Physica Scripta. Vol. T80, 205–206, 1999

Angular Differential Cross Sections for Slow Highly Charged Ions Interacting with C_{60}

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Received September 14, 1998; accepted in revised form December 1, 1998

PACS Ref: 34.70.+e

Abstract

Angular differential cross sections are presented for collisions between 26.4 keV Ar^{8+} ions and C_{60} molecules. Using a classical overbarrier simulation the deflection function is calculated for large impact parameters. To compare with experimental data the theoretical cross section values are convoluted with an instrumental function. Both the theoretical and experimental cross sections are absolute in magnitude and position. The experimental cross section for retaining one electron on the projectile is qualitatively well described by the theoretical cross sections for initially capturing one to four electrons from the target.

1. Introduction

Slow highly charged ions (HCIs) colliding with neutral matter can induce multielectron transfer between the target and the projectile. For many years two types of collisions have received a lot of attention: Slow HCI-atom collisions [1] and slow HCI-metal surface interactions [2,3]. The experimental studies have been stimulated by the advent of modern high-current ion sources. Lately, the focus has turned to the related fields of slow HCI-insulator surface interactions [3,4] and slow HCI-cluster collisions [5], the latter of which we will treat here. A cluster target of free fullerenes (C_{60}) provides an interesting intermediate between the atom target and the surface target. The large number of electrons in C_{60} can make the projectile a hollow atom, as in the case of using a metal surface target, but for the cluster target the hollow atom may survive the collision. As for an atom target the collision time is limited. For clusters a further field of study is the fragmentation of the target as a result of the collision.

Most of the modelling of the multielectron transfer, transfer ionization and electron emission in slow HCI-cluster collisions has been done under the assumption that classical overbarrier (COB) transitions dominate. Taking into account the specific structure of the targets these COB-models have been successful [6] in that they have yielded results explaining experimental data.

In this paper we will first briefly review the COB-simulation model developed by U. Thumm [6], which is used to calculate the angular deflection function $\theta(b)$ (and scattering angle) of the projectile. We present theoretical absolute angular differential cross sections ($d\sigma/d\theta$) calculated from the deflection function and compare these to experimental data.

2 Classical overbarrier model

In the COB-picture the electrons in the target are strongly affected as the HCI approaches. When the potential barrier separating the projectile and the target is lowered below the lowest occupied state the electrons are assumed to be transferred. The present model, which is described in detail in Ref. [6], treats the time evolution of the occupancy of both projectile and target levels. The COB-model so far only describes the electron transfer for distant collisions, i.e. for large impact parameters.

In the simulation of the electron flow between the target and the projectile the electron charge is treated as a continuous parameter. However, for the calculation of the trajectory, the charge in each step is rounded off to the nearest integer value. The deflection function $\theta(b)$ for 26.4 keV Ar^{8+} is shown in Fig. 1 for large impact parameters. The stepwise structure of the deflection function will give rise to rainbow scattering peaks and other singularities in the non-convoluted theoretical differential cross section. Most of this structure will disappear in the convoluted spectra.

3. Results and discussion

The angular differential cross sections $d\sigma/d\theta$ are calculated from

$$\frac{d\sigma}{d\theta} = \sum_j \frac{2\pi b_j}{|d\theta/db_j|} \quad (1)$$

where $\theta(b)$ is the deflection function obtained from the COB simulation. The cross sections are convoluted by an instrumental function consisting of a Gaussian weighted

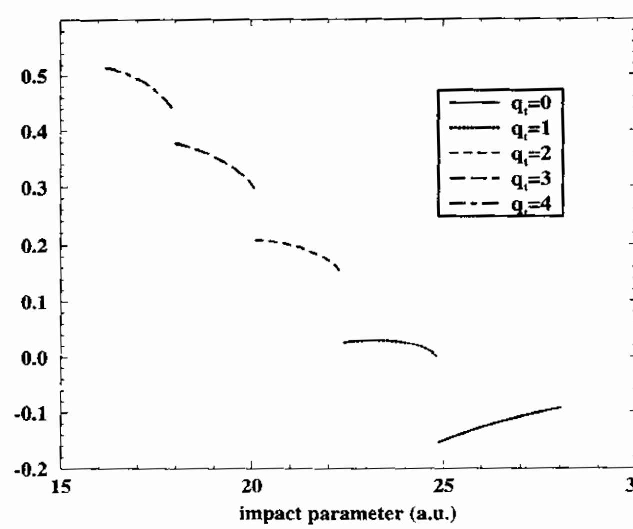

Fig. 1. Deflection function for 26.4 keV Ar^{8+} producing $C_{60}^{q_t+}$, with $q_t = 0$–4.

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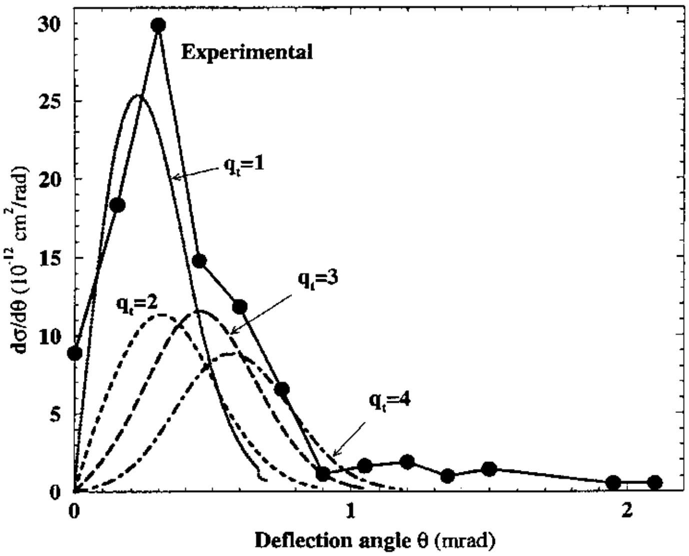

Fig. 2. Experimental angular differential cross section for 26.4 keV Ar^{8+} to end up as Ar^{7+} in collisions with C_{60}. Also shown are COB simulations of production of $C_{60}^{q_t+}$, with $q_t = 1$–4.

by $|\sin(\theta)|$. The FWHM of the Gaussian is estimated from the experimental data [7] to be around 0.3 mrad.

In the experiment the outgoing ions in the process 26.4 keV $Ar^{8+} + C_{60} \rightarrow Ar^{(8-s)+} + \ldots$ are detected, where the C_{60} can fragment or become multiply charged. From the COB model we calculate convoluted theoretical cross sections $d\sigma/d\theta$ for 26.4 keV $Ar^{8+} + C_{60} \rightarrow C_{60}^{q_t+} + \ldots$ ($q_t = 1$–4). The relaxation of the projectile after the collision is not included. In Fig. 2 the experimental $d\sigma/d\theta$ for $s = 1$, i.e. one retained electron on the projectile, is compared to the theoretical $d\sigma/d\theta$ for $q_t = 1$–4, i.e. one to four electrons removed from the target. Both the experimental and the theoretical values are absolute in magnitude and position (in contrast to Ref. [8]) and the excellent agreement, obtained without adjustment or normalization, should be stressed. As can be seen from Fig. 2 the contribution from $q_t = 1$ describes the low angle part very well. Only a small fraction of $d\sigma/d\theta$ for processes where C_{60} has lost more than one electron is needed in addition. The exact contributions, though, require knowledge of the branching ratios for the relaxation of the projectile.

In Ref. [8] it is shown that the polarizability of C_{60} plays an important role in the description of the angular distributions. This is illustrated by comparing calculations with and without image potentials, affecting the positions of the angula distributions significantly, with experiments. The energy o the Ar ions used here is an order of magnitude higher thai what is used in Ref. [8] and excluding the image potentia in our calculations would only produce a negligble shift o the position of $d\sigma/d\theta$.

In comparison to other applications of the overbarrie model, which one could use to calculate $d\sigma/d\theta$, the presen scheme has the advantage that extensions can be quite easil incorporated. Future developments of the code which coul affect the angular differential cross sections include thorough modelling of the relaxation of the projectile. Fu thermore the effect on $d\sigma/d\theta$ of a localized charge on the su face of the C_{60} should be investigated by incorporation i the present model.

In summary, we have shown that the COB-simulatio model successfully can reproduce the angular differenti cross section of slow HCI interacting with C_{60}.

Acknowledgements

This research was supported by the Swedish Natural Science Research Cou cil (NFR) and, in part, by the Division of Chemical Sciences, Basic Ener Sciences, Office of Energy Research, U.S. Department of Energy.

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