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Investigation of the negative ionization of hydrogen particles on metal surfaces with low work function

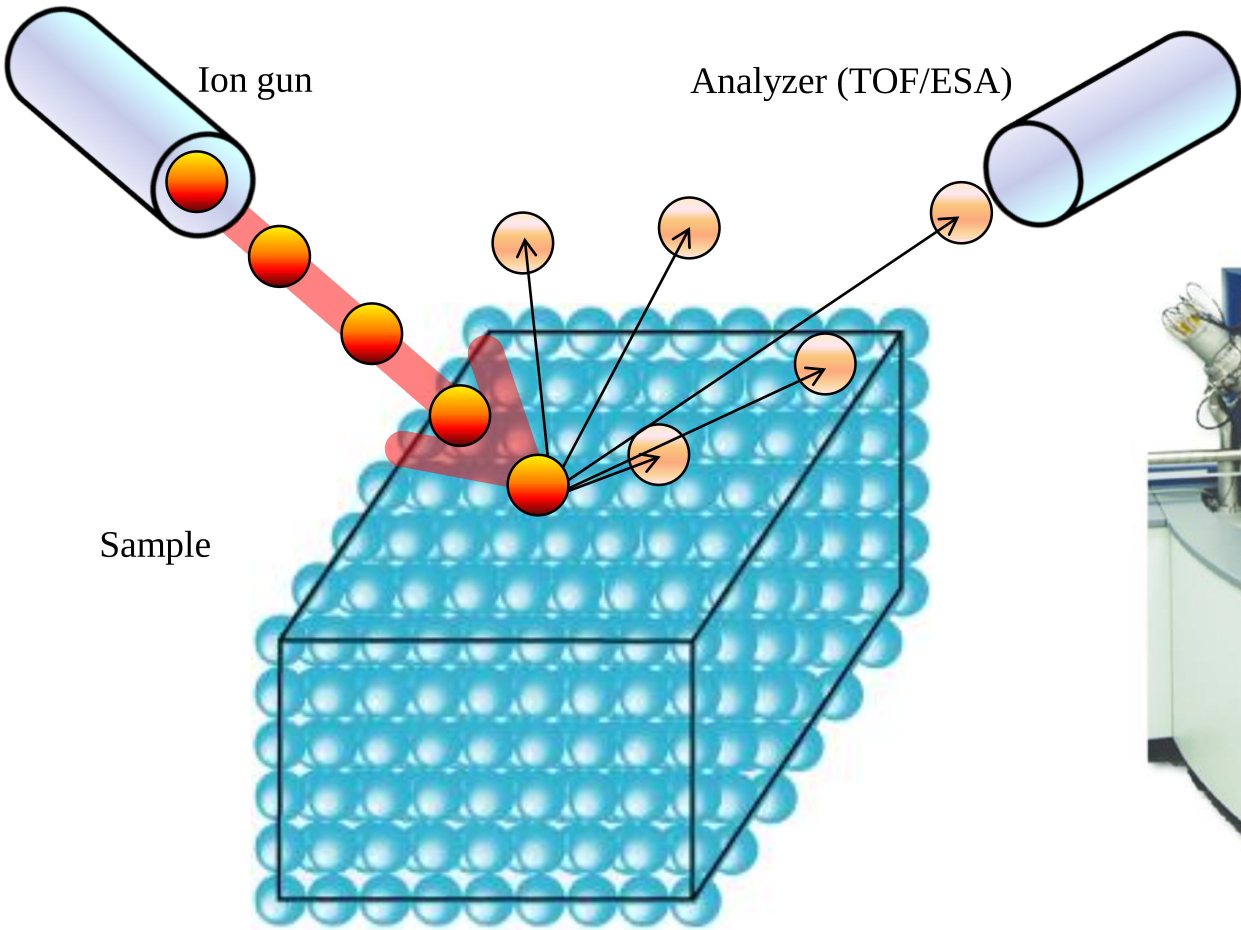
Outline

- Introduction
- Physical model and numerical method
- Results and discussion
- Conclusion

Atomic units $$m_e = e = \hbar = 1$$

l – 0.53 Å; E – 27.211 eV; t – $2.419 \cdot 10^{-17}$ s; v – $2.188 \cdot 10^{8}$ sm/s

Low energy ion scattering (LEIS)



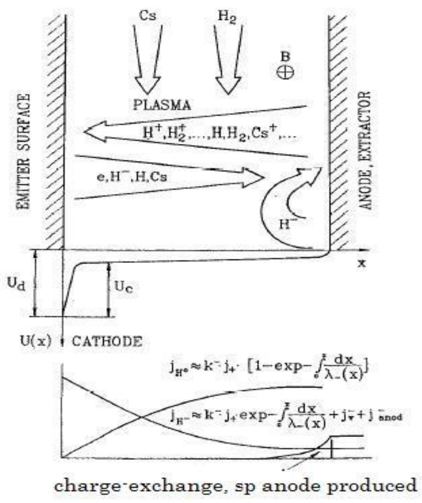
Sketch of LEIS experiment

Photo of «TOF.SIMS 5 and Qtac 100» setup, used in LEIS experiments

LEIS is powerful technique for negative ionization investigation

Muons, Inc.

General diagram of the Surface-Plasma Generation of negative ions in a gas discharge



Surface plasma generation of H^- on the anode often is the dominant process of H^- formation in discharges without Cs, as well as with Cs.

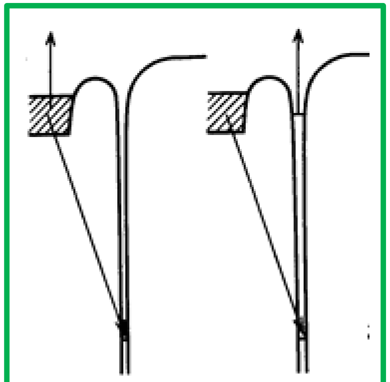
Accumulation of elements with low ionization potential on the emission surface is important. The negative potential of this surface helps this accumulation

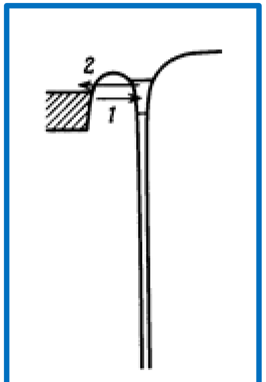
As negative ions pass through the plasma and gas to the anode, the weakly bound electrons are easily removed creating accelerated neutral atoms. The majority of accelerated negative ions will **survive** to reach the beam forming region **only if the layer of plasma** and gas between the emitter and the beam forming system **is very thin**.

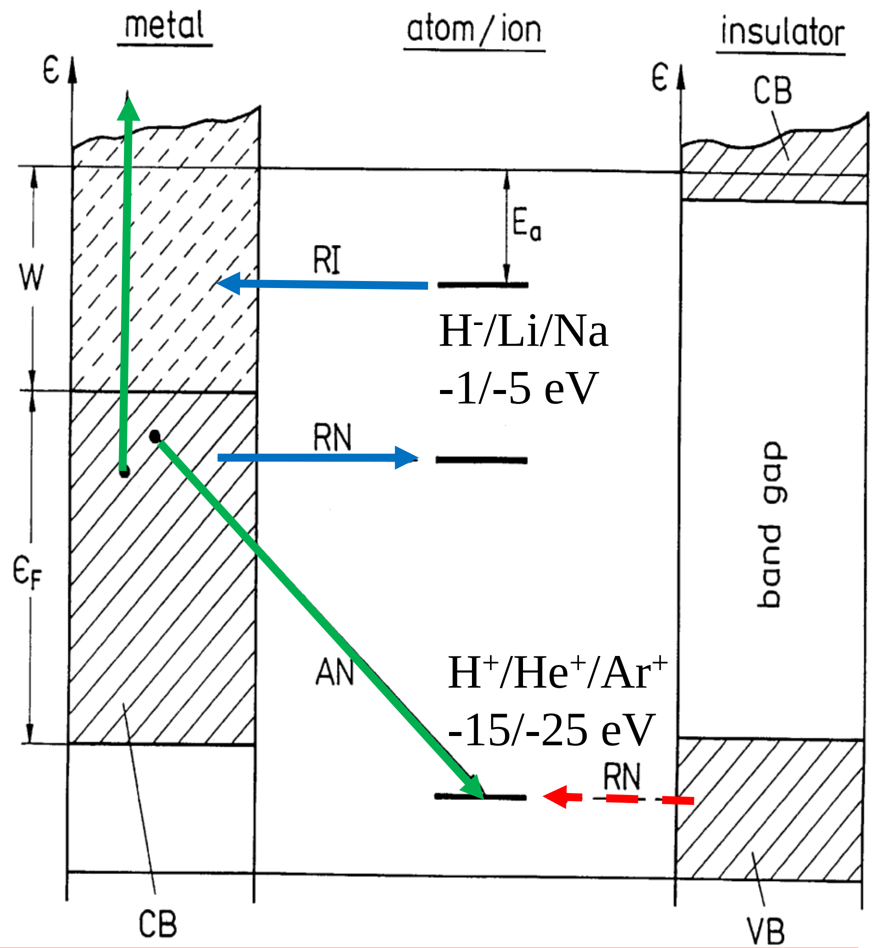
Charge exchange processes

Velocity	Process
0-1 a. u.	Collision-induced charge transfer
2-4 a. u.	Auger-processes
5-10 a. u.	Resonant charge transfer (RCT)

z







RCT is the main charge exchange channel for the metallic surfaces

H. Winter, Phys. Rep. 367 (2002), 387.
H. H. Brongersma et al. Surf. Sci. Rep. 62 63 (2007)

Basic approaches to RCT calculation

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$$i\frac{\partial \Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N,t)}{\partial t} = \hat{H}(\mathbf{r}_1,\ldots,\mathbf{r}_N,t)\Psi(\mathbf{r}_1,\ldots,\mathbf{r}_N,t)$$

- Anderson-Newns model

$$\hat{\mathrm{H}}\left(z(t)\right)=\sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}n_k+\varepsilon_a\left(z(t)\right)n_a+\sum_{\mathbf{k}}\left(\mathrm{V}_{\mathbf{k}}\left(z(t)\right)\mathrm{c}_k^{+}\mathrm{c}_a+\mathrm{V}_{\mathbf{k}}^{*}\left(z(t)\right)\mathrm{c}_a^{+}\mathrm{c}_k\right)$$

- Rate equation (adiabatic approximation)

$$\frac{dP}{dt}=-\Gamma_{loss}\cdot P+\Gamma_{capture}\cdot(1-P)$$

- Wave-packet propagation method

$$i\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=\left[-\frac{\Delta}{2}+V_{e-ion}(\mathbf{r})+V_{e-surf}(\mathbf{r})\right]\Psi(\mathbf{r},t)$$

Rate equation is suitable for low ion energies

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Parallel velocity effect

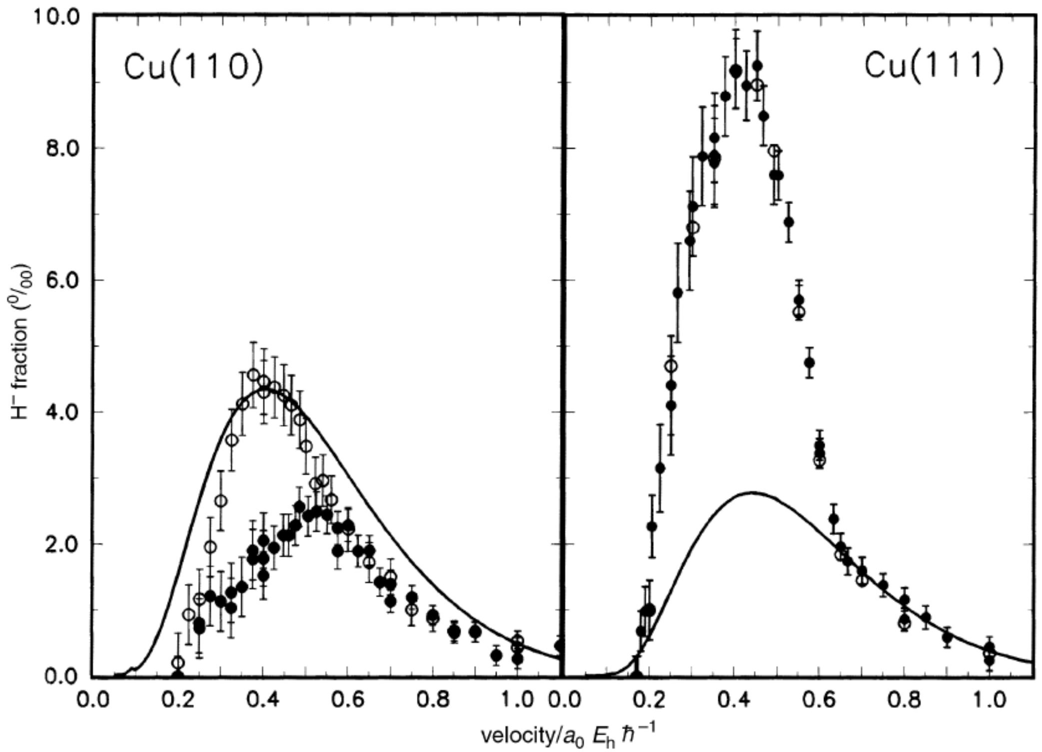
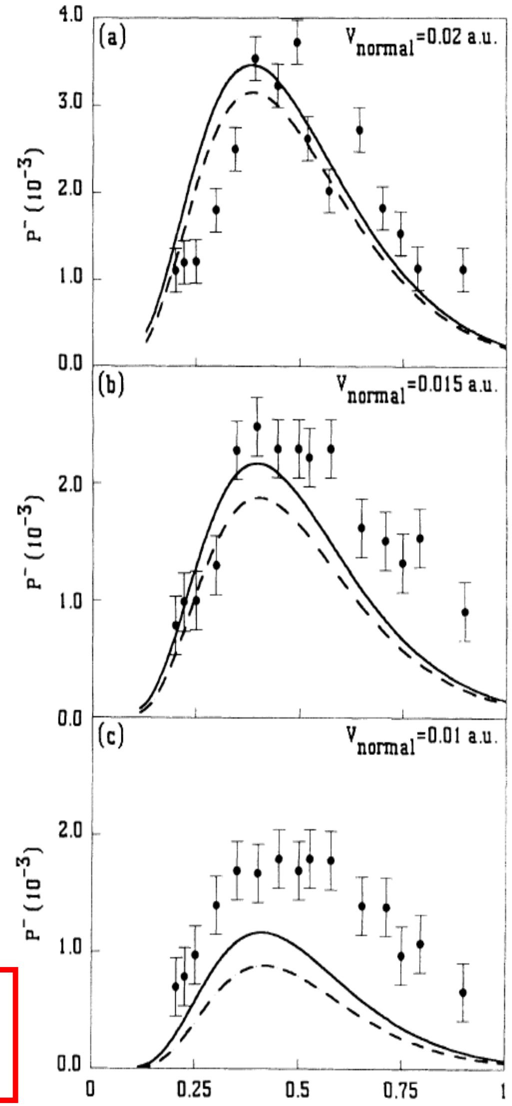


Fig. 5 Left panel: H^- fraction as function of parallel velocity for scattering from Cu(110) surface with a normal velocity component of 0.02 $a_0 E_h \hbar^{-1}$. Calculations within the jellium model, (●) and (○) experimental data for azimuthal settings close to ⟨001⟩ and ⟨1$\bar{1}$0⟩ directions, respectively. Right panel: Same as left panel, but for Cu(111) surface. (——) Calculations within the jellium model, (●) and (○) experimental data for azimuthal settings close to ⟨1$\bar{1}$0⟩ and ⟨1$\bar{2}$1⟩ directions, respectively.



Due to the parallel velocity effect P^- increases by order of magnitude

T. Hetch, H. Winter, A.G. Borisov, J.P. Gauyacq and A.K. Kazansky, Faraday Discuss. 117, 27 (2000).

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Rate equation for calculation of negative ionization probability

$$\frac{dP^-}{dt} = -\Gamma_{loss}(z)\cdot P^- + \Gamma_{capture}(z)\cdot(1-P^-)$$

$$\Gamma_{loss}(z) = g_{loss}\cdot\Gamma(z)\cdot F_{loss}$$

$$\Gamma_{capture}(z) = g_{capture}\cdot\Gamma(z)\cdot F_{capture}$$

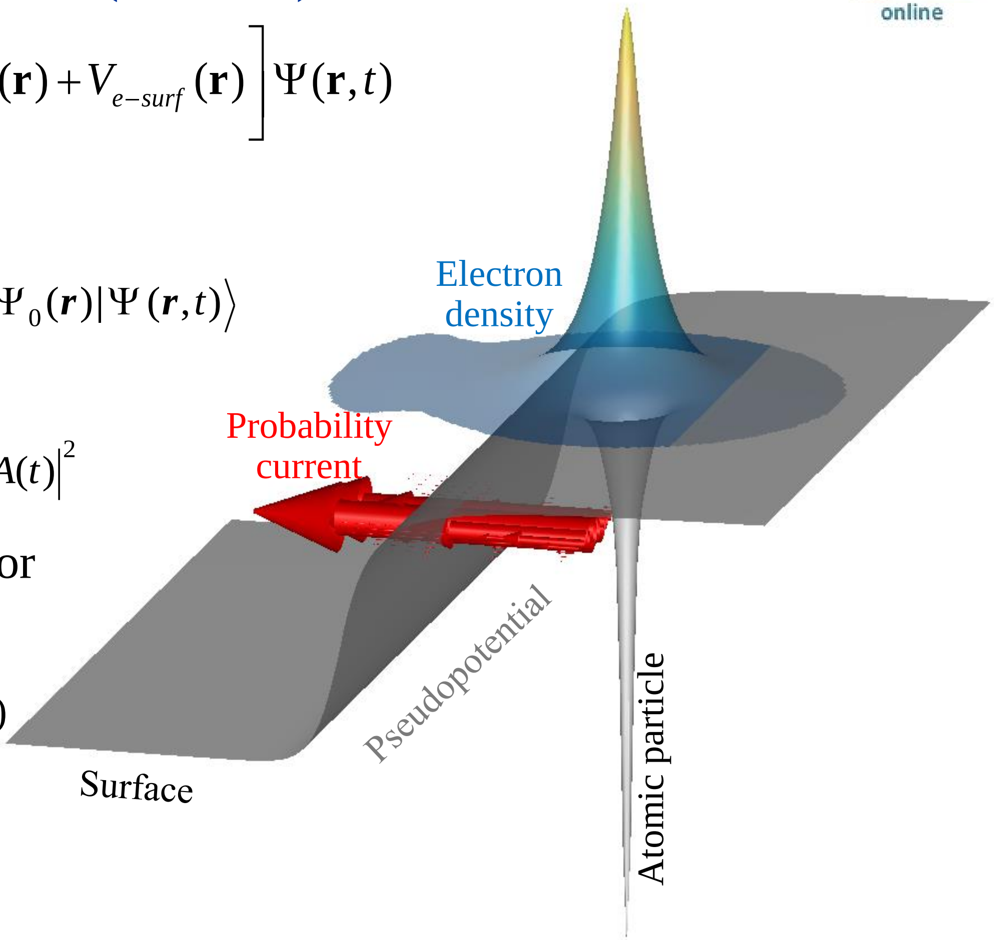
Ermoshin V. A., Kazansky A. K.
Phys. Lett. A. 218 99 (1996)

Wave-packet propagation (WPP) method

$$i\frac{\partial \Psi(\mathbf{r},t)}{\partial t} = \left[-\frac{\Delta}{2} + V_{e-ion}(\mathbf{r}) + V_{e-surf}(\mathbf{r})\right]\Psi(\mathbf{r},t)$$

- Wave function evolution $\Psi(\boldsymbol{r},t)$
- Autocorrelation function $A(t) = \langle \Psi_0(\boldsymbol{r}) | \Psi(\boldsymbol{r},t) \rangle$
- Atomic particle occupation for the "dynamical" problem $P(t) = |A(t)|^2$
- Atomic energy level and level width for the "static" problem

$$A(t) = \langle \psi_0(\boldsymbol{r}) | \psi(\boldsymbol{r},t) \rangle \approx \exp(-i\,E\cdot t)\cdot\exp(-\Gamma\cdot t)$$



WPP method allows to calculate ion level width $\Gamma(z)$ and electron density distribution

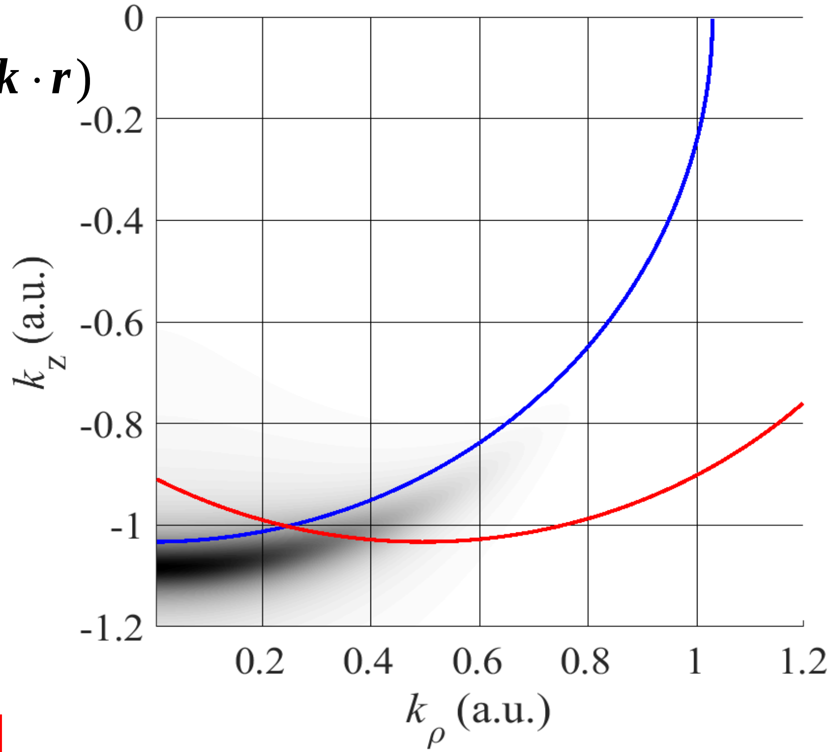
Ermoshin V. A., Kazansky A. K.
Phys. Lett. A. 218 99 (1996)

Calculation of electron loss and capture weights

$$f(\mathbf{k},\, t) = \frac{1}{(2\pi)^{3/2}} \cdot \int\limits_{z<0} d\mathbf{r}^3 \cdot \psi(\mathbf{r}, t) \cdot \exp(-i\mathbf{k}\cdot\mathbf{r})$$

$$F_{loss} = \int\limits_{|\mathbf{k}|>k_f} d\mathbf{k}^3 \cdot |f(\mathbf{k})|^2$$

$$F_{capture} = \int\limits_{|\mathbf{k}|<k_f} d\mathbf{k}^3 \cdot |f(\mathbf{k})|^2$$



Our approach accounts parallel component of ion velocity

Illustration of electron loss and capture weights calculation. The shaded area figure shows electron distribution f(k) in k-space for the H- active electron. The blue solid line corresponds to the Fermi sphere for W(110) in the static case; the red solid line to the Fermi sphere for vpar = 0.5 a.u.

Approach for the affinity level

$$E_a(z) = \left(1 - g(z)\right)\left(E_a(\infty) - 1/4z\right) + f(z)E_0$$

$$g(z) = 1/\left(1 + \exp\left(\alpha(z - \beta)\right)\right)$$

$$E_a(z) = E(\infty) - 1/4z$$

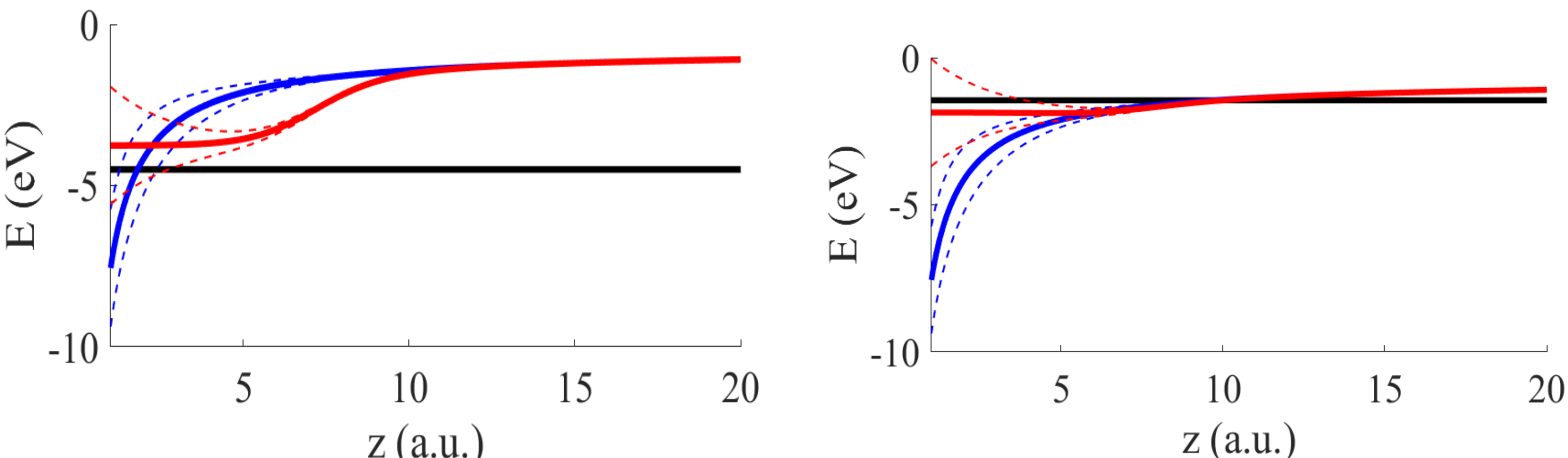


Illustration of the affinity level Ea(z) and level broadening. The blue solid line shows H- affinity level, which is calculated by means of classical image potential. The red solid line shows the form of H- affinity level dependence on ion-surface distance, which is used in this article. Black straight line shows the Fermi level of the metal. Thin dashed lines depict the level broadening near the surface. Left panel - Ef = -4.5 eV and E0 = -3.75 eV, right panel - Ef = -1.45 eV and E0 = -1.85 eV

1) The only approximation parameter E_0.

2) No critical dependence on initial distance z_0.

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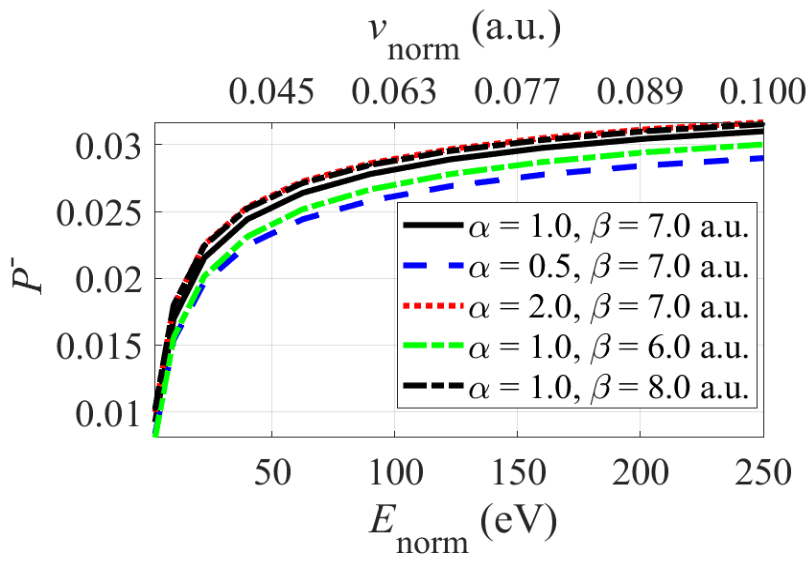
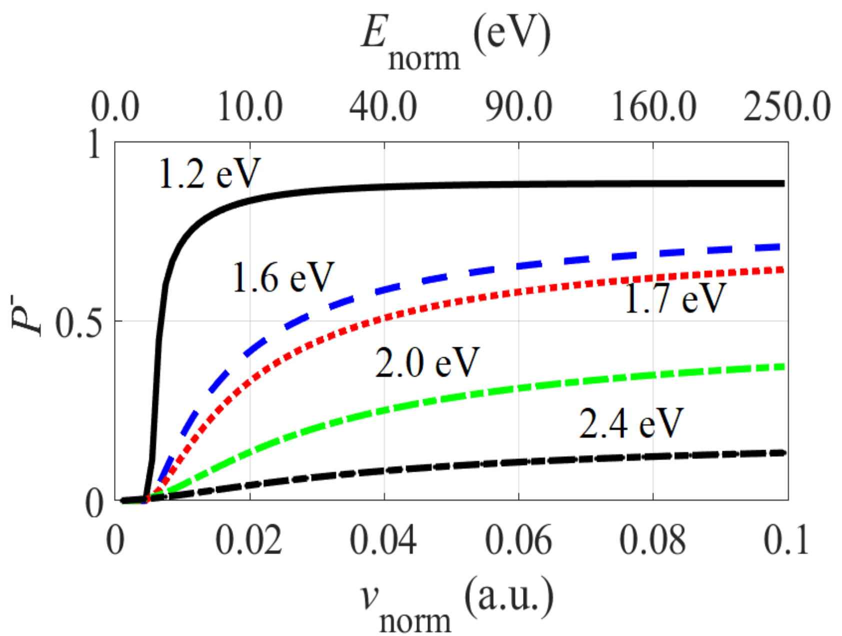
Main factors, influencing the P^-



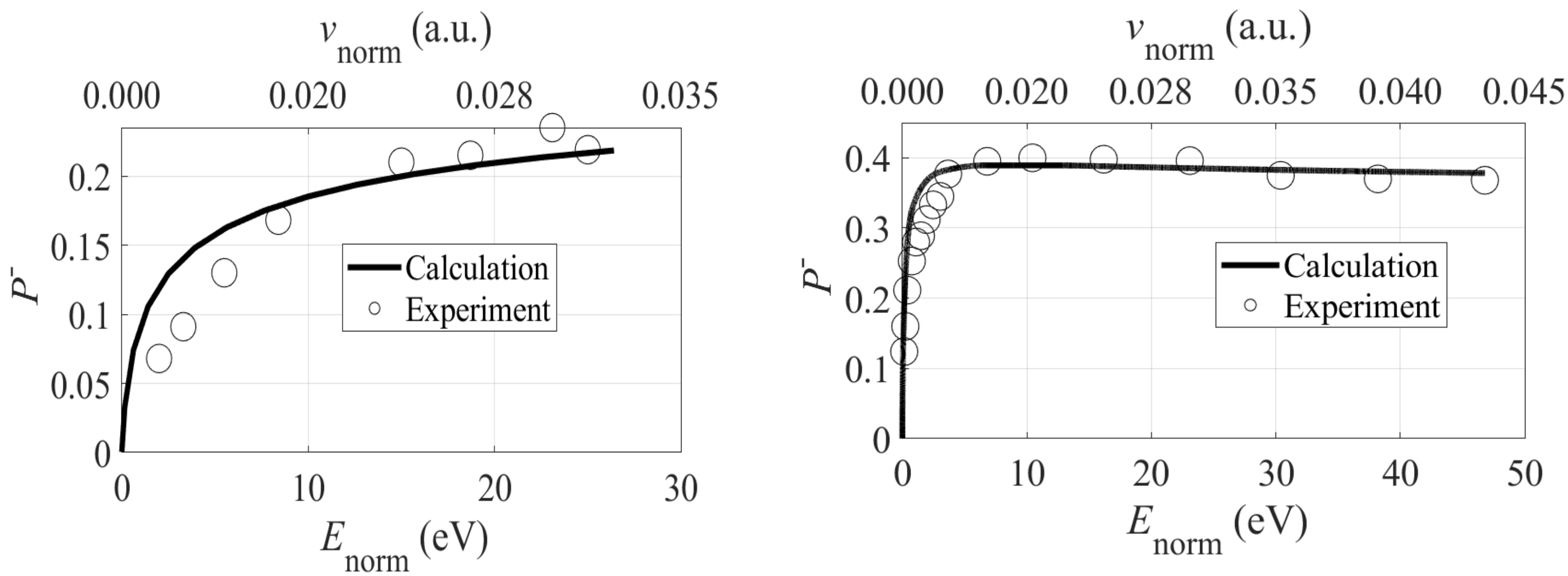
Negative ionization probability on W(110) converter surface (φ=5.21 eV). Figure shows the negative ionization probability of hydrogen as function of normal exit energy/velocity for different parameters (see legend).



Influence of surface work function on negative ionization probability. Figure shows the negative ionization probability of hydrogen as function of initial normal exit energy/velocity for different work functions.

Negative ionization probability mainly depends on surface work function and ion velocity

Comparison to experiment

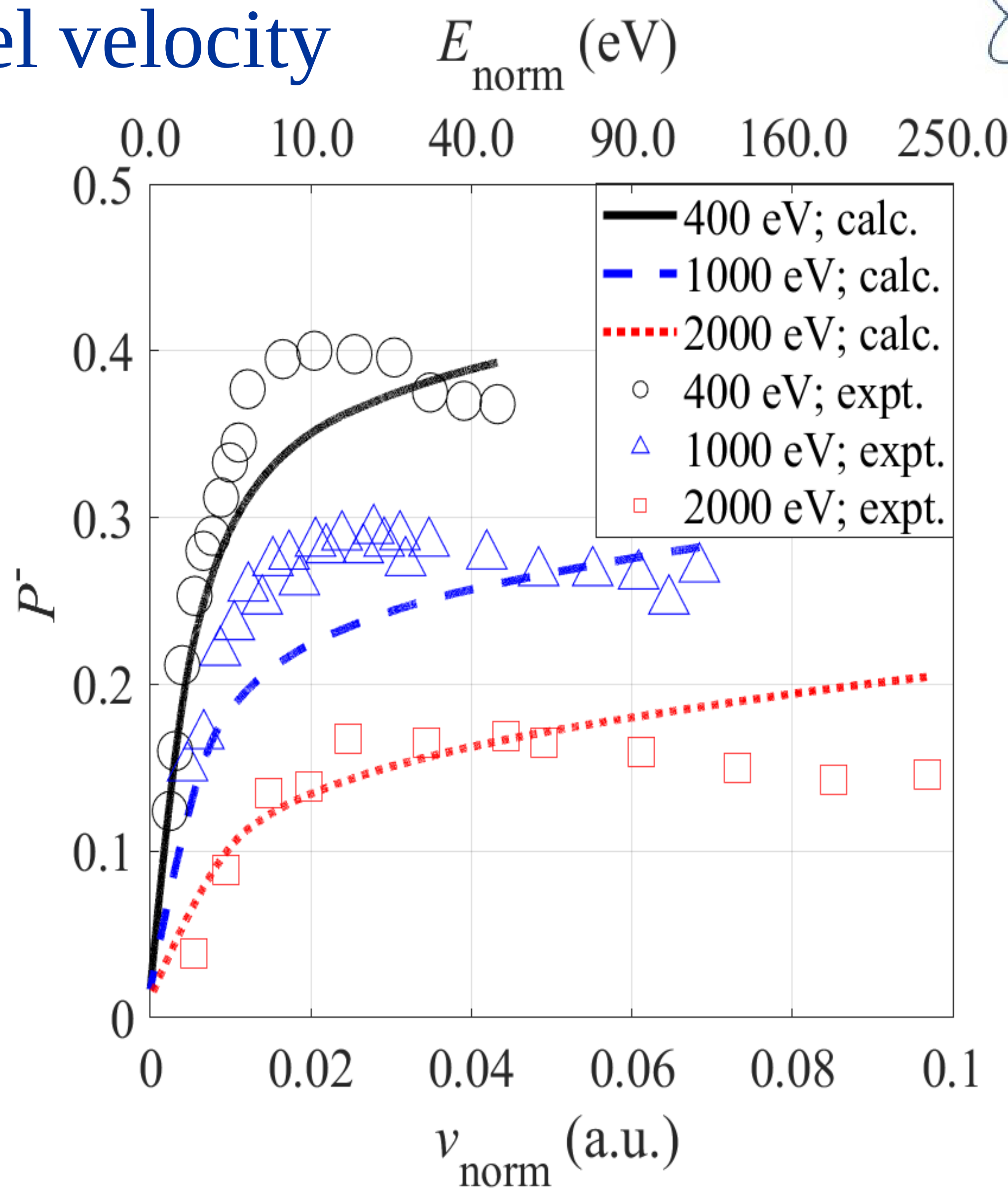


Negative ionization probability of hydrogen on different converter surfaces as function of exit normal energy/velocity. The calculations were done according to the model, presented in Section 2. Left side – for the cesiated Mo (φ=1.5 eV) [Newns D.M., Makoshi K., Brako R. and van Wunnik J. N. M. 1983 Physica Scripta 1983 5]; right side – for cesiated W(110) (φ=1.45 eV) [Van Wunnik J. N. M., Gerrlings J. J. C. and Los J. 1983 Surface Science 131 1].

Presented approach reasonably well describes experimental data

Influence of parallel velocity

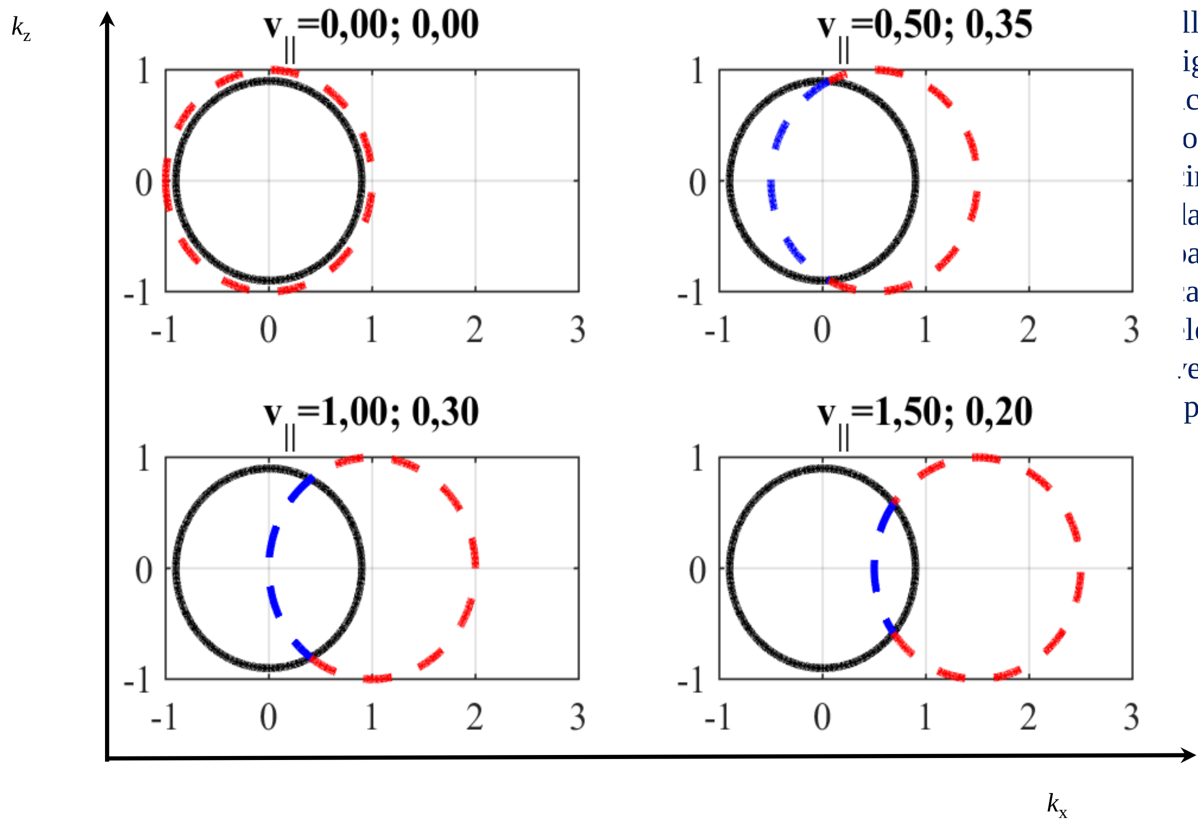
Negative ionization probability of hydrogen on cesiated W(110) converter surface (φ=1.45 eV) as function of exit normal velocity/energy for different ion beam energies (see legend). The experimental data is taken from ref. [Van Wunnik J. N. M., Geerlings J. J. C. and Los J. 1983 Surface Science 131 1]. The incident angle of primary H+ beam is 100 from the surface, the exit angle is varying in the range 0-200.



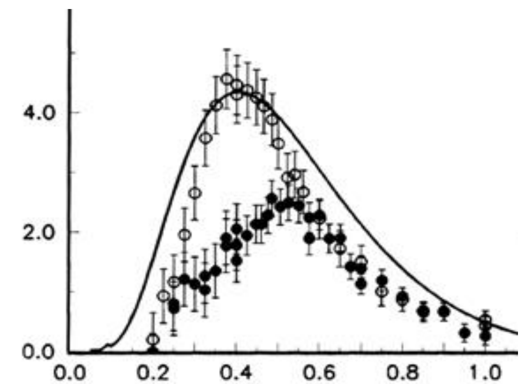
Presented model accounts parallel velocity component

$v_{par} = 0.14 – 0.25$ a.u.

Influence of parallel velocity

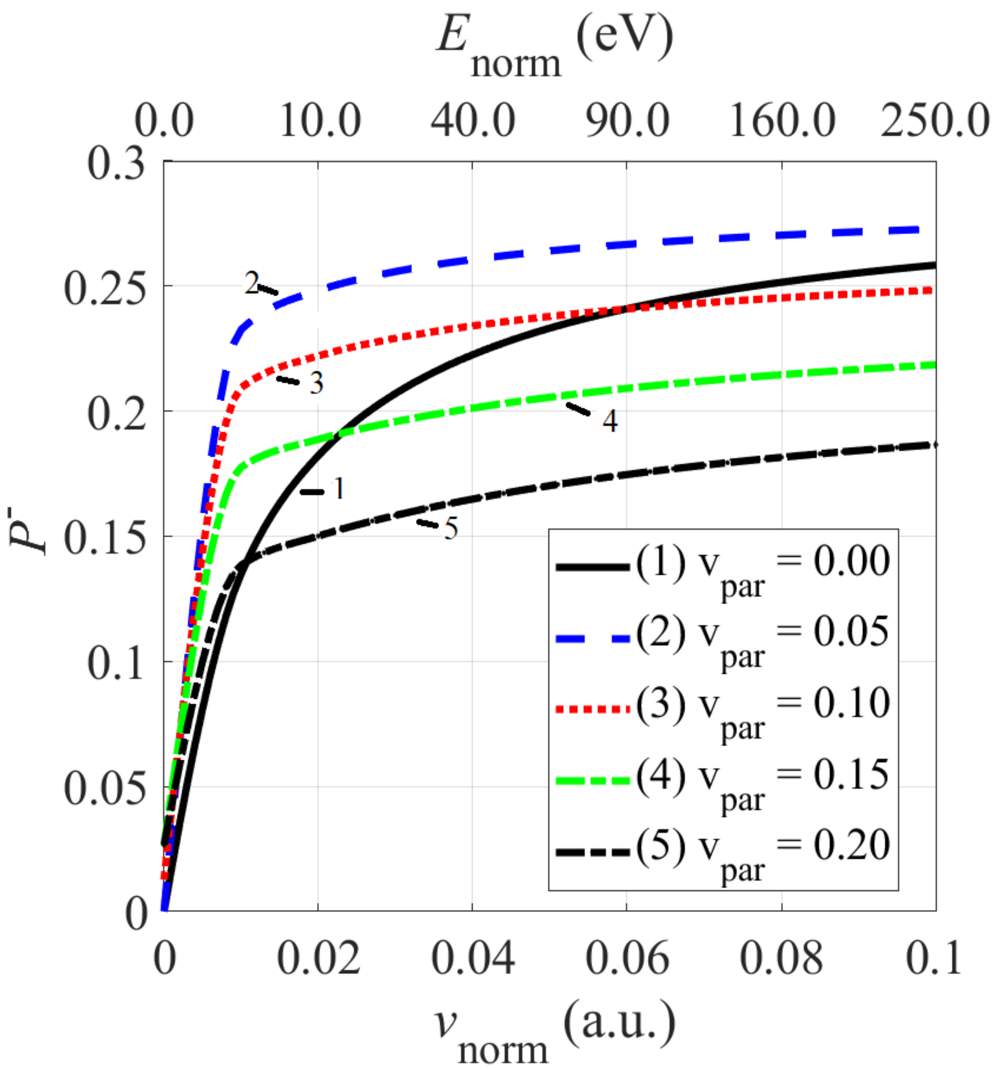


llustration of shifted Fermi spheres model. The igure shows intersection between sphere of ctive electron and Fermi sphere of the metal or different parallel velocities. Black solid ircle – Fermi sphere of the metal. Color lashed circle – sphere of active electron; blue art (inside Fermi sphere) denotes the electron apture, red part (outside Fermi sphere) – lectron loss. The legend shows the parallel elocity value and intersection between the pheres.



Shifted Fermi spheres model explains the parallel velocity effect

Estimation of $P^{-}(v_{par})$



Negative ionization probability of hydrogen on cesiated Mo converter surface (φ=1.5 eV) as function of exit normal velocity/energy, calculated for different parallel velocities (see legend).

The parallel velocity effect can enhance the negative ionization probability up to ~33%

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Conclusions

- Theoretical model has been presented for the negative ionization probability calculation:
  - Only one approximation parameter - E_0.
  - No critical dependence on z_0.
  - Accounts parallel component of ion velocity.
- The presented model gives quantitative correspondence to wide range of experimental data.
- Numerical estimations show, that the negative ionization probability of hydrogen can be enhanced up to ~33% due to the parallel velocity effect.

Thank you for your attention