{4}$$

for $i = 1, 2$. The lower part of the blocking cone can be estimated from $\psi_{down} = k\psi_{up}$, where k is in the range 1.0–1.3 and is dependent on the same variables as ψ_{up}. We do not provide a universal fitting formula for ψ_{down} here since its fitting coefficients represent surfaces whose analytical forms in the space of the parameters are not that straightforwardly determinable as in case of ψ_{up}.

4 Conclusions

Our MD simulations reveal the asymmetry in the blocking cone size with respect to the interatomic axis. For small d and E, the asymmetry of the blocking cone is maximum and decreases with increasing d and E. At small interatomic distances and low projectile energies, the difference in the blocking cone sizes can be as large as 15 %. This is important in the low energy range when the critical angles are large and the displacements of the virtual source from the first atom cannot be neglected. We note that although in the double alignment experiments in the Rutherford Backscattering technique this asymmetry is small enough to be neglected, care must be taken in Low Energy Ion Scattering when drawing conclusions about surface relaxation based on the shape of the blocking cone.

References

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