# ON THE POSSIBILITY TO DETERMINE REPULSIVE POTENTIALS IN eV REGION FROM FAST MOLECULAR BEAM SCATTERING EXPERIMENTS

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For many years the fast molecular beam (energy $E$~1 keV) small-angle ($10^{-4}$ – $10^{-2}$ rad) scattering experiments were used to determine repulsive interaction potentials. Traditionally the collisions in such experiments were considered to be of the elastic nature. It is usually true for scattering in rare gases but if the colliding particles are molecules the inelastic processes may take place too. An experimental set up built at the Institute for Problems in Mechanics of Russian Academy of Sciences measures not only the scattering angle but the fast particle energy as well. Such experiments measure the differential cross sections and energy loss spectra that allows to deduce the elastic and inelastic differential cross sections. A procedure to find the interaction potential from these differential cross sections is proposed.

The paper discusses the problem of experimental determination of repulsive interaction potentials in the 0.1-10 eV energy range by fast molecular beam scattering method. It worth mentioning that the fast molecular beam technique is obviously the only experimental one giving information about the repulsive interaction potential in eV energy range. The collisions in such experiment were traditionally considered to be the elastic ones. Back in 1977 we found [1] that the He-$N_2$ system differential cross section has some peculiarities. Farther investigation [2] demonstrated that such peculiarities were present for many other systems which include molecules. We put forward a hypotheses [2], [3] that these peculiarities were connected to electronic or vibrational excitation of molecules. To solve this problem we have designed and built up an experimental apparatus measuring not only the scattering angle (differential cross sections) but also capable of obtaining the energy of fast scattered particles (energy loss spectra). The simplified version of this apparatus is presented in Fig.1. Here 1 is the ion source, AM – the analyzing magnet, MR – the modulation area, CC – the charge-exchange chamber, SC – the scattering chamber, PSD – the position sensitive detector, PC – the personal computer. A detailed description of this apparatus can be found in paper [4], and very shortly this experimental set up is discussed in [5].

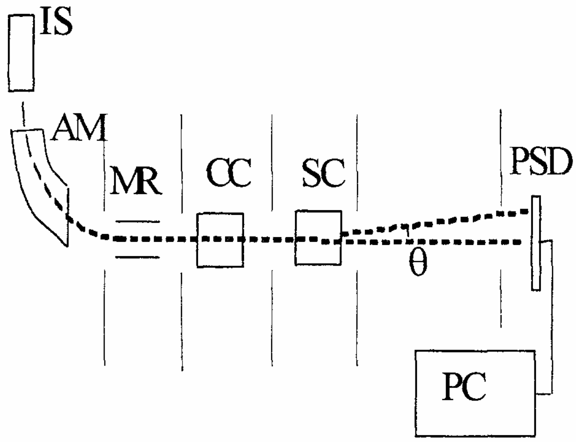


Fig. 1. A simplified version of experimental setup.

As an example of the obtained results the differential cross sections and the energy loss spectra for He-$N_2$ systems are shown in Figs. 2 and 3 (the reduced coordinates $\tau=\theta\cdot E$ and $\rho=\sigma\cdot\theta^2$ are used, where θ- is the scattering angle, σ – is the differential cross section).

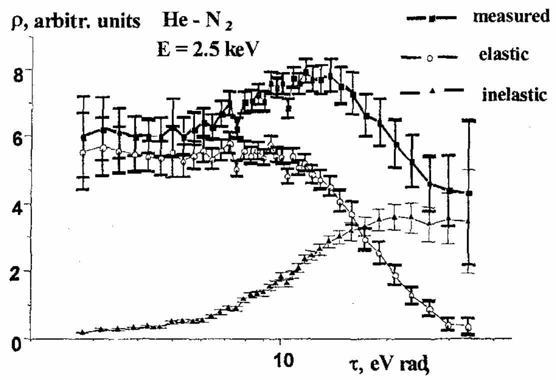


Fig.2. Differential cross sections of He-$N_2$ system.

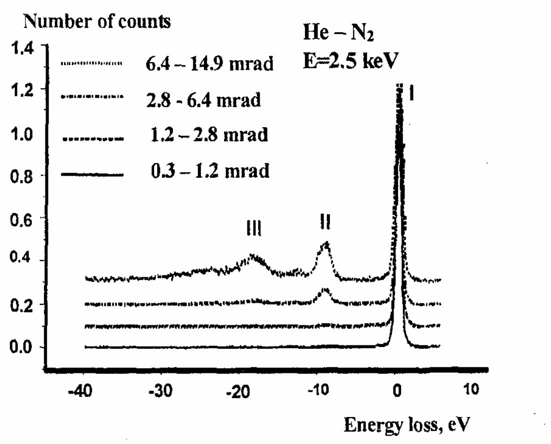


Fig.3. Energy loss spectra of He-$N_2$ system.

The measured differential cross section in Fig.2 (solid squares) is the one which was measured by the position-sensitive detector provided by the scattering angle obtained per every scattered particle. This differential cross section is a sum of elastic and inelastic cross sections which can be restored via the energy loss spectra. The cross sections restoration procedure is based on the amount of counts in peaks shown in Fig.3 as described in [6]. Such extracted cross sections are also shown at Fig.2 (elastic –open circles, inelastic – solid triangles). Such elastic and inelastic differential cross sections make it more realistic to find the interaction potentials.

The inversion procedure of the repulsive interaction potential out of the elastic differential cross sections is considered in terms of the classical mechanics and is based on the definition of σ(θ) differential cross section for the monotonous function of the scattering angle θ on the impact parameter *b*:

$$\rho(\tau) = \frac{b(\tau)}{\left|\frac{d\tau}{db}\right|} \tag{1}$$

The integral cross section for a monotonous τ(*b*) function is:

$$Q(\tau, E) = \pi b^2(\tau) \tag{2}$$

τ(*b*) is related to *V(R)* potential by a simple equation:

$$\tau(b) = -\frac{\partial}{\partial b}\int_b^\infty \frac{V(R)RdR}{\sqrt{R^2 - b^2}}\,. \tag{3}$$

This equation can be converted to:

$$V(R) = \frac{2}{\pi}\int_R^\infty \frac{\tau(b)db}{\sqrt{b^2 - R^2}}\,. \tag{4}$$

To calculate the integral (4) Gauss-Mehler formulas can be used:

$$V(R) = \frac{2}{n}\sum_{j=1}^{n}\frac{\tau(R/\upsilon_j)}{\upsilon_j},$$

where $\upsilon_j = \cos\left(\frac{2j-1}{2n}\pi\right)$. (5)

In this respect the problem of V(R) restoration is related to finding of τ (b) function. The τ (b) can be found from ρ(θ) differential cross section by numerical solution of the first order differential equation (1):

$$b_i^2 = b_k^2 - 2\int_{\tau_i}^{\tau_k}\rho(\tau)\,d\ln\tau\,. \tag{6}$$

The measurements of differential cross sections are relative therefore we used measurements of absolute integral cross sections carried our earlier for detector with the aperture angle of 5 $10^{-3}$ rad to restore the absolute b value (2)

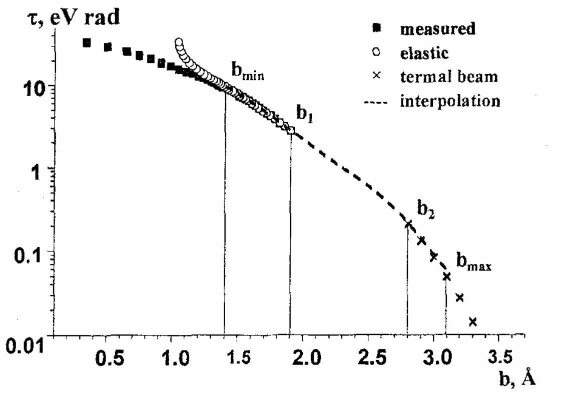


Fig. 4. The dependence of reduced angle τ on impact parameter b for He-$N_2$ system.

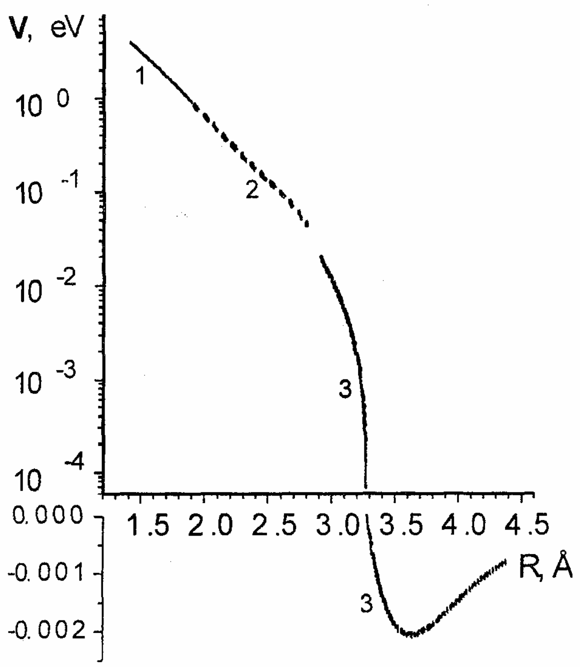


Fig.5. The He-$N_2$ potential.

Nevertheless the procedure of finding the interaction potential out of the restored elastic differential cross section is not that easy. The point is that the elastically scattered particle can be a subject of two transitions during the collision. First transition from the ground to excited state at the oncoming trajectory and the second one from the excited to ground state when the particles fly away. Such double transition in this case distorts the elastic differential cross section measurement. To overcome this ambiguity we calculate two τ (*b*) functions using formulae (6)– one for elastic and another for measured ρ(θ). Open circles in Fig.4 show the He-$N_2$ system function τ (*b*) calculated for elastic differential cross section. Solid squares demonstrate the function restored from measured ρ(θ) for the same system. From Fig.4 one can see that this two dependencies begin to differ at the point of $b$=1.4 Å. And to the right from this point the function can be considered to imply only elastic collisions. The V(R) potential inversion needs the τ (b) dependence of up to $b \to \infty$ (see equation (4)). To solve this problem we decided to take into account the apriori potentials found for the well region and the attractive part (theoretical results [7], [8] for He-$N_2$ and $N_2$-$N_2$ systems). The τ (*b*) calculation for the He-$N_2$ potential from [7] is presented by crosses in Fig.4. The united τ (*b*) curve may be found from the interpolation curve connecting these two parts of the restored and calculated results (dot lines on Fig.4). The method allows to gain the τ (*b*) function for the values of *b* up → ∞ while V(R) is derived using equation (5). The results for He-$N_2$ is presented in Fig.5, and for $N_2$-$N_2$ – in Fig.6. Here 1 is our inversion of high energy results, 2- is the potential found from the interpolation curve, 3- is the potential from [7] for He-$N_2$ and from [8] for $N_2$-$N_2$. The potentials 1 and 2 can be approximated by analytic formulae:

1) for Ne-$N_2$

$$V(R) = \begin{cases} 253 \cdot \exp(-2.95 \cdot R) & 1.4 < R < 1.9\,\text{Å} \\ 435 \cdot \exp(-3.26 \cdot R) & 1{,}9 < R < 2{,}8\,\text{Å} \end{cases}$$

2) for $N_2$-$N_2$

$$V(R) = 1197 \cdot \exp(-2.91 \cdot R)$$
$$2.0 < R < 3.0 \ \text{Å}$$

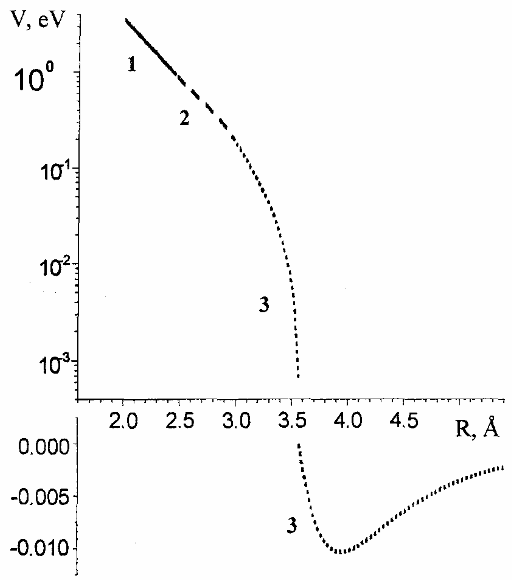


Fig.6. The $N_2$-$N_2$ potential.

It should be noted in conclusion that the procedure of inversion the potentials from fast molecular beam double differential cross sections measurements is proposed. The potentials for He-$N_2$, $N_2$-$N_2$ systems are taken as examples

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# ПРО МОЖЛИВІСТЬ ВИЗНАЧЕННЯ ПОТЕНЦІАЛІВ ВІДШТОВХУВАННЯ В ЕЛЕКТРОНВОЛЬТНОМУ ДІАПАЗОНІ З ЕКСПЕРИМЕНТІВ З РОЗСІЮВАННЯ ШВИДКИХ МОЛЕКУЛЯРНИХ ПУЧКІВ

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Багато років експерименти з малокутового ($10^{-4}$ - $10^{-2}$ рад) розсіювання швидких молекулярних пучків (енергія $E$~1 кеВ) використовувалися для визначення відштовхувальних потенціалів взаємодії. Традиційно вважалося, що зіткнення в таких експериментах пружні. Це зазвичай правильно для інертних газів, але якщо в зіткненнях беруть участь молекули, можуть мати місце і непружні процеси. Експериментальна установка, створена в Інституті проблем механіки Російської академії наук, вимірює не тільки кут розсіювання, а й енергію швидких частинок. У таких експериментах вимірюються диференціальні перерізи та спектри енергетичних втрат, що дає змогу отримати диференціальні перерізи для пружних і непружних процесів. Пропонується процедура знаходження потенціалу взаємодії з цих диференціальних перерізів.