Supplementary Material to the article "Dissipative Van der Waals and mirror-image forces of atoms with keV energies at glancing reflections from the metal surface"

The Bonham-Strand model [1] of the electron density of atoms with $1 \leq Z \leq 36$ operates with the expression (atomic units $e = \hbar = m_e = 1$ are used)

$$\rho_e(r) = -\frac{Z}{4\pi r}\sum_{i=0}^{n} {}^{a}\gamma_i \, {}^{a}\lambda_i^2 \exp(-{}^{a}\gamma_i r) - \frac{Z}{4\pi r}\sum_{j=0}^{m} {}^{b}\gamma_j \, {}^{b}\lambda_j({}^{b}\gamma_j r - 2)\exp\left(-{}^{b}\gamma_j r\right) \quad \text{(S1)}$$

By rearranging (S1), we can write it in the form of Eq. (1) with the parameters

$$c_i = \begin{cases} {}^{a}\lambda_i\,, \text{ for } i = 0,1 \\ -2\,{}^{b}\gamma_j / {}^{b}\gamma_j\,, \text{for } j = 0,1\ldots m \text{ and } i = j+2 \end{cases} \quad \text{(S2)}$$

$$\lambda_i = \begin{cases} {}^{a}\gamma_i\,, \quad \text{for } i = 0,1 \\ {}^{b}\gamma_j\,, \text{for } j = 0,1\ldots m \text{ and } \; i = j+2 \end{cases} \quad \text{(S3)}$$

$$d_j = {}^{b}\lambda_i \text{ and } \gamma_j = {}^{b}\gamma_j \quad \text{for } j = 0,1..m \quad \text{(S4)}$$

For Na and K atoms, parameters c_i, λ_i, d_j and γ_j are given in Table S1.

Table S1. Parameters of atomic electron distributions

Atom	i, j	c_i	λ_i	d_j	γ_j
Na	0	1.1353	1.2009	-1.7781	2.013
	1	-0.1353	25.776	-3.576	11.463
	2	1.7667	2.013		
	3	0.6239	11.463		
K	0	1.4523	2.32	-5.045	5.439
	1	-0.4523	32.78	-10.448	20.656
	2	1.855	5.438	0.047	0.6328
	3	1.0116	20.656		
	4	-0.14855	0.6328		

When solving Eq. (2), the $\rho(x,y,z,t)$ and $\Phi(x,y,z,t)$ are represented in the form

$$\rho(x,y,z,t) = \int \frac{d\omega}{2\pi}\int \frac{d^2k}{(2\pi)^2}\rho_{\omega\mathbf{k}}(z)\exp(-i(\mathbf{k\rho} - \omega t)) \quad \text{(S5)}$$

$$\phi(x,y,z,t) = \int \frac{d\omega}{2\pi} \int \frac{d^2k}{(2\pi)^2} \phi_{\omega\mathbf{k}}(z) \exp(-i(\mathbf{k\rho} - \omega t)) \quad \text{(S6)}$$

where $\mathbf{k} = (k_x, k_y)$ and $\boldsymbol{\rho} = (x, y)$. Substituting (S5) and (S6) into Eq. (2) yields

$$\left(\frac{d^2}{dz^2} - k^2\right) \phi_{\omega\mathbf{k}}(z) = -4\pi\rho_{\omega\mathbf{k}}(z) \quad \text{(S7)}$$

Table S2 presents the fundamental frequencies of electronic transitions and oscillator strengths corresponding to Na and K atoms [31].

Table S2. Parameters of electronic transitions of Na and K atoms

Atom	f_i	ω_i, atomic units
Na	0.324	0.0772
	0.648	0.0772
	0.167	0.0206
	0.335	0.0206
K	0.347	0.059
	0.684	0.0593
	0.051	0.0366
	0.102	0.0366

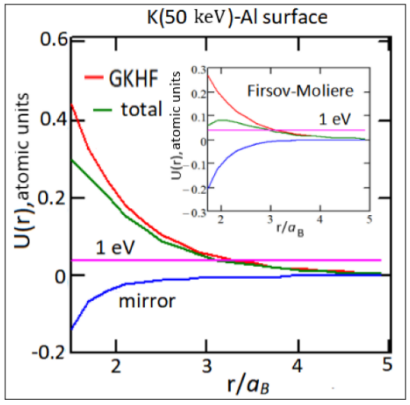

Fig. S1(a) (Color online) Interaction potential of a K atom with an aluminum surface. Designations are the same as in Fig. 2a.

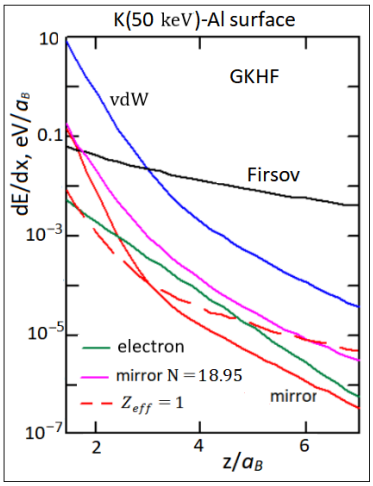

Fig. S1(b) (Color online) Stopping power of a K atom with an initial energy of 50 keV depending on the distance to the surface. Designations are the same as in Fig. 2b.

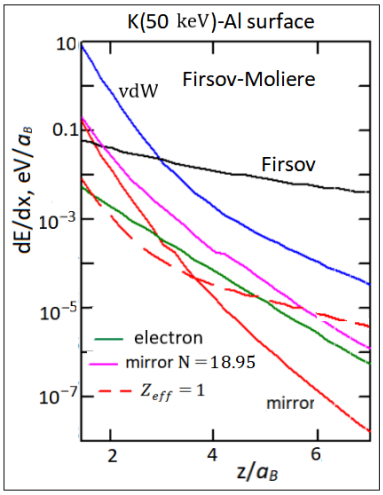

Fig. S2 (Color online) Same as in Fig. S1(b) in the Firsov-Moliere approximation.

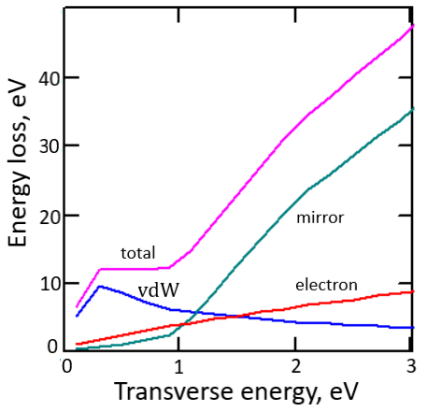

Fig. S3 (Color online) Resulting energy loss of a K atom upon reflection from an aluminum surface as a function of transverse energy.

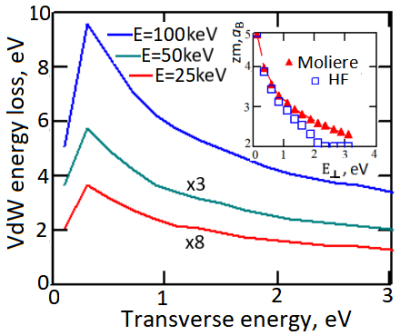

Fig. S4 (Color online) Dissipative van der Waals energy loss of a K atom. The data of the two bottom curves are magnified by 8 and 3 times.

The Firsov-Moliere approximation for the interatomic interaction potential $V_a(r)$ reads

$$V_a(r) = \frac{Z_1 Z_2}{r}\sum_i \alpha_i \exp(-\beta_i r/a_F)\,, a_F = 0.8853\left(\sqrt{Z_1}+\sqrt{Z_2}\right)^{-2/3} \quad \text{(S8)}$$

where $\alpha_i = (0.1, 0.55, 0.35)$ and $\beta_i = (6, 1.2, 0.3)$. Averaging (S8) according to Eq. (13) yields

$$U_a(z) = 2\pi n Z_1 Z_2 a_F^2 \sum_i \frac{\alpha_i}{\beta_i^2}\exp(-\beta_i z/a_F) \quad \text{(S9)}$$

According to original Firsov's result [2], based on Eq. (20), the result of the integration reads

$$\Delta E(b,v) = \frac{0.35(Z_1+Z_2)^{5/3}v}{\left(1+0.16\sqrt[3]{Z_1+Z_2}\,b\right)^5} \quad \text{(S10)}$$

where b is the impact parameter. When an atom is moving above the surface, $b = \sqrt{z^2+\rho^2}$ (see Fig. 1). Then, unlike Eq. (23), the electronic energy loss per unit path length is given by

$$\frac{dE}{dx} = F_x(z) = 2nv\int_z^\infty d\rho\rho \arccos\left(z/\sqrt{z^2+\rho^2}\right)\Delta E\left(\sqrt{z^2+\rho^2}\right). \quad \text{(S11)}$$

where n is the atomic volume density of the target. Assuming that $\arccos\left(z/\sqrt{z^2+\rho^2}\right) \approx 1$ and performing the integration in (S11) yields

$$\frac{dE}{dx} \approx 2.28n(Z_1+Z_2)\frac{\left(1+0.64\sqrt[3]{Z_1+Z_2}\,z\right)}{\left(1+0.16\sqrt[3]{Z_1+Z_2}\,z\right)^4} \quad \text{(S12)}$$

Formula (S12) has been used when calculating the curves "Firsov" in Figs. (2b) and (S1). Moreover, in the case of the Firsov-Moliere approximation, formulas (8)–(10) in the main text can be used with the substitutions $c_i \to \alpha_i$, $\lambda_i \to \beta_i/a_F$, $d_j \equiv 0$.

[1] R. Bonham, T.G. Strand, "Analytical expressions for the Hartree—Fock potential of neutral atoms and for the corresponding scattering factors for X rays and electrons", J. Chem. Phys. **39**, 2200 (1963).

[2] O. B. Firsov, "Calculation of the interaction potential of atoms", Soviet Phys. JETP **6**(3), 534 (1958).