Supplementary Material to the article "On channeling of atomic beams of keV energies in flat and cylindrical channels"

In the Firsov-Moliere approximation, the interatomic interaction potential $V_a(r)$ reads (here and in what follows, the atomic units with $e = \hbar = m_e = 1$ are used)

$$V_a(r) = \frac{Z_1 Z_2}{r}\sum_i \alpha_i \exp(-\beta_i r/a_F)\,,\, a_F = 0.8853\left(\sqrt{Z_1}+\sqrt{Z_2}\right)^{-2/3}, \tag{S1}$$

where $\alpha_i = (0.3, 0.55, 0.35)$ and $\beta_i = (6, 1.2, 0.3)$. For a planar surface, using (S1) and the continuum approximation

$$U_a(z) = 2\pi n \int_z^\infty dy \int_0^\infty d\rho\rho V_a\left((\rho^2+y^2)^{1/2}\right), \tag{S2}$$

we obtain

$$U_a(z) = 2\pi n Z_1 Z_2 a_F^2 \sum_i \frac{\alpha_i}{\beta_i^2}\exp(-\beta_i z/a_F), \tag{S3}$$

where n and z are the bulk atomic concentration and the distance between an atom and a surface.

For a cylindrical channel (a thick-walled tube) we first obtain the continuum interaction potential, assuming that the walls are infinitely thin, with a surface atomic density $n_s = ndR$:

$$U_a^{(thin)}(\rho, R) = n_s R \int_0^{2\pi} d\varphi \int_{-\infty}^{\infty} V_a(z,\rho,\varphi,R)\, dz. \tag{S4}$$

In (S4), the function $V_a(z,\rho,\varphi,R)$ is defined by (S1) with $r = \left(z^2 + |\boldsymbol{\rho} - \boldsymbol{R}|^2\right)^{1/2}$; $\boldsymbol{\rho}$ and $\boldsymbol{R}$ are the transverse radial vectors relative to the center of the cylinder cross-section (Fig. S1), z is the longitudinal coordinate along the symmetry axis. Taking this into account, the integral (S4) is explicitly calculated, yielding

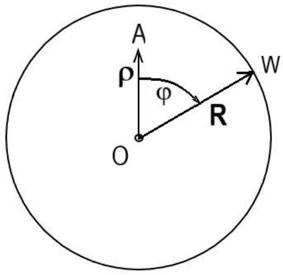

Fig. S1. Cylindrical coordinates of the incident atom A and the atom W of the channel wall.

$$U_a^{(thin)}(\rho, R) = 4\pi n_s Z_1 Z_2 R \sum_i \alpha_i\, K_0(\beta_i \rho/a_F) I_0(\beta_i R/a_F), \tag{S5}$$

where K_0 and I_0 are the modified Bessel functions. Finally, integrating (S5) yields

$$U_a(\rho) = \int_a^\infty U_a^{(thin)}(\rho, R) dR = 4\pi n Z_1 Z_2 a a_F \sum_i \frac{\alpha_i}{\beta_i} K_1(\beta_i a/a_F) I_0(\beta_i \rho/a_F). \tag{S6}$$

Equation (S6) corresponds to the interaction potential between an atom and the walls of a cylindrical tube with an internal radius a.

In the limit of a flat wall, $a, \rho \to \infty, a-\rho \to z$, taking into account the asymptotics of the functions K_0 and I_0, Eq. (S6) is reduced to (S3). Next, according to [1], the expressions for the "mirror" interaction potential $U_m(z)$ and stopping force $F_m(z)$, van der Waals friction force $F_{\text{vdw}}(z)$ and electronic stopping force $F_e(z)$ are given by [1] (v is the atom velocity)

$$U_m(z) = -\frac{Z_1^2}{2\pi}\int_0^\infty dkY(k,z)f_1(kv)\,, \tag{S7}$$

$$F_m(z) = -\frac{Z_1^2}{\pi}\int_0^\infty dkkY(k,z)f_2\,(kv)\,, \tag{S8}$$

$$Y(k,z) = q^2e^{-2kz} + q(1-q)e^{-kz}B(k,z) + \frac{(1-q)^2}{4}B(k,z)^2, \tag{S9}$$

$$f_1(x) = \int_0^\pi d\varphi \mathrm{Re}(\Delta(x\cos\varphi)), \tag{S10}$$

$$f_2(x) = \int_0^\pi d\varphi\cos\varphi \mathrm{Im}(\Delta(x\cos\varphi)), \tag{S11}$$

$$B(k,z) = \sum_i c_i \frac{\lambda_i^2}{\tilde{\lambda}_i(\tilde{\lambda}_i - k)} e^{-\tilde{\lambda}_i z} \tag{S12}$$

where $q = 1 - N/Z$, $\Delta(\omega) = \frac{\varepsilon(\omega)-1}{\varepsilon(\omega)+1}$, $\lambda_i = \beta_i/a_F$, $\tilde{\lambda}_i = \sqrt{\lambda_i^2 + k^2}$; moreover,

$$F_{vdw}(z) = -\frac{1}{\pi}\sum_n \frac{f_{0n}}{\omega_{0n}}\left(\frac{\omega_{0n}}{v}\right)^4 f_3(\omega_{0n}, 2\omega_{0n}z/v)\,, \tag{S13}$$

$$f_3(x,y) = \int_1^\infty dtt^3\mathrm{Im}[\Delta(x(t-1))](K_0(yt) + K_2(yt))\,, \tag{S14}$$

$$F_e(z) = \frac{3.54}{\pi}(Z_1+Z_2)^{5/3}nv\int_z^\infty d\rho\rho\arccos\left(z/\sqrt{z^2+\rho^2}\right)I(\sqrt{z^2+\rho^2})\ , \tag{S15}$$

$$I(x) = \sum_i\sum_j \alpha_i\alpha_j f\left(\left(\beta_i+\beta_j\right)x/2a\right), a = 0.8853/\sqrt[3]{Z_1+Z_2}\ , \tag{S17}$$

$$f(x) = \int_x^\infty dyK_1\,(y)/y\,. \tag{S18}$$

1. G. V. Dedkov, "Dissipative van der Waals and mirror interaction of keV-energy atoms at glancing reflections from the surface of metal", JETP Lett. **123**, 257 (2026).