On the Theory of Pore Formation at the Passage of High Charged Ions Through a Carbon Nano-Membrane

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Abstract
The change in the size of projectile’s wave field during the passage through the set of parallel solid films is considered. The possibility to explain the experimental data is found.

Keywords: High charged ion; Thin carbon film; Polarization phenomena; Wave packet; Ehrenfest equations; Electric forces; Carbon nano-membrane; Porous structures

Introduction

Sometimes, especially in experimental studies, when a particle beam bombards the surface of a solid, each particle is considered as a classical material point moving along a certain classical trajectory. This approach is natural also in those mathematical models of physical phenomena that use the method of molecular dynamics. But in the last three decades experimentators also in the technique of beam-solid interactions attain the high level of measurement accuracy. In the modern experiments the physicists actually can observe individual atoms. In this case for to have the possibility of correct theoretical estimations of experimental data the theoreticians should take into account all the quantum-mechanical properties of projectiles as well as the target. On the picture (Figure 1) is shown the porous structure created by the high charged atomic ions (HCI) Xe+35 having energies 40keV and 12 keV. The pores created in the stack of four parallel carbon nano-membrans (CNM). Each CNM is produced with the help of a specific technique (the details contains in [q,2]) and contains mainly the carbon atoms. After the some estimations we have found that the films which have been used in experiments [1,2] are much more friable in comparison to the graphene. It is seen as individual atoms sequentially pierce the pores in each of the membranes.

Figure 1: Passage of HCl through a stack of four carbon nano-membranes (CNM) foils [2].

Theoretical explanation of the effect
The basic idea which is proposed here is to explain the experiments with suggestion that the wave packet of each HCI
produce the pore in carbon nano-membrane because of their great electric field. For solve the problem of passage of HCl through CNM is appropriate to use the semi-classical approximation based on the Ehrenfest’s theorems. The wave packet does very depend on the interaction with the other parts of matter. The mostly simple description of change in wave packet’s properties can be obtained with the help of the density matrix (DM). DM changes very sufficient yet in the elastic collision, but in this case the breaking of the wave packet usually didn’t concerned with the loss of phase correlation between different parts of the wave field. The elastic collision usually happens sufficiently seldom because the non-avoided inelastic processes. The analysis of inelastic collisions lead us to the conclusion that the wave field can rapidly loss his spatial coherence [3].

$$\delta_j^2(t) \approx \delta_0 2 \frac{1}{1 + 4 \delta_0^2 \Delta^2 k_j} + \frac{t^2}{4 \delta_0^2 m^2}$$

Here the quantities $\Delta^2 k_j$, equal to the squared mean momentum fluctuations for the projectile arisen in course of interaction with a solid. As we see, the fluctuations of momentum inside the solid during the time $t < \frac{\delta_0}{m}$ influence on a projectile’s states in opposite manner compared with the dispersive dependence of the projectile’s energy on the momentum. Within the solid the progressive momentum and energy fluctuations sufficiently changes all the picture. Especially it is important for the particle obeying a great mass. In this case during the comparatively long distance we can observe the rapid contracting in particle’s coherence length. This behavior is mostly significant if an initial width of a packet is great [4]. If a momentum fluctuation stops to increase, then, according to information received, in course of time the process resumes the dispersion broadening of the packet’s width. At the first time of interaction , when $t < \frac{\delta_0}{m^2}$, in consequence of inelastic events the coherence length diminishes in correspondence to the rule

$$\delta_j \approx \frac{\delta_0}{\sqrt{1 + 4 \delta_0^2 \Delta^2 k_j \delta_0^2}}$$

where $\Delta^2 k_j$ is the squared fluctuation of j-th component of the wave vector, $\delta_0$ is the Gauss width of the packet before the foil, $\delta_j$ is the same after the foil. The crude approximation for $\delta_0^2$ is $jL\lambda_B$ where L is the distance which the ion passes from accelerator to foil, $\lambda_B$ is the de-Broglie wavelength of the projectile.

For to get estimations presented in the above formula we have used the electron gas theory presented by Lindhard & Winter in the well known work [5]. The electron gas parameters was previously estimated in the works [3,5] $r_0 \approx 3.8$. Application of Lindhard-Winter approach in our case was generalized with taking into account the fluctuation of the projectile’s momentum (instead of energy loss) and the non-point charge behavior of the wave packet electric field. In the low velocity regime the estimation of the wave vector fluctuations can be obtained with the usage the following formula

$$\frac{d \Delta k^2}{dx} = \frac{4 \pi Z^2 e^4}{m e^2} \bar{n} \frac{L_{k2}}{\lambda^2}$$

where (in atomic units)

$$L_{k2} = 3 \frac{\lambda^4}{2} \text{ sr} \left( \frac{dz}{r_F^2 \bar{n} \exp \left(-4 \frac{k_F^2 \delta^2}{\lambda^2} \right)} \right)^{1/2}$$

Here we follow to all the nominations applied by Lindhard and Winter in their work. Result of our comparison of the theoretical and experimental data presented in the Table 1. Here the first number in the first column in the experimental data is used as the starting point for the theoretical preliminary estimations. The initial size of the wave packet is found in correspondence to the vacuum behavior of the wave function. The previous estimations [6,7] have shown that the radius of the pore which is produced with the Gauss wave packet is proportional to the Gauss width, and approximately following to the relation $R \approx 1.5 \cdot \delta$. It is noteworthy to mention that between the data for 40 keV and 12 keV the relationship is very close to the one between $E_2^{1/4}$ and $E_1^{1/4}$. This conclusion immediately follows from $\delta_0 \approx \sqrt{L \lambda_B}$. This circumstance is important in verification of the theory presented here.

Table 1: The comparison between exp. and theor. estimations of Gauss widths of the wave packets of Xe+35 for two energies.

|          | Column1 | Column2 | Column3 | Column4 |
|----------|---------|---------|---------|---------|
| $\delta_j$, a.u., exp | 40 keV  | 70      | 67      | 48      | 29      |
| $\delta_j$, a.u., th  | 40 keV  | 67      | 61      | 55      | 47      |
| $\delta_j$, a.u., exp | 12 keV  | 87      | 73      | 59      | 52      |
| $\delta_j$, a.u., th  | 12 keV  | 85      | 71      | 51      | 46      |

**Conclusion**

a. The theory of pore formation at the passage of HCl through a carbon nano-membrane, which assumes a mechanism created by the moving ion wave packet electric forces, correctly describes the event.
The results of investigations allowed us to make an additional conclusion about the possibility of measuring some properties of wave packets with the help of its passage through the specific carbon films.

The more less diminishing of the theoretical estimations signals us on the existence of additional physical circumstances which should be taken into account in calculations.

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