Excitation of atomic hydrogen at metal surfaces promoted by proton motion

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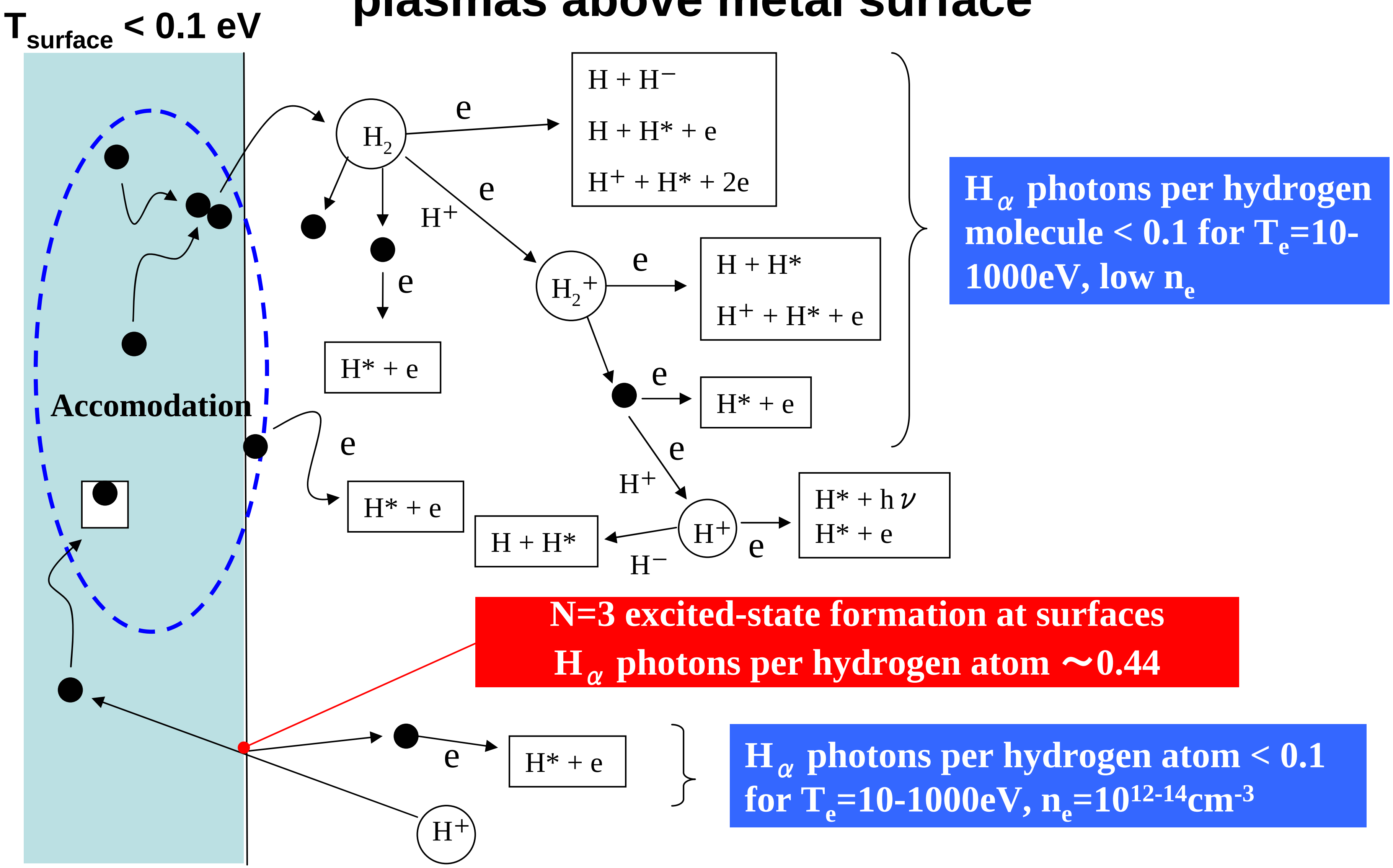
NIFS

OUTLINE

- Behavior of excited states in neutral H atoms reflected at metal surfaces in edge plasmas.
- Excited state abundance investigated in 1D model calculations.
- Mechanisms of the excited state formation.
- Conclusion

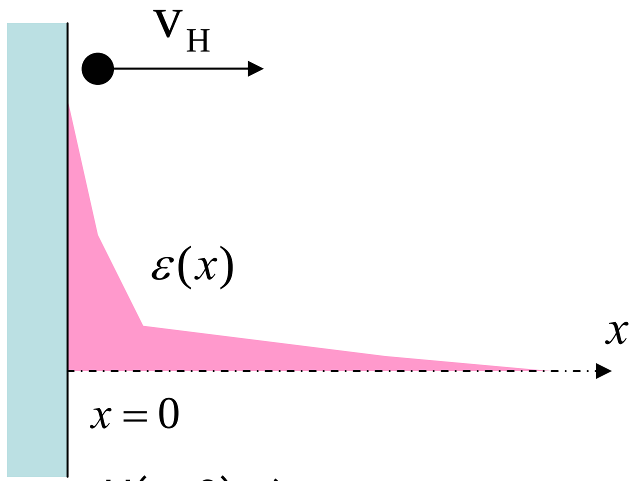
Excited state formation and H_α emission in low density plasmas above metal surface



Radiation of excited state formed at surface

Emission coefficient and line integrated intensity

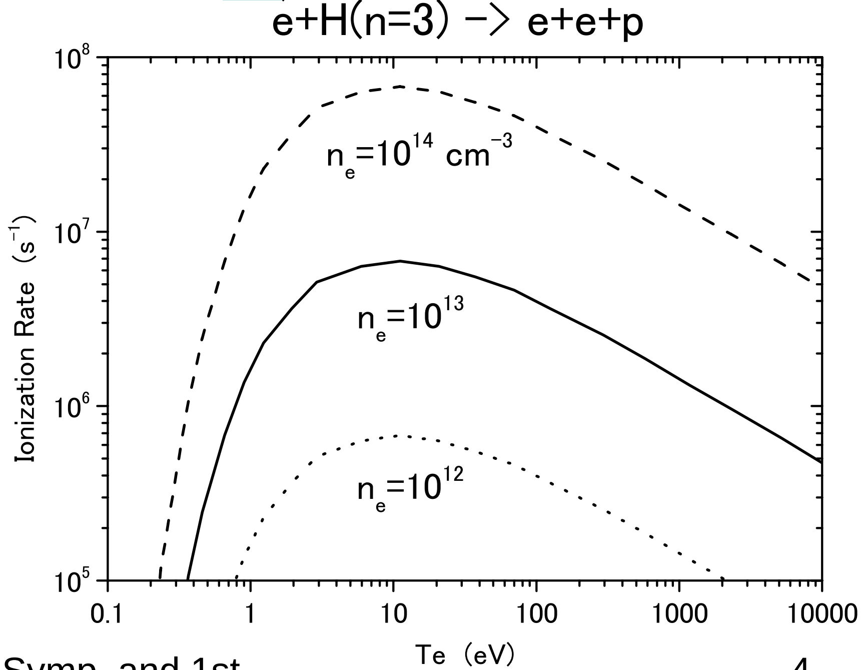
$$\varepsilon^{s}(x)=\frac{1}{4\pi}\,\overline{n}_{H}^{*s}(x)A_{i\to k}=\frac{A_{i\to k}}{4\pi}\,\overline{n}_{H}^{*s}(0)\exp\left[-\frac{\sum_{k}A_{i\to k}}{v_{H}}x\right]$$



$$I^{s}=h\nu\int_{0}^{\infty}\varepsilon^{s}(x)dx=\frac{h\nu}{4\pi}\Gamma\Phi_{H}^{*s}(0)$$

$$\Phi_{H}^{*s}(0)=v_{H}\overline{n}_{H}^{*s}(0)$$

$$\Phi_{H}^{*s}(\infty)=0$$

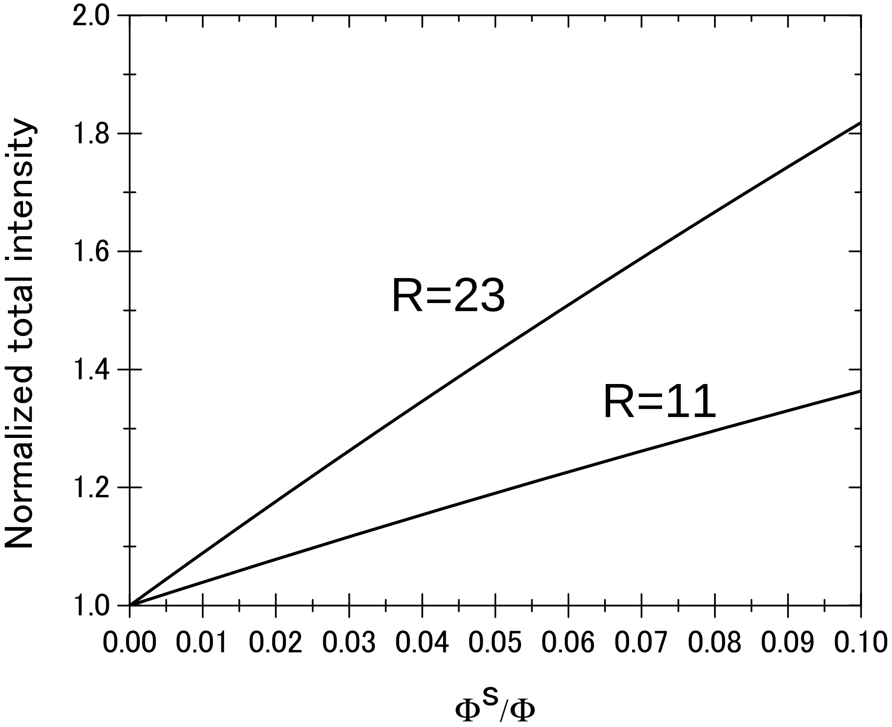


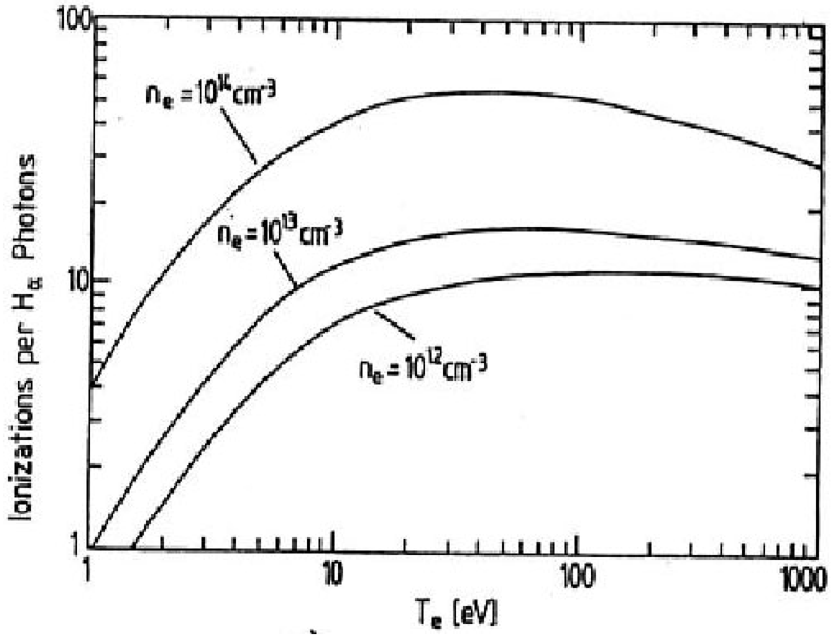
Depopulation of excited states by collision is unimportant for low density.

Charge exchange with impurity ions might affect the depopulation significantly.

H_α intensity may change significantly, while total flux is unchanged

(assuming all of excited H atoms created at surfaces decay by photon emission)

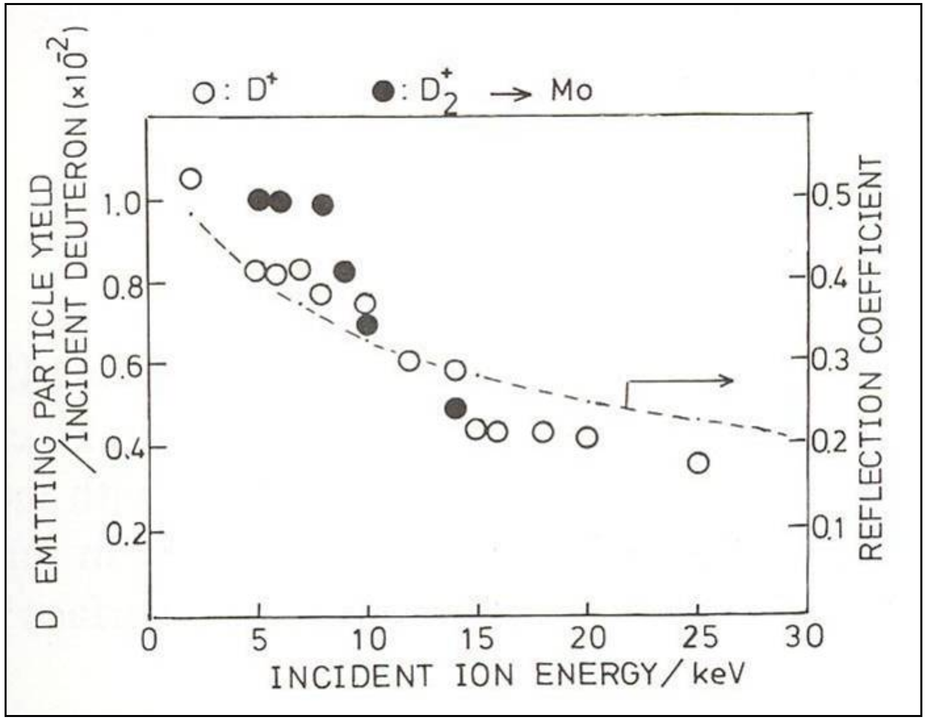




Plot of $R = \dfrac{\int_0^\infty \bar{n}_\mathrm{H} C_\mathrm{ion} dx}{\Gamma \int_0^\infty \bar{n}_\mathrm{H} C_\mathrm{exc} dx}$

$(\Gamma \approx 0.44 : \mathrm{branchingration\ for\ H}_\alpha)$

D $_{\alpha}$ (656.1 nm) emission from neutrals of a deuteron beam reflected at Mo surfaces



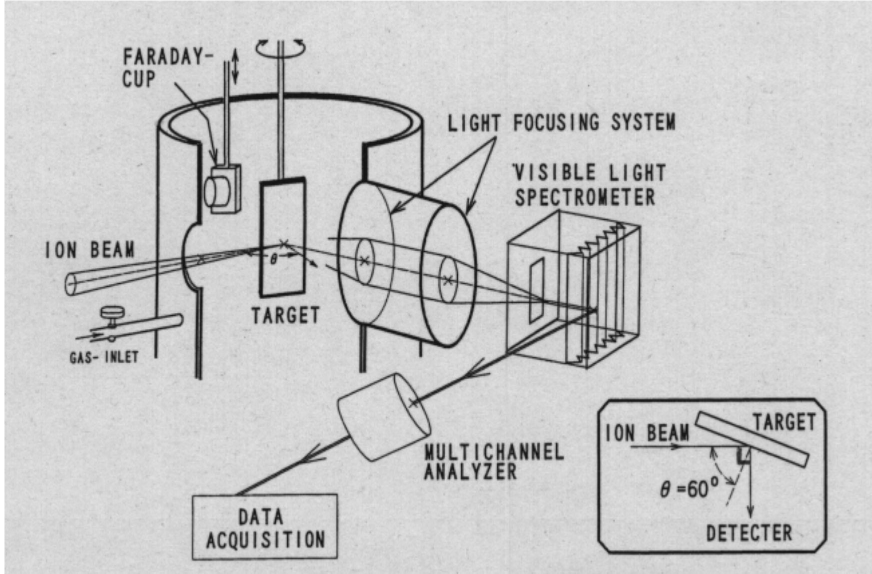


Fig. 1. Schematic diagram of the experimental apparatus.

T. Tanabe et al.; J. Nucl. Mater. 220-222 (1995) 841.

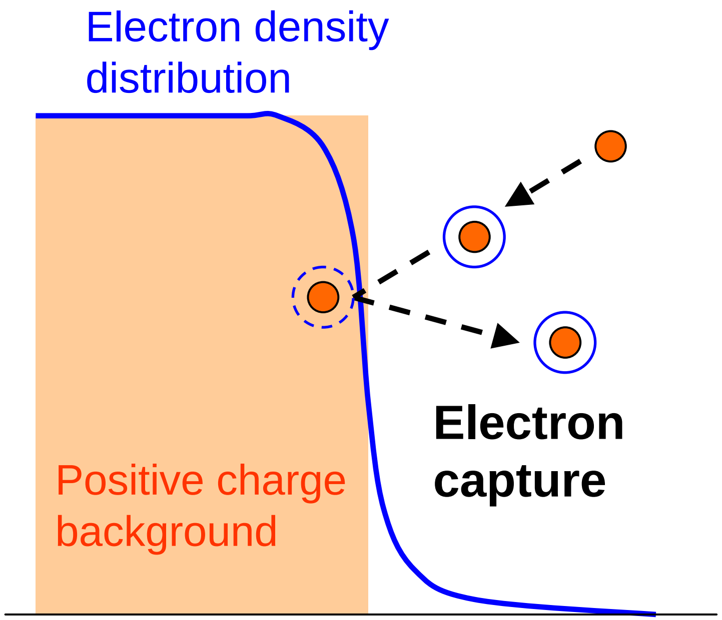
D $_{\alpha}$ emission intensity is nearly proportional to reflection coefficient of Mo for E > 1 keV.

About 2 % of reflected particles emit D $_{\alpha}$ photons. -> about 4 % of reflected particles in N=3 state.

Excited hydrogen atoms are not stable in metals

High electron density $\approx 10^{22-23} cm^{-3}$

Short screening distance in Thomas-Fermi approximation
$\approx 0.64\sqrt{r_s} < 1$Å



Excited states are formed by electron capture above the surface.

The semi-classical theory for single electron capture by an receding proton from metal slab

Electronic transition is treated by quantum mechanics

Ion motion is represented by classical trajectories

De Broglie wavelength of ion << extent of electron wavefunction

(= proton kinetic energy $\geq$ 1eV)

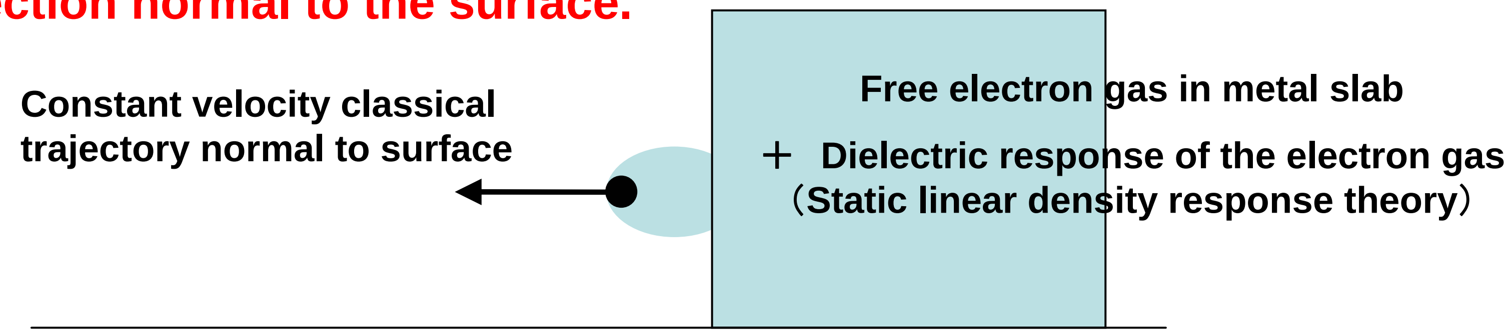
Ion kinetic energy >> Electronic transition energy

For electrostatic dielectric response of solids,

Ion velocity $\leq 10^{-8}$ cm × plasma frequency (10^{16} s^{-1} for $n_e=10^{23}$ cm^{-3})

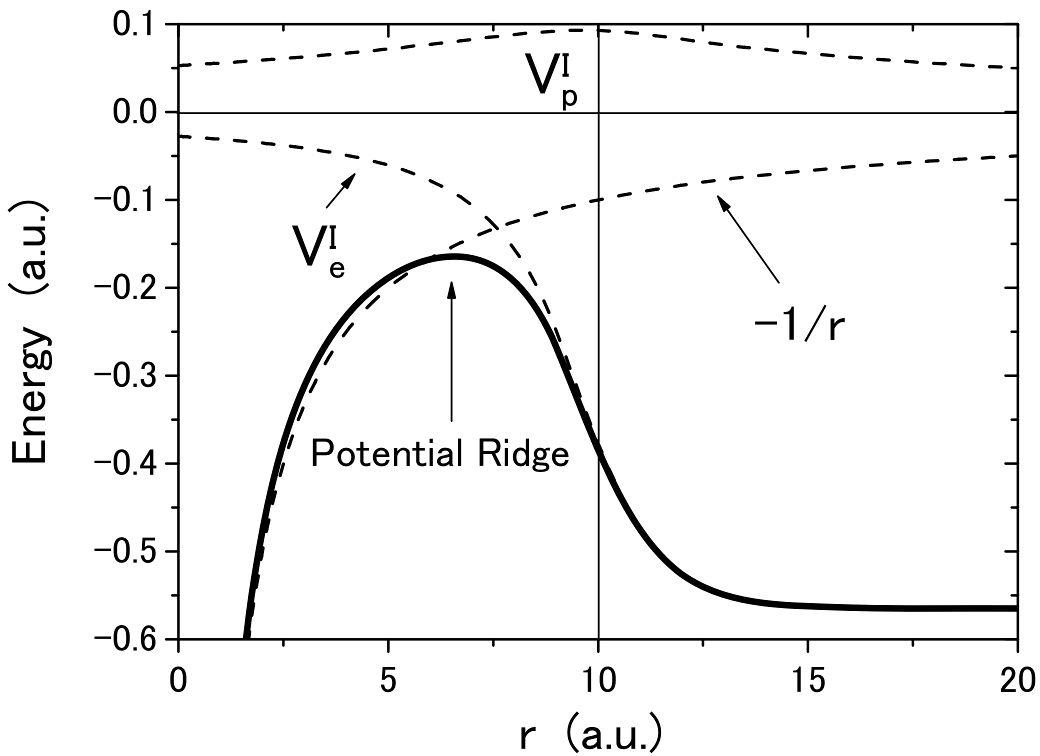
(= proton kinetic energy $\leq$ 25 keV)

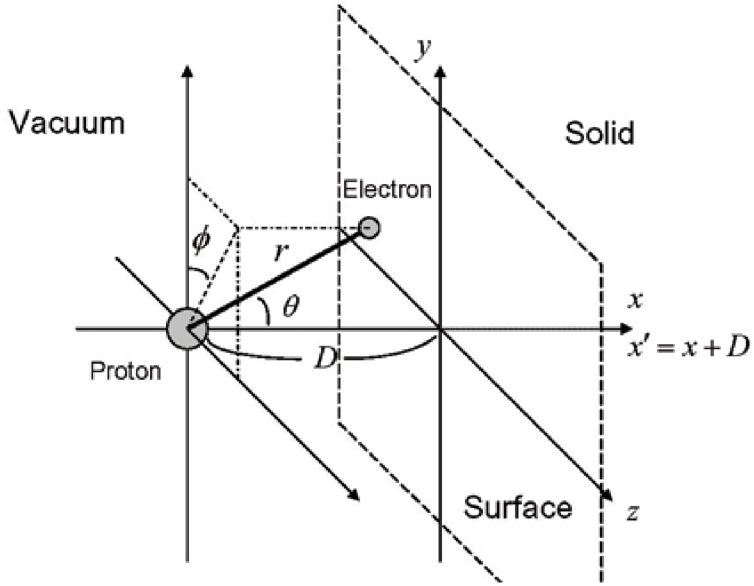
1D model: degrees of freedom of electron motion are restricted to the direction normal to the surface.



Effective interaction potential of electron + proton + metal surface

- Coulomb attractive potential of proton: -1/r,
- Attractive potential of the surface dipole layer and the exchange-correlation effect: V_e^I,
- Repulsive potential of a pile of electron density at the surface induced by proton: V_p^I.

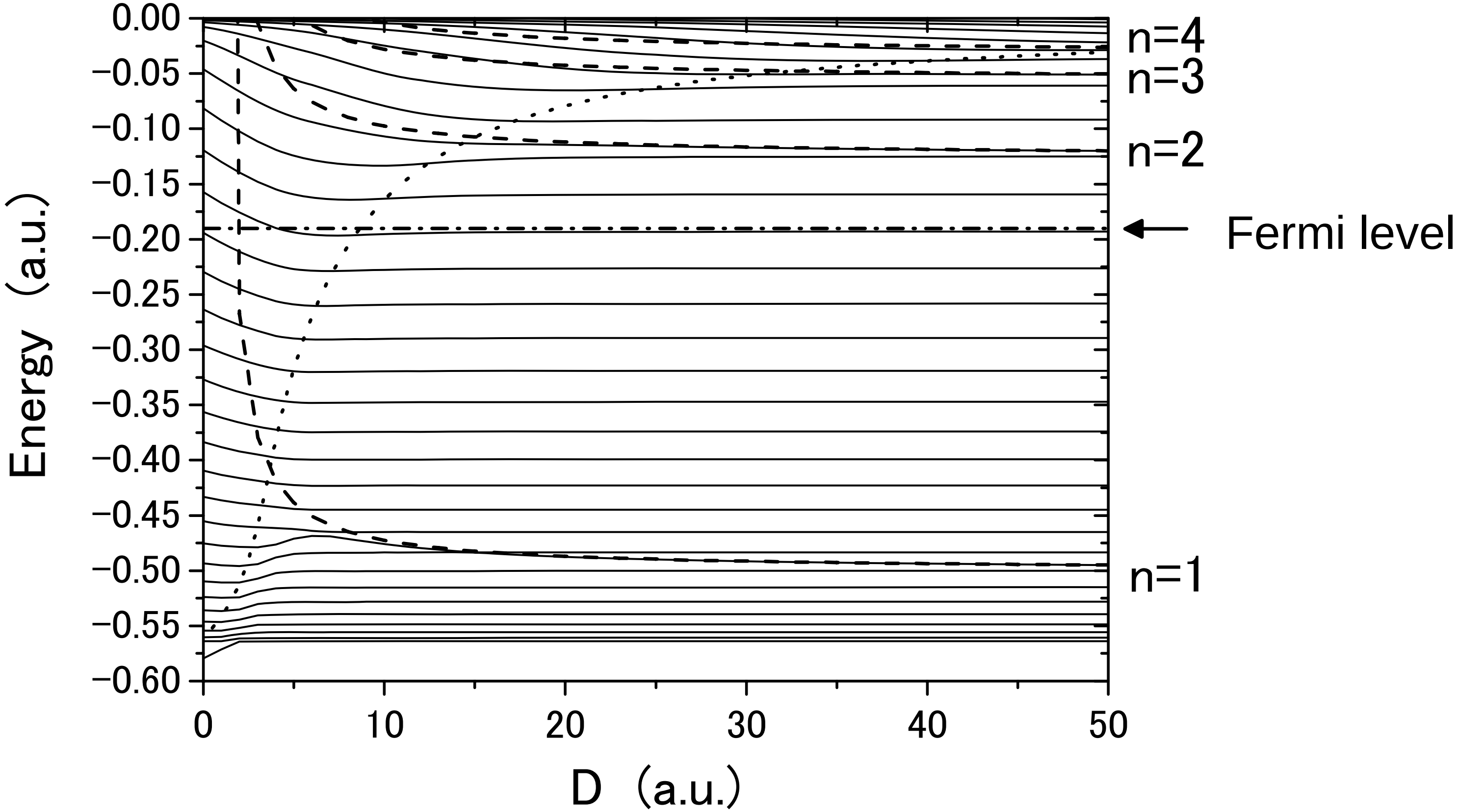




Proton is located at the origin, 10 a.u. distant from surface.

Energy level curves of H-Metal as a function of distance from surface (Fermi energy and workfunction of W)

Dashed curves are H levels shifted by the classical image potential, a dotted curve the top of the potential ridge, and a dashed-dotted line the Fermi level of W (about -0.19 a.u.).

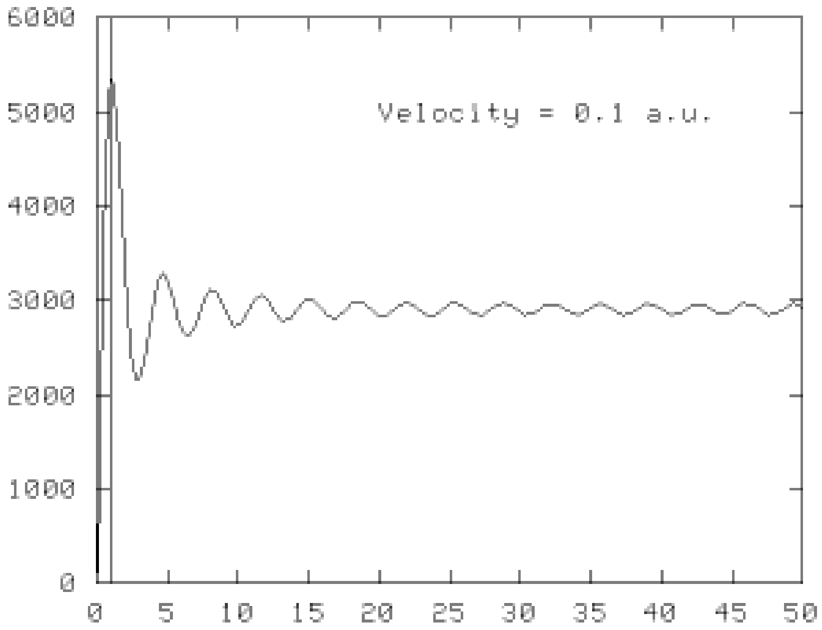


Electron density distribution for H-Metal

(Fermi energy and workfunction of W)

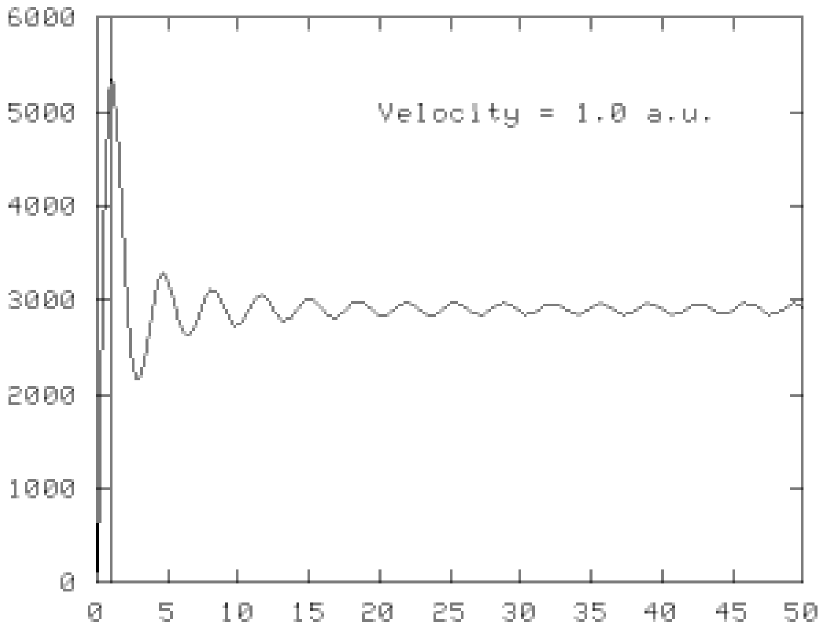
(rest frame of moving proton: proton is located always at the origin)

v=0.1 a.u. **Ten times slower than Fermi velocity.**



r (a.u.)

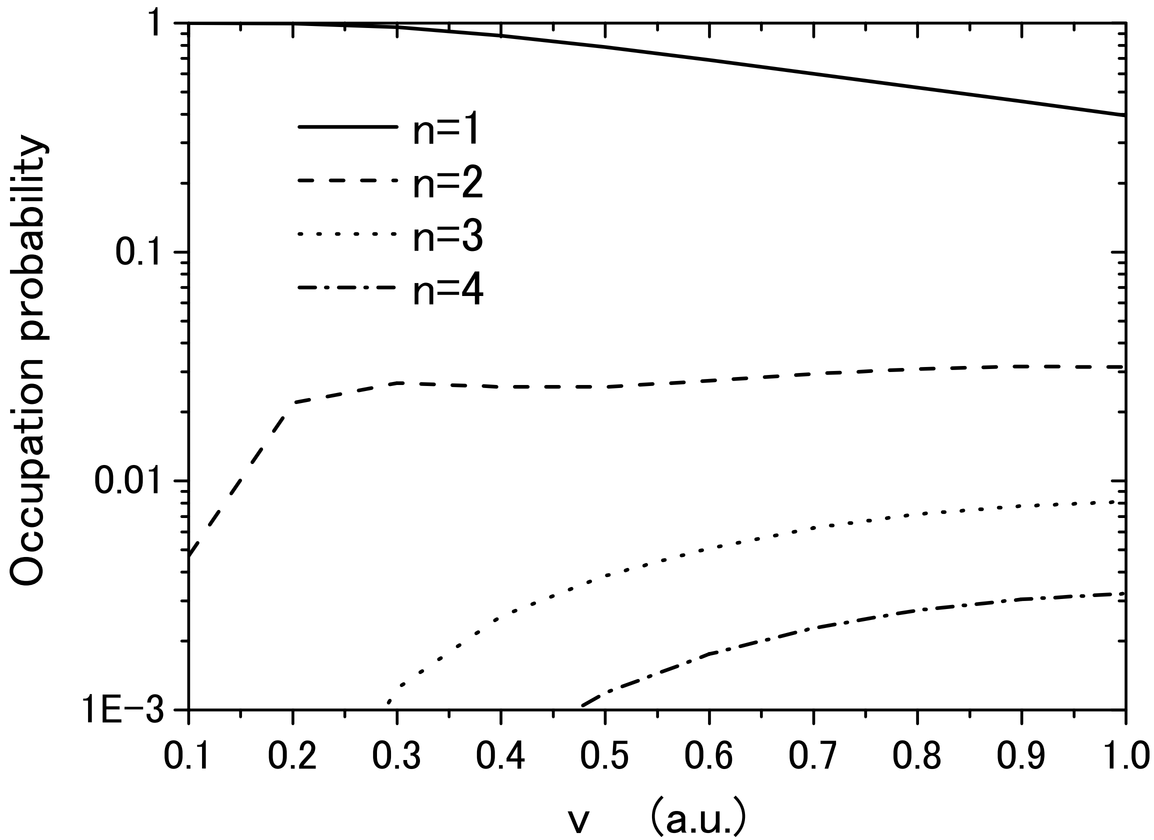
v=1.0 a.u. **About Fermi velocity.**



r (a.u.)

Occupation probabilities of H levels by single-electron capture

A hump is seen in the n=2 occupation probability at low velocities. It may be attributed to the oscillatory transition between quasi-resonant states of the n=2 level and a discrete conduction level of the tungsten slab.



Electron transfer between atomic levels and conduction band

Neutralization, ionization and total transition rates

$$\Delta^+(D) = 2\pi \sum_k f_k \left|M_{ka}\right|^2 \rho(\varepsilon_k - \varepsilon_a),$$

$$\Delta^-(D) = 2\pi \sum_k (1 - f_k)\left|M_{ka}\right|^2 \rho(\varepsilon_k - \varepsilon_a)$$

$$\Delta(D) = g^+\Delta^+(D) + g^-\Delta^-(D)$$

Master equation for occupation probability:

$$\frac{dP_a}{dD} = \frac{\Delta(D)}{v}\left(P_a^{EQ}(D) - P_a(D)\right)$$

Equilibrium occupation probability

(ion kept at a fixed position):

$$P_a^{EQ}(D) = g^+\Delta^+(D) \big/ \left(g^+\Delta^+(D) + g^-\Delta^-(D)\right)$$

Occupation probability:

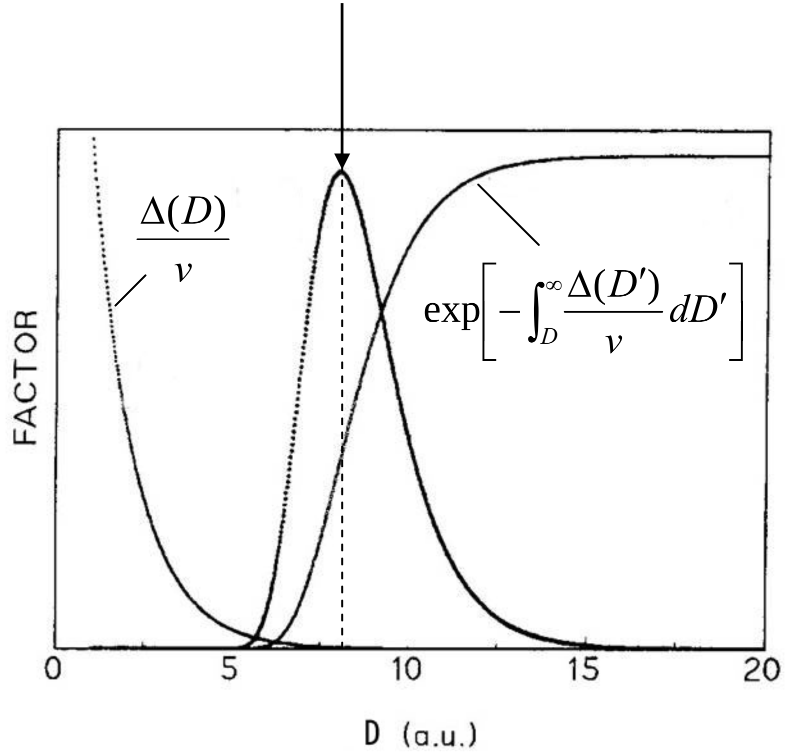
$$P_a(\infty) = P_a(D_0)\exp\left[-\int_{D_0}^{\infty}\frac{\Delta(D)}{v}dD\right]$$

$$+\int_{D_0}^{\infty} dD \frac{\Delta(D)}{v} P_a^{EQ}(D) \exp\left[-\int_{D}^{\infty}\frac{\Delta(D')}{v}dD'\right]$$

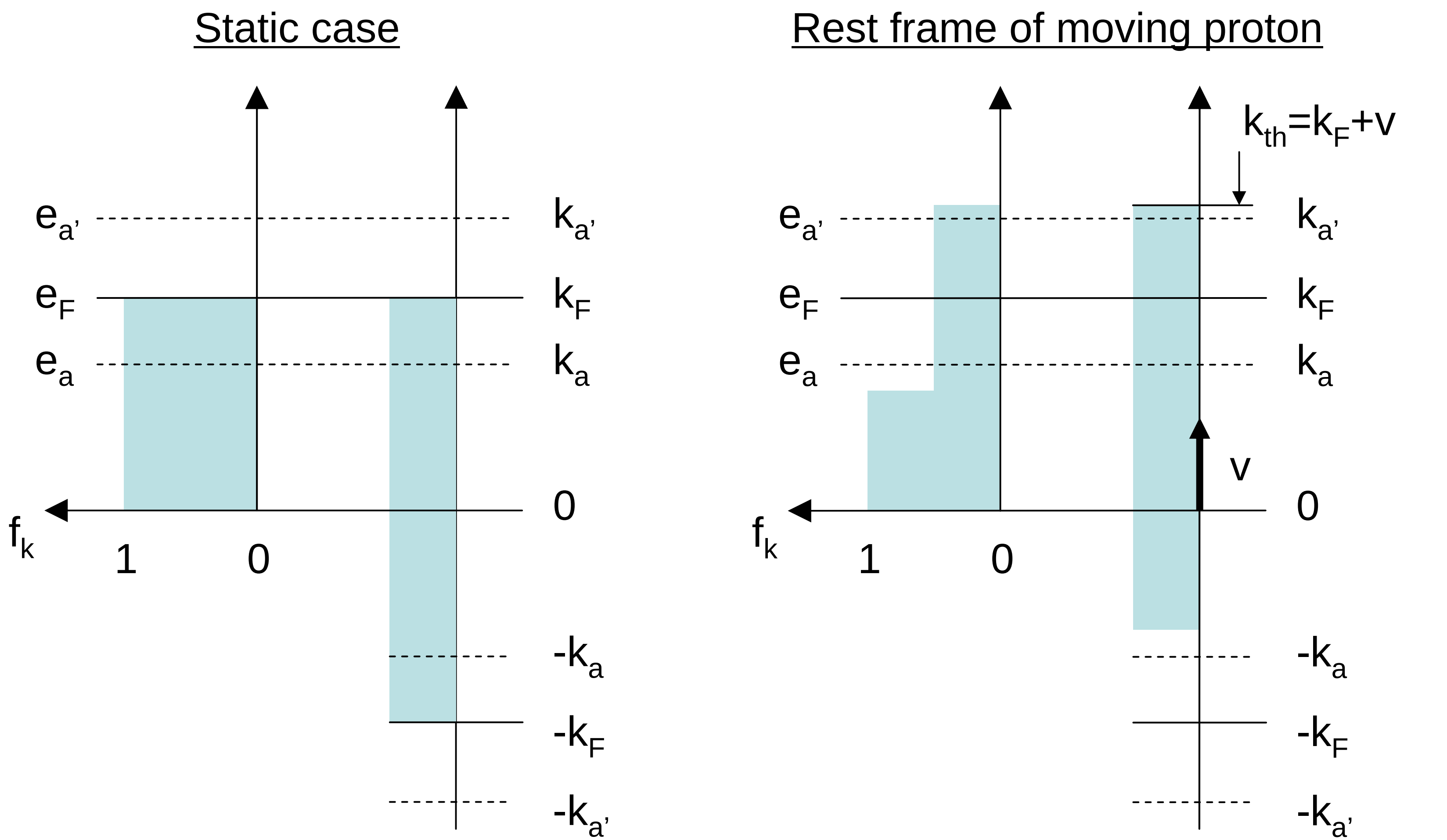
Freezing distance

$$\Delta(D) = \Delta_0 \exp(-D/L)$$

$$X = L\ln(\Delta_0 L/\hbar v)$$



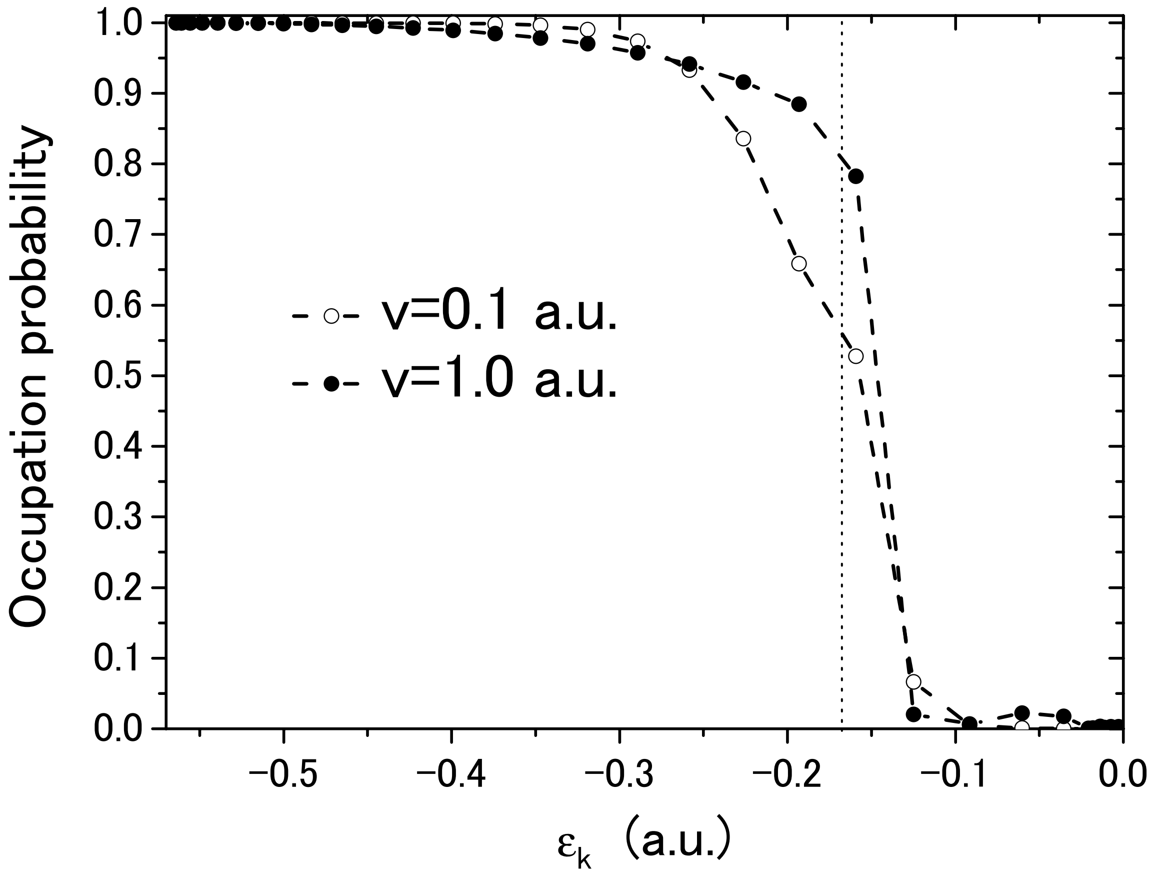
Shifted Fermi level by proton motion and Doppler-Fermi-Dirac distribution (1D model case)



Low proton velocities, say 0.1 a.u. (250 eV), compare with surface temperature in the 10^4 K range for the static case.

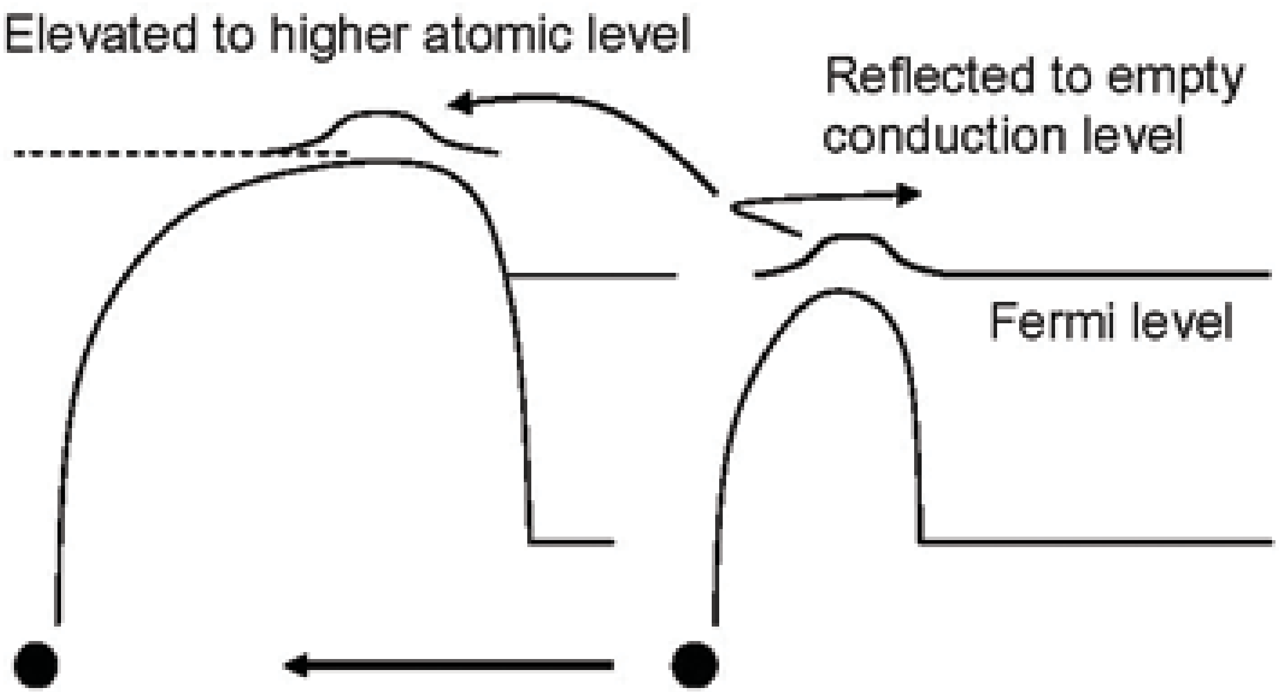
Occupation probabilities of conduction levels after single-electron capture by a proton

At higher velocities, electron capture from deeper conduction levels. Population above the Fermi level cannot be explained by the shift of the Fermi level.



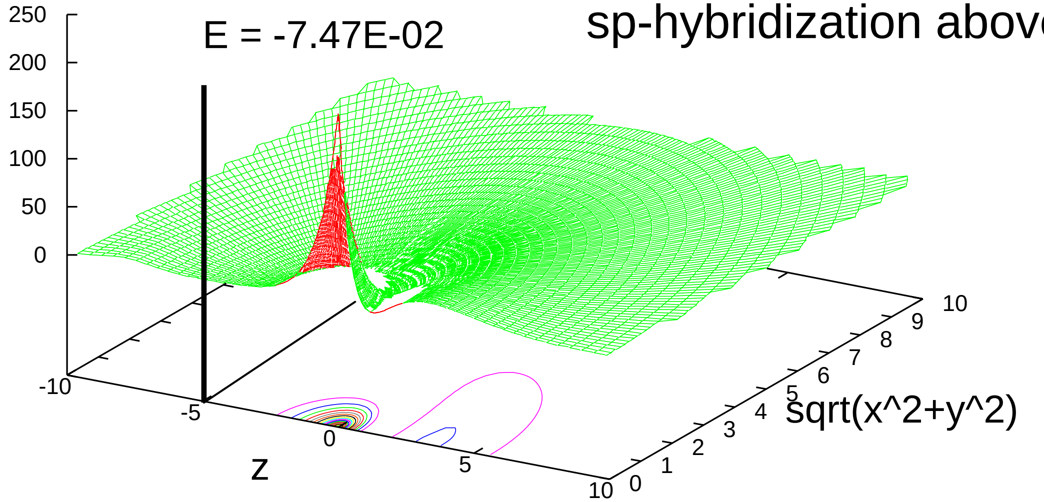
Non-adiabatic transition to higher levels

As the proton recedes from the surface, the top of the ***potential ridge*** rises out of the Fermi level. Faster the proton recedes from the surface, more the electronic wave function is kept sitting astride of the ridge and elevated to the higher atomic level. The wave function astride of the ridge represents a ***diabatic state*** which is promoted to the higher excited levels along the top of the ridge.



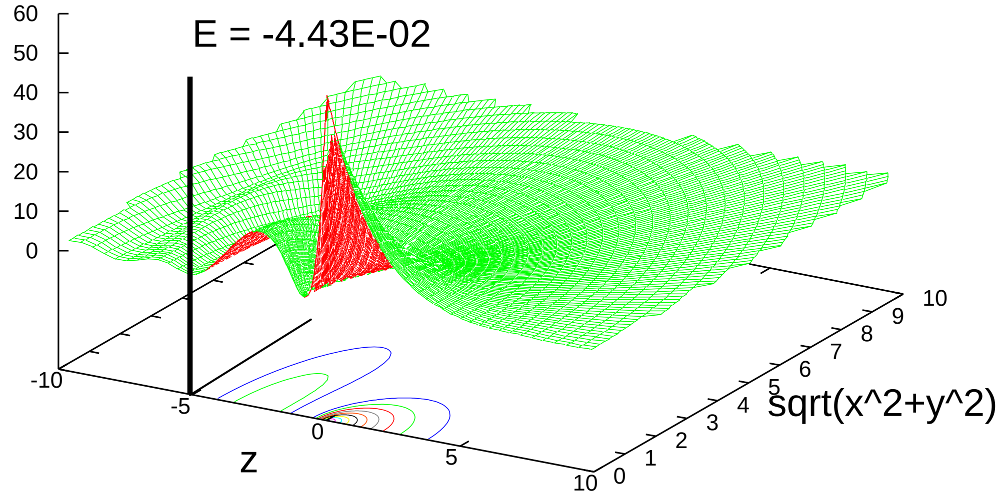
More accurate treatment of interaction and electron transfer between atoms and metal surfaces: Developing 3D model.

Squared of wavefunction for resonance states of H(n=2) sp-hybridization above Al surface.



Electron stays far side.
Narrow energy width, stable.

Stronger coupling with conduction band. Larger energy width.



conclusion

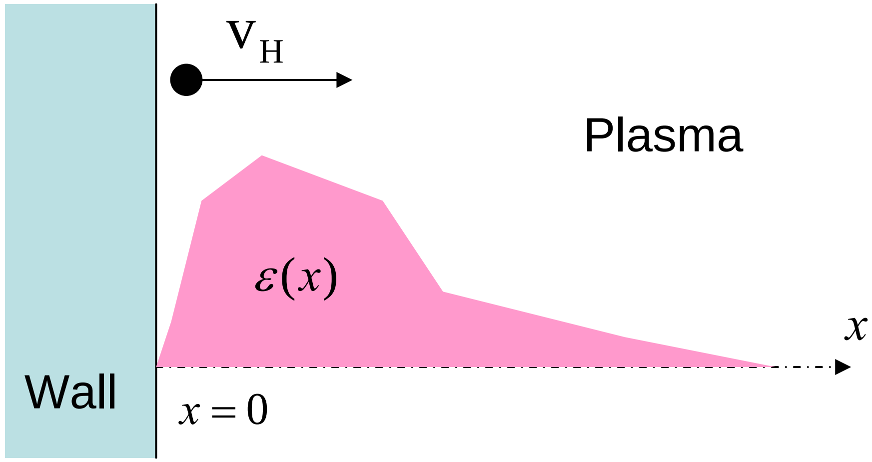
- Existence of excited states in neutral H atoms reflected at metal surfaces increase photon emission and charge exchange in edge plasmas.
  – Recycling diagnostics and collisional sheath.
- Theories are being developed based on atomic and solid state physics.
- Theories may be verified by PSI experiments in laboratory devices. Material selection is important.
  – Metals of higher energy reflection, larger fraction of excited states.
  – Excited state abundance depends on profile of Fermi surfaces.

Radiation by electron-impact excitation

Steady state in low density plasma
(Corona model)

$$\bar{n}_{\mathrm{H}}^{*}(x)\sum_{k} A_{i\to k} = \bar{n}_{\mathrm{H}}(x)C_{\mathrm{exc}}(x)$$

$$\bar{n}_{\mathrm{H}}(x) = \bar{n}_{\mathrm{H}}(0)\exp\left[-\frac{1}{\mathrm{v}_{\mathrm{H}}}\int_0^x C_{\mathrm{ion}}(x')dx'\right]$$



Emission coefficient and line integrated intensity

$$\varepsilon(x) = \frac{1}{4\pi}\bar{n}_{\mathrm{H}}^{*}(x)A_{i\to k} = \frac{\Gamma C_{\mathrm{exc}}}{4\pi}\bar{n}_{\mathrm{H}}(0)\exp\left[-\frac{1}{\mathrm{v}_{\mathrm{H}}}\int_0^x C_{\mathrm{ion}}dx'\right]$$

$$I = h\nu\int_0^\infty \varepsilon(x)dx = \frac{h\nu}{4\pi}\Gamma\int_0^\infty \bar{n}_{\mathrm{H}}C_{\mathrm{exc}}dx = \frac{h\nu}{4\pi}\frac{\Gamma\int_0^\infty \bar{n}_{\mathrm{H}}C_{\mathrm{exc}}dx}{\int_0^\infty \bar{n}_{\mathrm{H}}C_{\mathrm{ion}}dx}\Phi_{\mathrm{H}}(0)$$

$$\Phi_{\mathrm{H}}(0) = \mathrm{v}_{\mathrm{H}}\bar{n}_{\mathrm{H}}(0),\ \ \Phi_{\mathrm{H}}(\infty) = 0$$