Theory/simulation tasks for photo-emitter developments

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Photocathode development and simulation

- **Theory/Simulation tasks**
- **NEA photocathodes**
- **Electron escape depth**
- **Pillar simulation**
- **Angular dependence of Gain, TTS**
- **Time Drift Simulation**
- **Aging effect can be studied by MC/MD**

Simulation Tasks

- **Existing technologies**

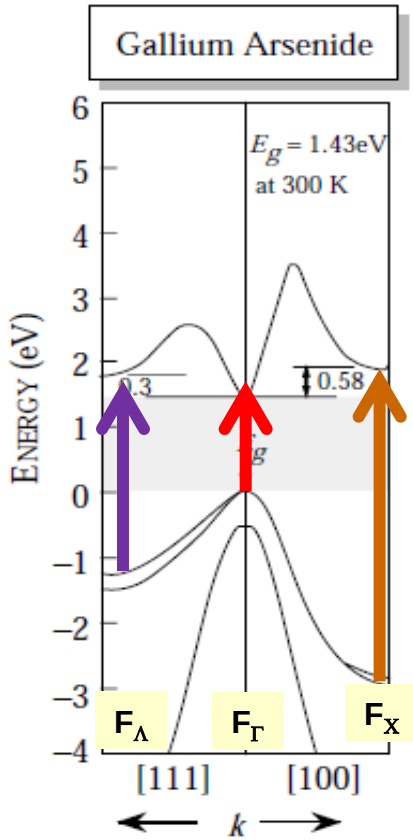
1. **Electron/hole diffusion lengths in the bulk semi-conductors**
2. **Surface roughness vs reflectivity**
3. **Trajectories of PE to the MCP surface - Valentin**

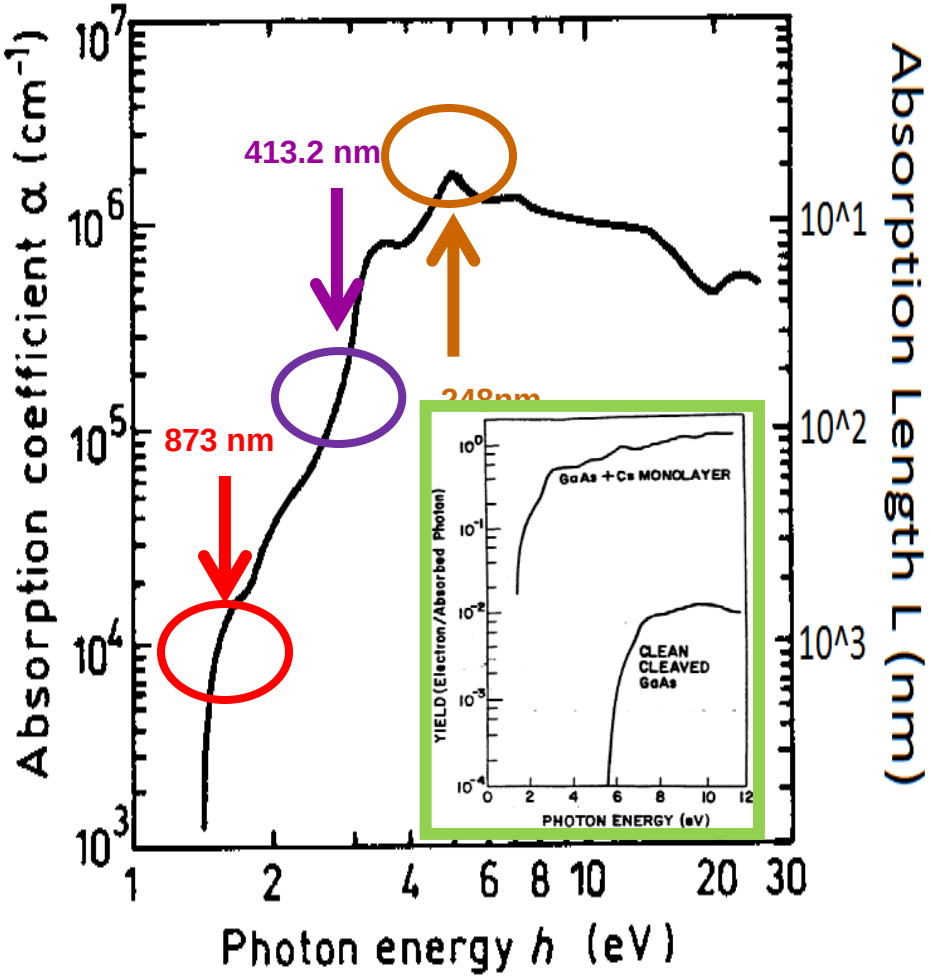
- **Prospective technologies**

1. **Ab-initio F_X, F_G, F_L (Bernhard)**
2. **Optimization of the NEA of the photo-cathode materials (Bernhard)**
3. **Electron / hole diffusion lengths in the heavily doped GaAs (Klaus)**
4. **Dopant profiles, electric fields by using a software (Klaus)**
5. **Surface roughness influence on the photon reflectivity or transmission (Klaus)**
6. **Trajectory studies for new materials and new morphology - Valentin**

Ab-initio simulations

- **Ab-initio studies of photonic, electronic, and defect properties of the nano-, multi-layered, mono- and poly-crystalline GaAs-Cs-O, doped CsO, TiO2 and NEA materials - Bernhard**
- **The overall structure of the photocathode will be optimized by COMSOL multiphysics package**





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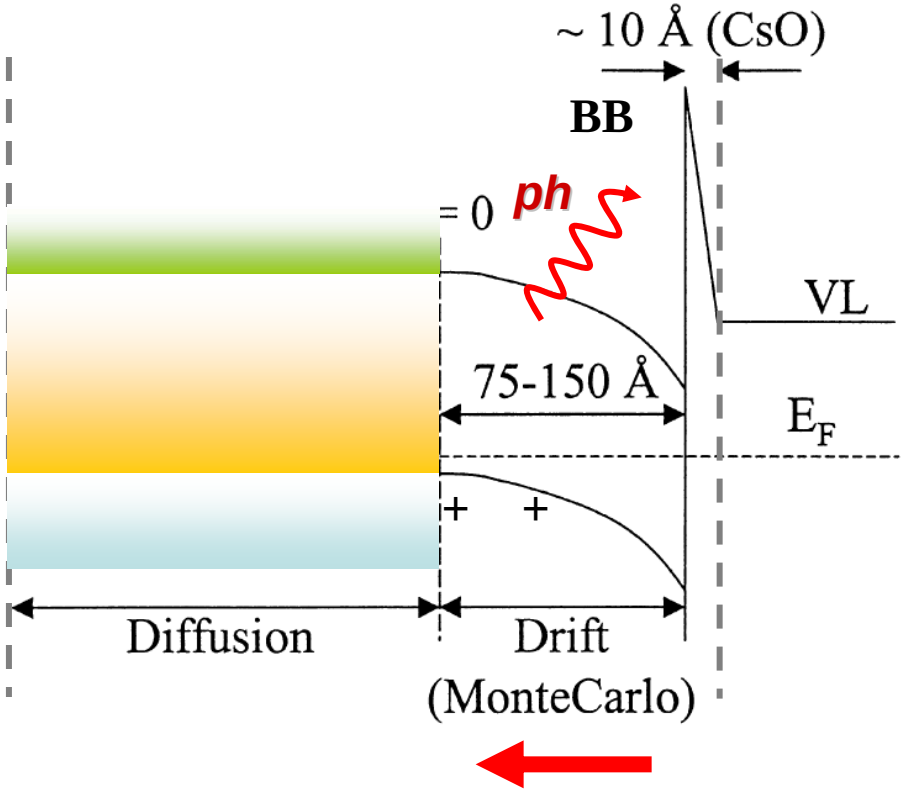
NEA photocathodes



CBM-conduction band minimum
VBM-valence band minimum
BB - band bending
VL - vacuum level
E_F - Fermi energy

E – very high
Hot electrons

[G. Vergara et al., Surf. Sci (1999)]

Theory of NEA device.

$$Y_X = \frac{P_X F_X}{1+(1/\alpha L_X)}(1-R),$$

$$Y_\Gamma = (1-R)\frac{P_\Gamma}{1+(1/\alpha L_\Gamma)}\left\{F_\Gamma + \frac{F_X L_\Gamma}{\alpha L_X (L_\Gamma + L_X)(1+(1/\alpha L_X))}\right\}.$$

$$L = \sqrt{D\tau} = \sqrt{\mu\tau(kT/e)},$$

$F_{X,\Gamma}$ – distribution of PE in X, Γ vallies (Ab-initio),

$P_{X,\Gamma}$ – probability to escape into vacuum (MC),

τ - recombination lifetime of Γ - electrons (MC),

R – reflection coefficient (MC).

[James, Mall (1969)]

e-LO-phonon scattering – main mechanism of energy relaxation in GaAs
e-plasmon collision – relaxation of energy in the bulk p^+-GaAs volume
e-charged impurity relaxation – in depleted region
e-h pair generation – in depleted region

Theory, simulation vs exp for NEA-GaAs

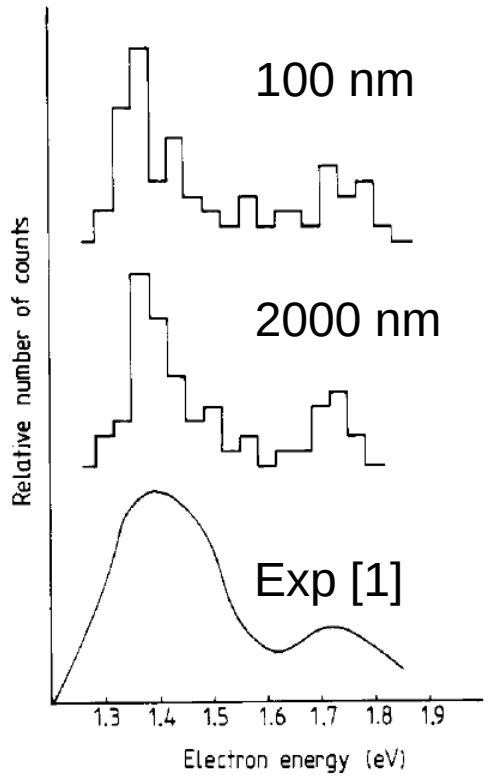
- James, Moll, Phys.Rev. (1969) – model and two peak energy distribution
- Escher, Schade, JAP (1973) – theory : Energy distribution of PE calculated
- Phillips, Hughes, Sibbett J. Phys. (1984) – one peak

Yang, Xu J. Phys. (1990) – Monte Carlo

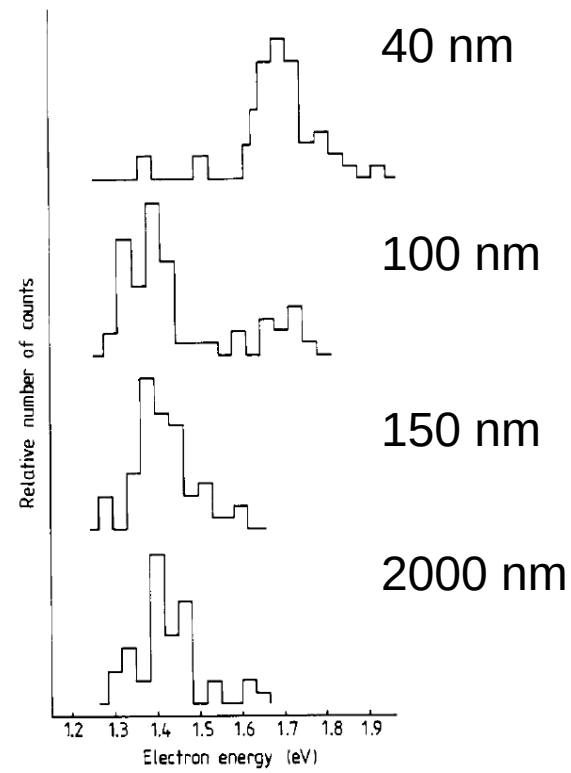
$N_A = 1\times10^{19}$ cm^{-3}

$h\nu = 2$ ev

Reflection mode



Transmission mode



[1] James, Moll (1969)

Tasks added by Bernhard

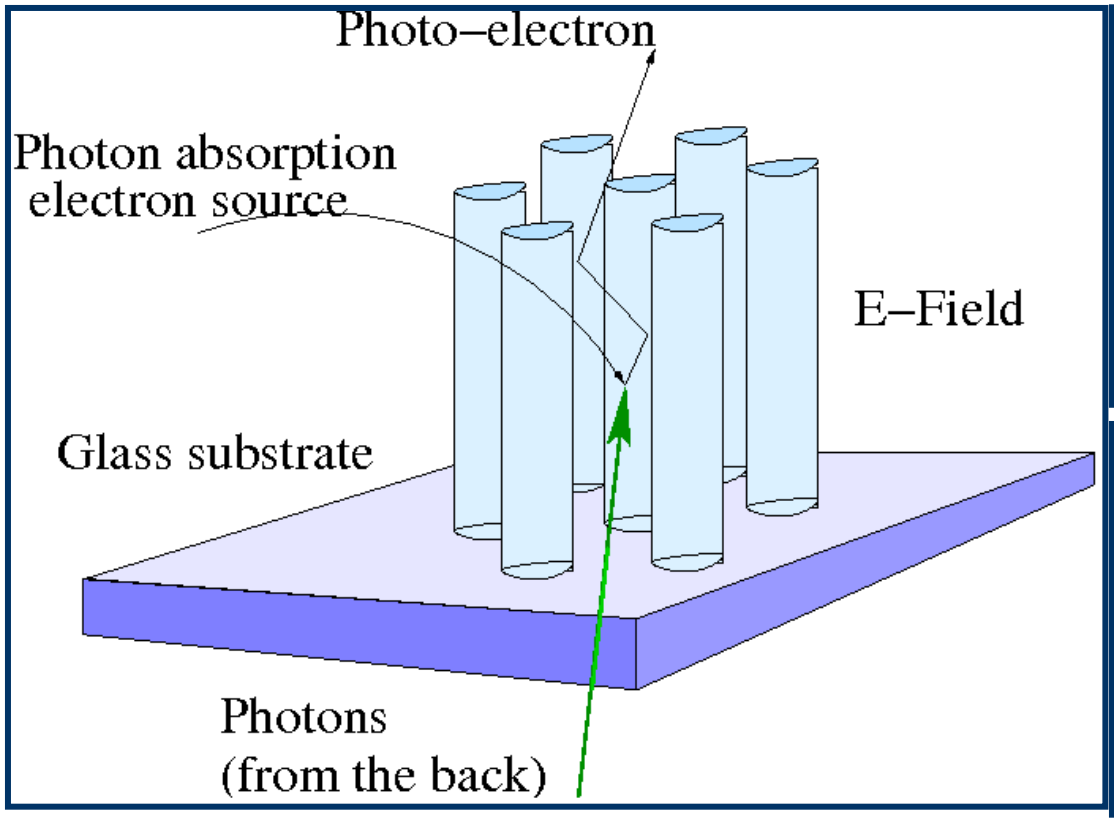
- **Optimization of Photocathodes for X-rays: how can we improve the X-ray stopping power while maintaining fast response?**
- **This is something fundamental, and just food for thought:**
  - ***we are assuming that a photon is absorbed in the photocathode, and an electron then has to diffuse (or be driven by E-field) from there to the surface***

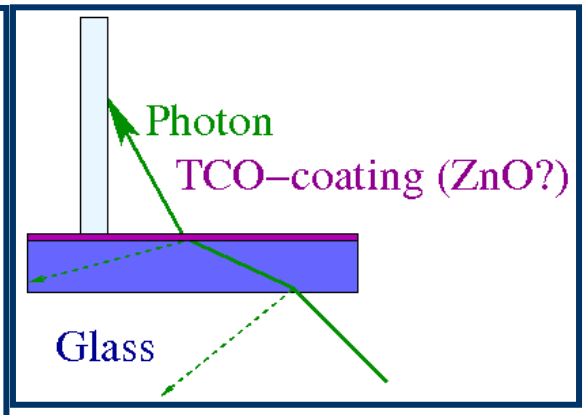
Question: are there other possibilities?

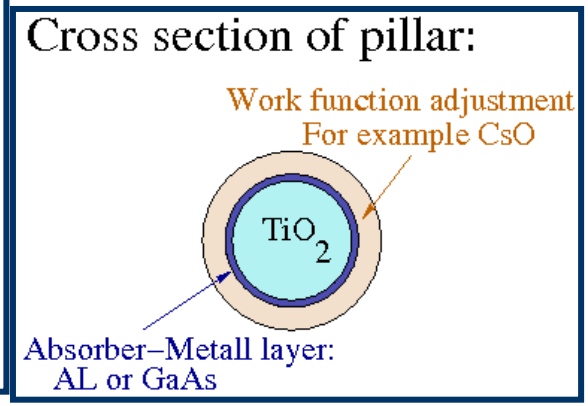
- Bernhard

- **Can electron emission work in other ways, such as can absorption of a photon deep in the cathode trigger release of an electron from the surface without electron diffusion – for example through E-fields inside the cathode? Enhancement vs noise**
- **Can we make a structure with internal gain? Pillar?**
- **Can electron emission be triggered from a nonlinear device, similarly to a laser diode operating right at the lasing threshold?**

Pillar structure

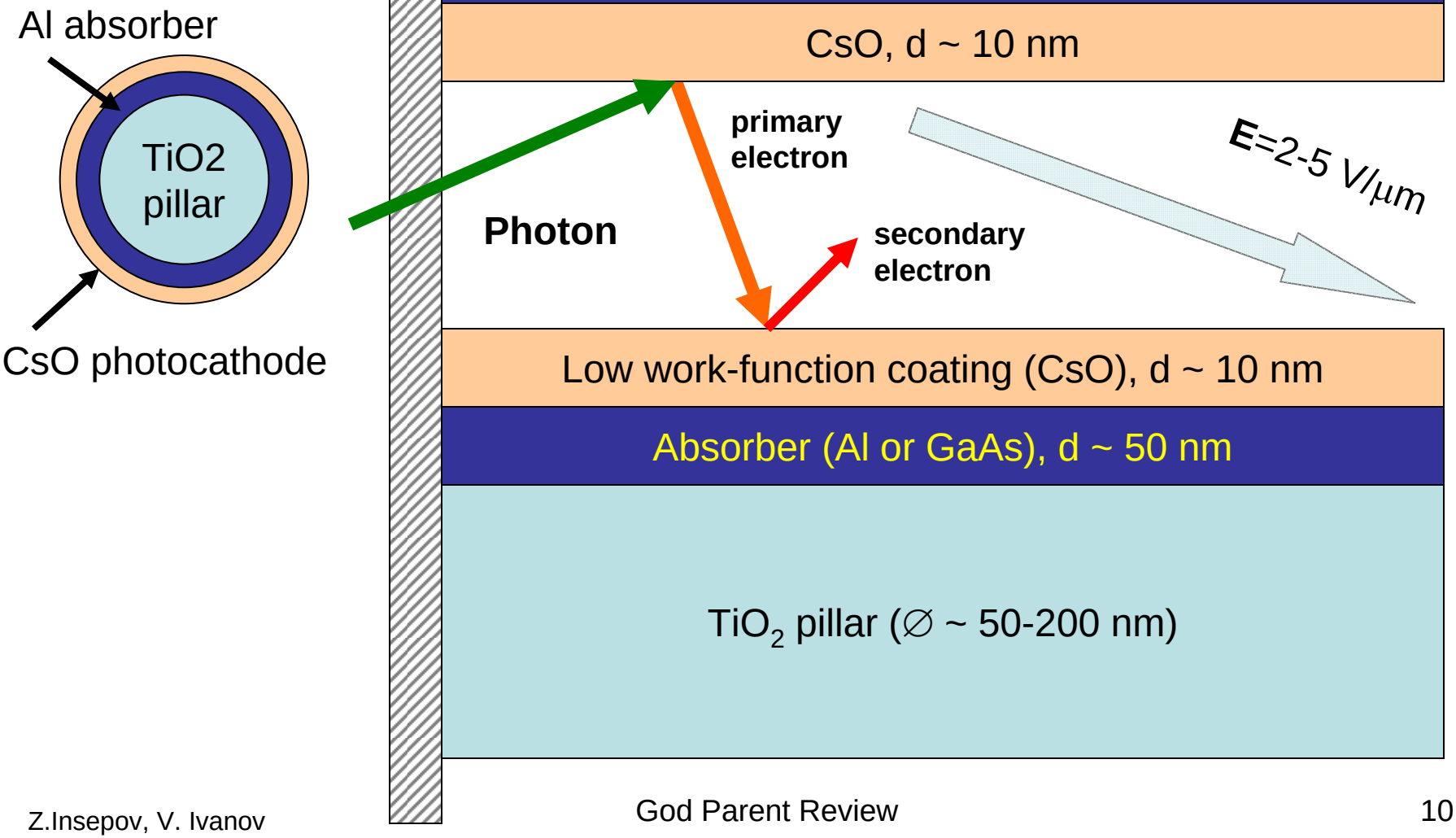




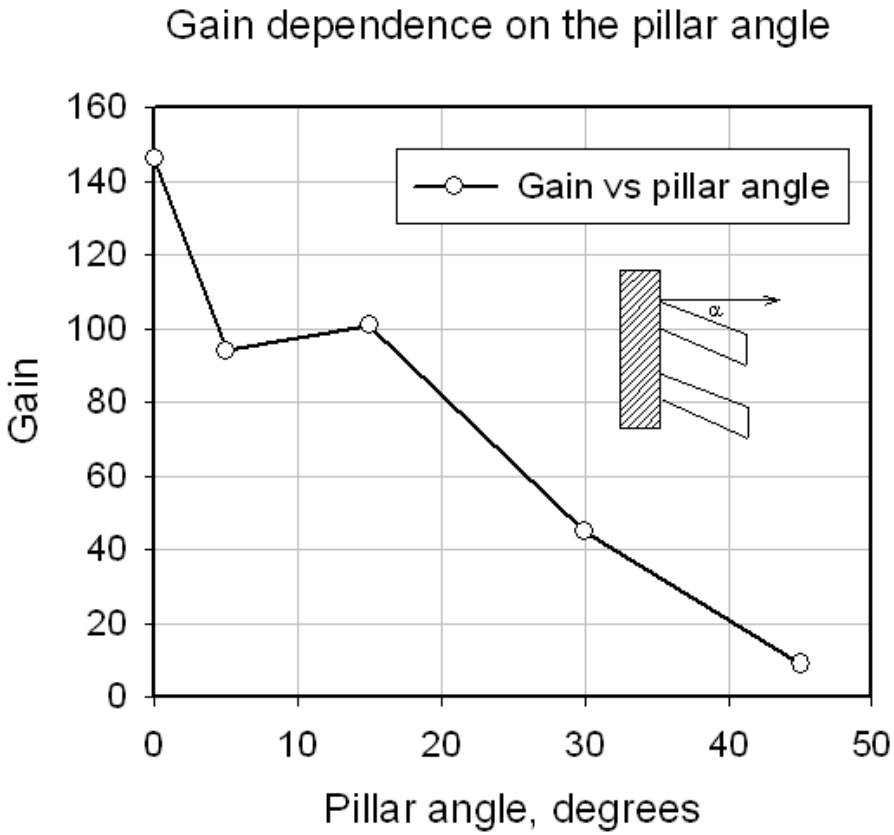


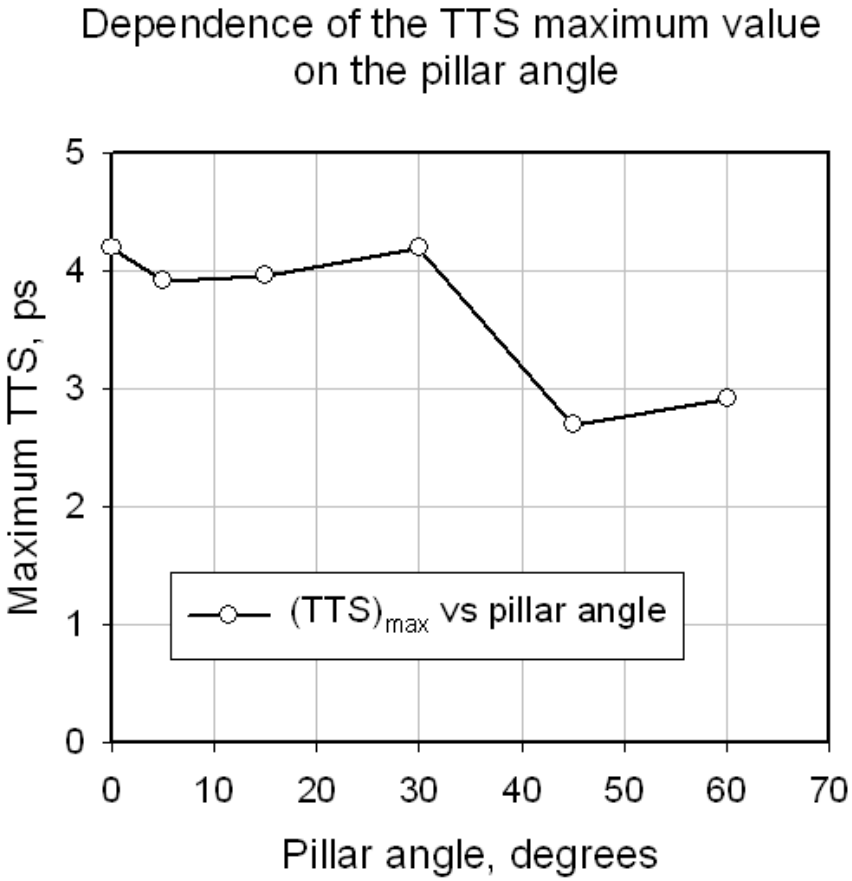
Pillar simulation

Cross-section of pillar

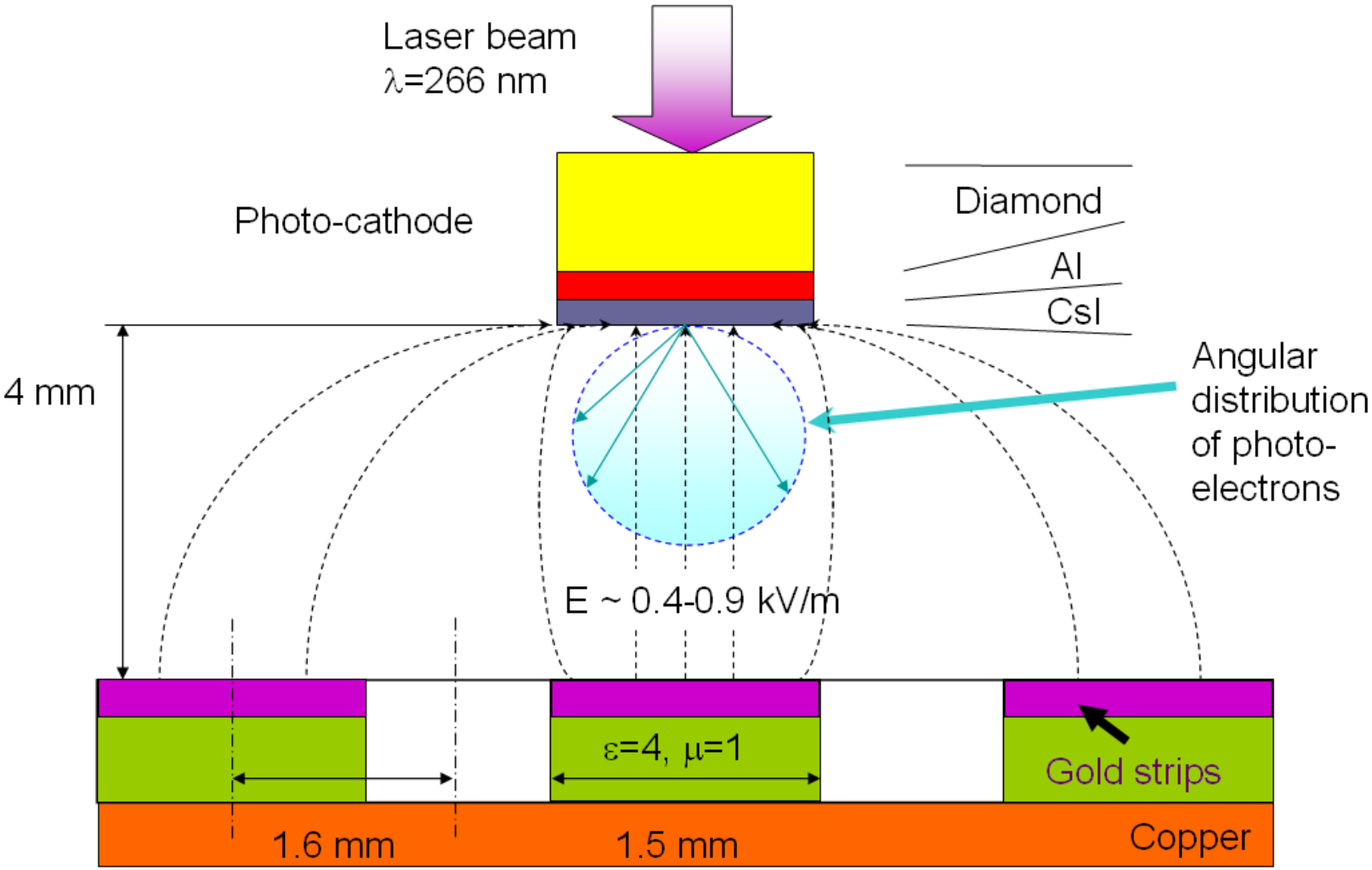


Gain

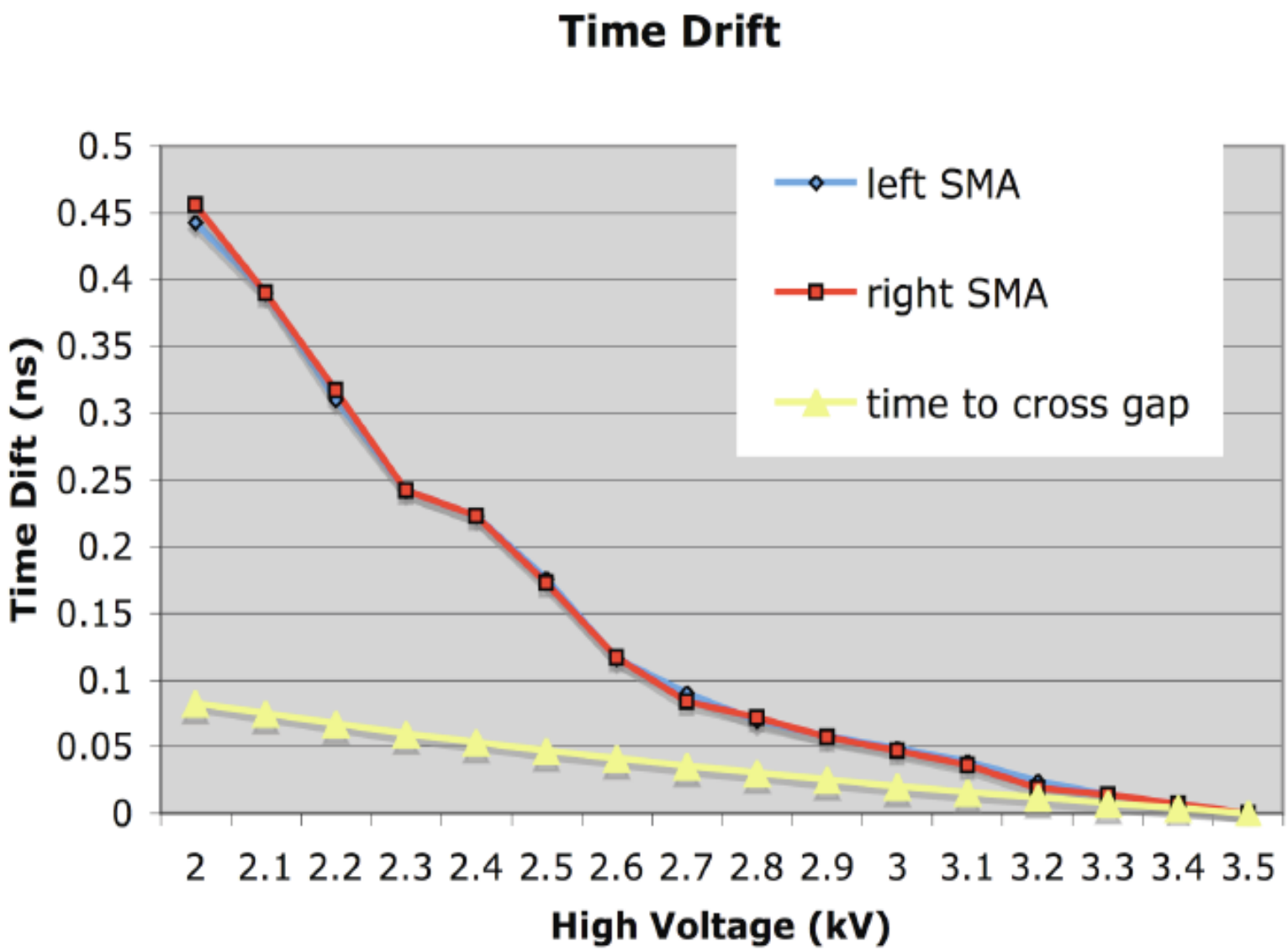

Gain dependence on the pillar angle
Gain vs pillar angle
α
Gain
Pillar angle, degrees
0
20
40
60
80
100
120
140
160
0
10
20
30
40
50


Dependence of the TTS maximum value on the pillar angle
(TTS)max vs pillar angle
Maximum TTS, ps
Pillar angle, degrees
0
1
2
3
4
5
0
10
20
30
40
50
60
70

Time Drift Simulation

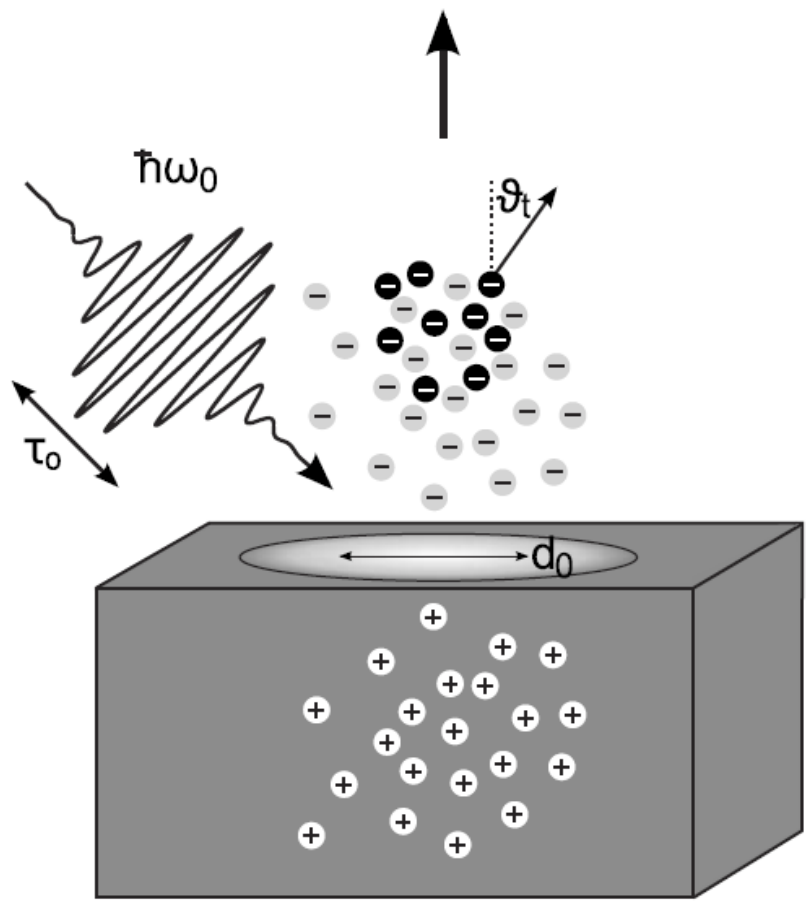


APS experiments



Space-Charge Effect in PC

- The higher the number of cloud electrons per pulse *Nc* the stronger is the space-charge effect.
- Non-negligible space-charge effects occur already at rather low values of *Nc* of about 1000*e* per pulse [1].
- APS experiments have estimated *Nc* per pulse >> 1000e [2].



APS experimental data

$Q = I_{max} * \tau_0 = 140\mu A * 80\ ps = 1.12e\text{-}14\ C$

Nc = 7e4 per pulse

[1] J. Zhou et al, J. El. Spectr.Rel.Phen. 2005.
[2] Matt Wetstein, APS, Nc=7e4 per pulse

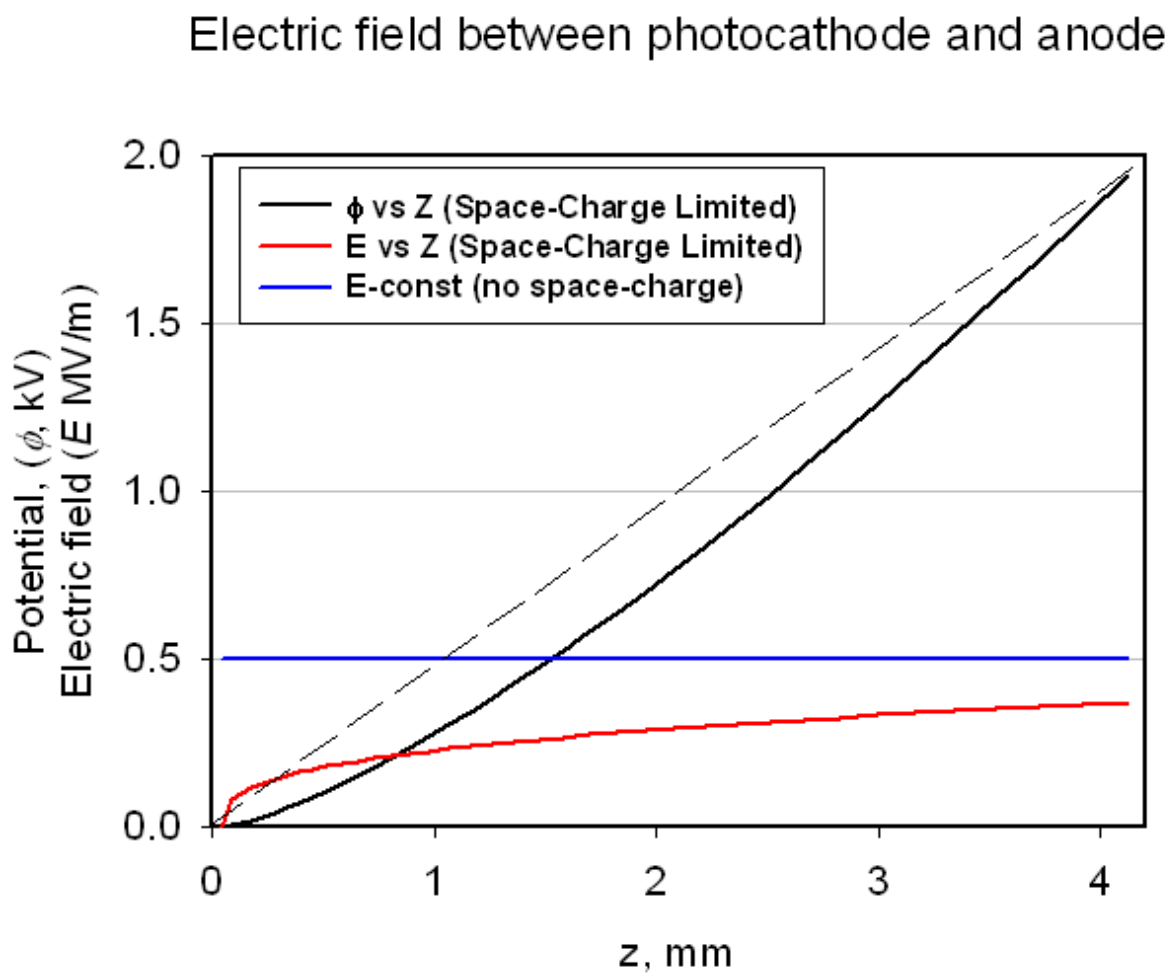
Space-Charge Limited Potential

Child-Langmuir equation

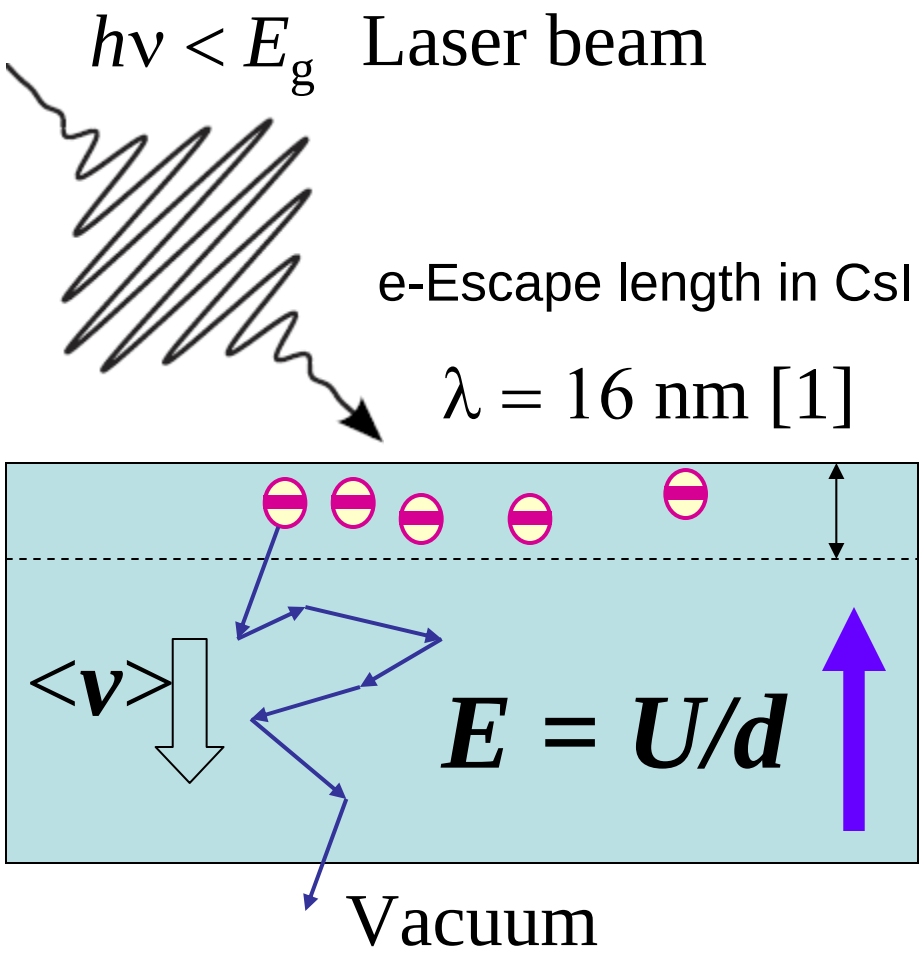
$$J_{SCL} = \frac{4}{9}\varepsilon_0 \sqrt{\frac{2e}{m}} \cdot \frac{V^{3/2}}{D^2},$$

$$\phi = V\left(\frac{z}{D}\right)^{4/3},$$

$$E = \frac{4}{3}\frac{V}{D}\left(\frac{z}{D}\right)^{1/3}.$$



Drift-diffusion model of electrons



Drift+Diffusion model

Langevin equation

$$\dot{\vec{v}}_i(t) = -\nabla U(\vec{r}_i)/m_e - \gamma \cdot \vec{v}_i(t) + \vec{R}_i/m_e,$$

γ – friction coefficient, $\vec{R}_i$ random force,

$$< R(t) >= 0,$$

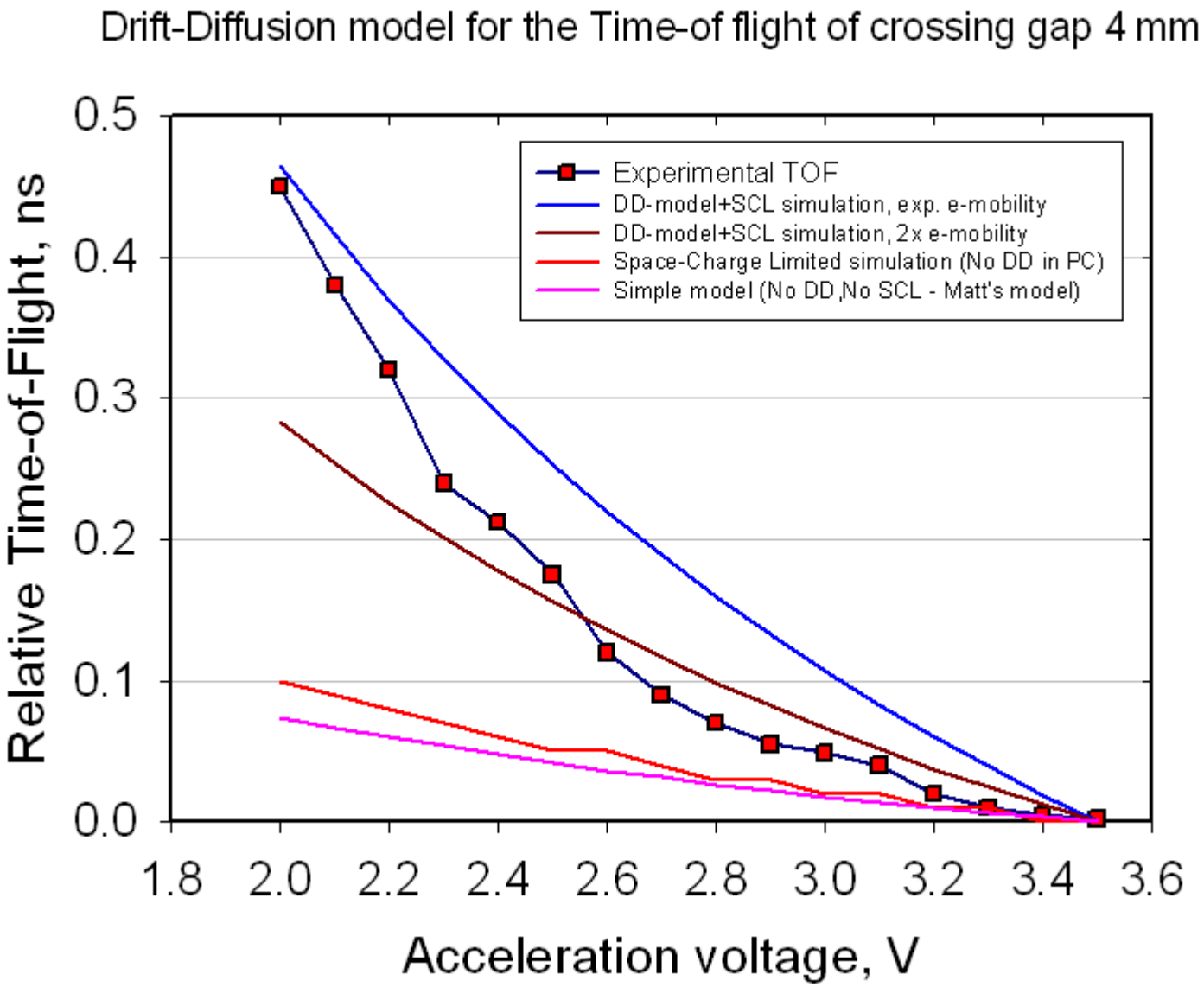
$$< R(t)R(t') >= 2\frac{\gamma k_B T}{m_e}\delta(t-t').$$

e – mobility

$$\mu_e = 8\times10^{-4} m^2/V\cdot s\,[2]$$

[1] Breskin, NIMA (1996)
[2] Aduev, Phys.Stat.Sol. B (1998)

Time to Drift in vacuum



Summary

- **NEA models will be modified (+L point)**
- **MC micro-code #1 will be developed for micro- PC modes (refl+tr)**
- **MC macro-code #2 will be developed for Gain, TTS**
- **PC coatings can be studied by MC**
- **Drift time can be calculated by MC and compared to Matt's experiment**
- **Ab-initio band structure calculations will be valuable addition to fundamental tasks (Bernhard + TBN) and for simulation parameters**
- **Dopand profiles, carrier mobility and defect properties will be calculated via a Klaus's software**