

Emittance Growth Caused by Surface Roughness

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**Photocathode Physics for
Photoinjectors 2016**

Motivation

What causes the emittance growth

- Dowell's equations of QE & emittance for bulk emission

Dowell, 2009, PRST

$$\text{QE}(\omega) \approx \frac{1 - R(\omega)}{1 + \frac{\lambda_{\text{opt}}}{\lambda_{e-e}(\omega)}} \frac{(\hbar\omega - \phi_{\text{eff}})^2}{8\phi_{\text{eff}}(E_F + \phi_{\text{eff}})}$$

$$\varepsilon_{n,x} = \sigma_x \sqrt{\frac{\hbar\omega - \phi_{\text{eff}}}{3mc^2}}$$

Motivation

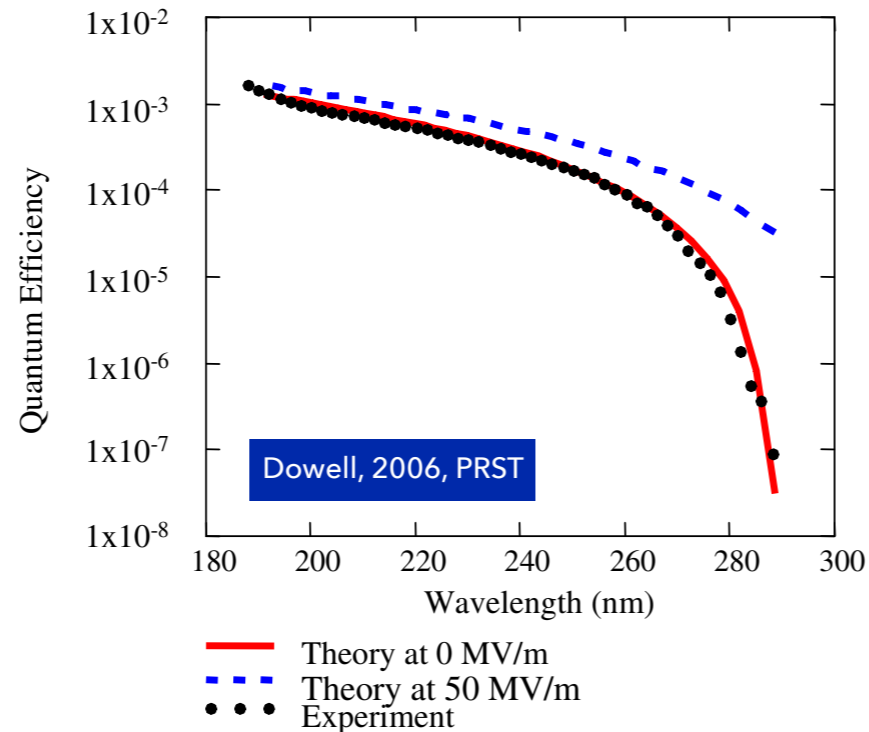
What causes the emittance growth

- Dowell's equations of QE & emittance for bulk emission

Dowell, 2009, PRST

$$QE(\omega) \approx \frac{1 - R(\omega)}{1 + \frac{\lambda_{opt}}{\lambda}} \frac{(\hbar\omega - \phi_{eff})^2}{8\phi_{eff}(E_F + \phi_{eff})}$$

QE: Theory vs. Measurement



Motivation

What causes the emittance growth

- Dowell's equations of QE & emittance for bulk emission

Dowell, 2009, PRST

$$QE(\omega) \approx \frac{1 - R(\omega)}{\lambda_{opt}} \frac{(\hbar\omega - \phi_{eff})^2}{8\phi_{eff}(E_F + \phi_{eff})}$$

Emittance: Theory vs. Measurement

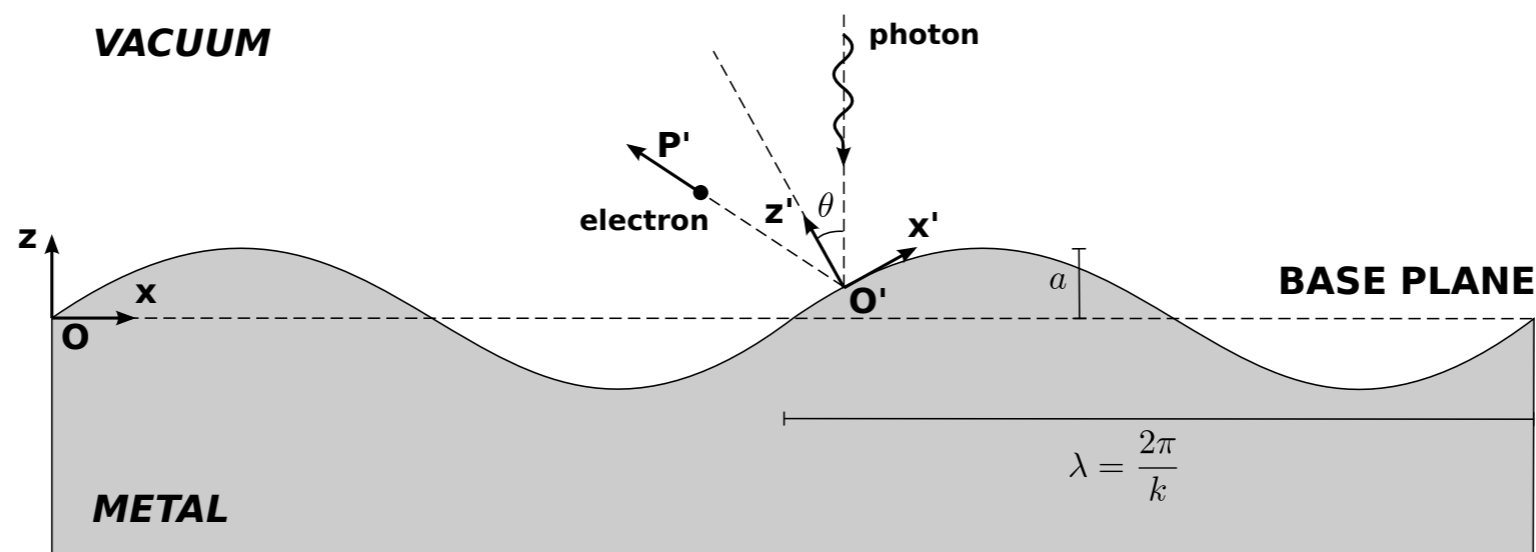
Qian, 2012, Ph.D.

$\epsilon_{n,x}$

Parameter	Unit	BNL	SLAC	PSI		
laser wavelength	mm	266	253	261	272	282
gun gradient	MV/m	95	115	/	/	/
gun phase	deg	/	15	/	/	/
launch electric field	MV/m	/	30	25	25	25
measured therm. emit.	$\mu\text{m}/\text{mm}$	0.92	0.9	0.68	0.54	0.41
theory therm. emit.	$\mu\text{m}/\text{mm}$	/	0.54	0.64	0.54	0.43
copper work function	$\mu\text{m}/\text{mm}$	4.59	4.65	4.3	4.3	4.3

Motivation

How people deal with the surface roughness effect



surface morphology $R = a \sin(kx)$

field distribution $E_x = E\xi \cdot e^{-kz} \sin kx$
 $E_z = E(1 + \xi e^{-kz} \cos kx)$
 $\xi = ak$

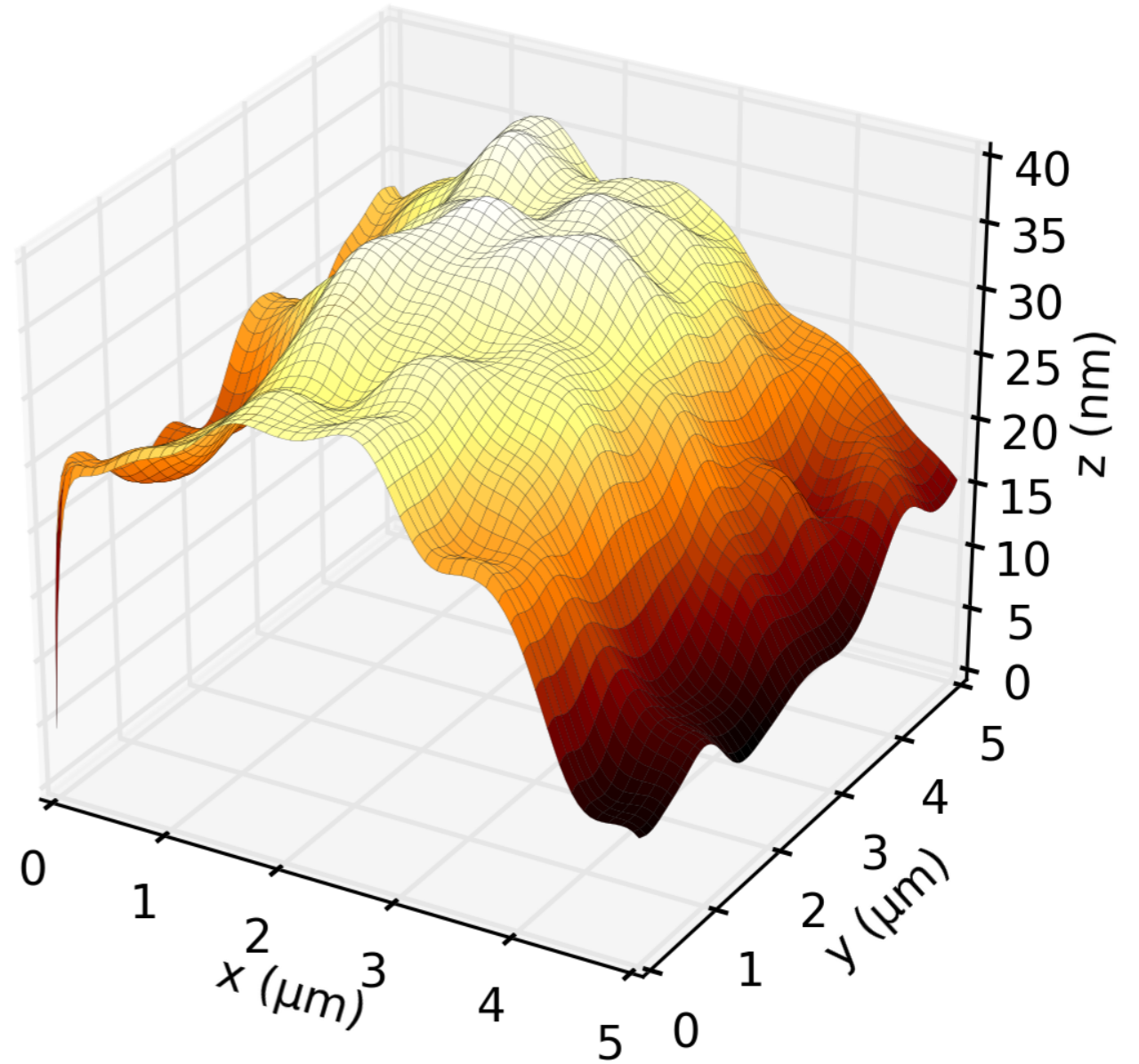
slope effect $\varepsilon_x^2 \approx \varepsilon_{D,x}^2 \left(1 + \frac{1}{2} \xi^2 \right)$

field effect $\varepsilon_x^2 \approx \varepsilon_{D,x}^2 \left(1 + \frac{3\pi e}{4} \cdot \frac{a^2 k E}{\hbar\omega - \phi_{\text{eff}}} \right)$

Motivation

Difficulties in 3D case calculation

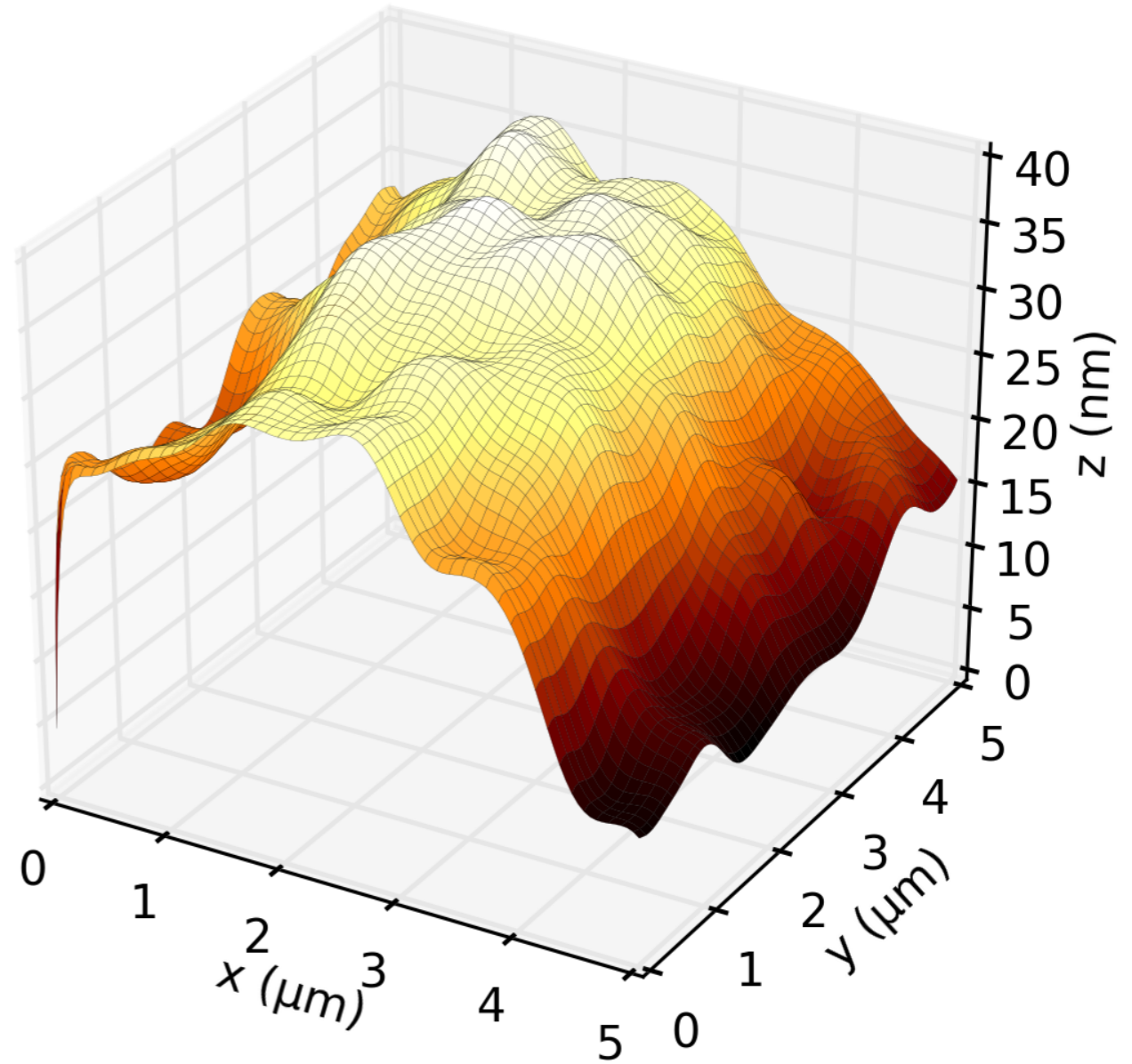
- Initial electron phase-space distribution (**slope effect**)
- EM field on an arbitrary surface (**field effect**)



Motivation

Difficulties in 3D case simulation

- Generate initial electron samples (**slope effect**)
- Simulation of the EM field near a real-life rough surface (**field effect**)



Motivation

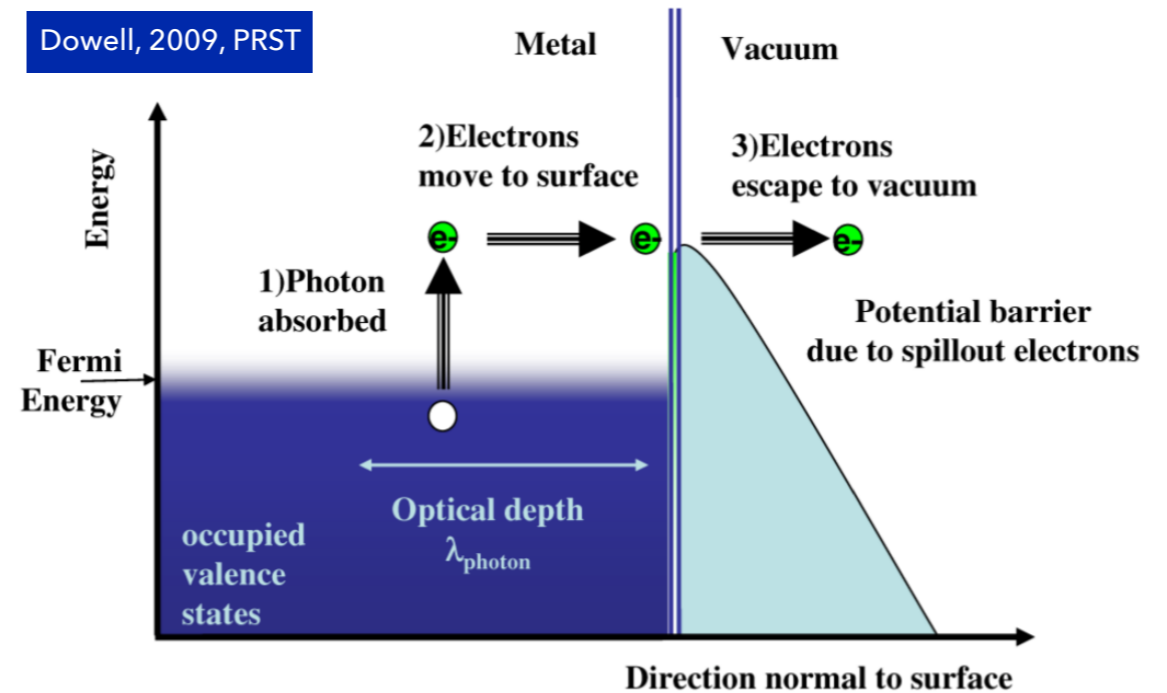
Difficulties in 3D case simulation

- Generate initial electron samples (**slope effect**)
- Simulation of the EM field near a real-life rough surface (**field effect**)

3-step Model

1. Absorption of the photon with energy $h\nu$
2. Migration including e-e scattering to the surface
3. Escape for electrons with kinematics above the barrier

Could sampling by applying the Monte-Carlo method.



Motivation

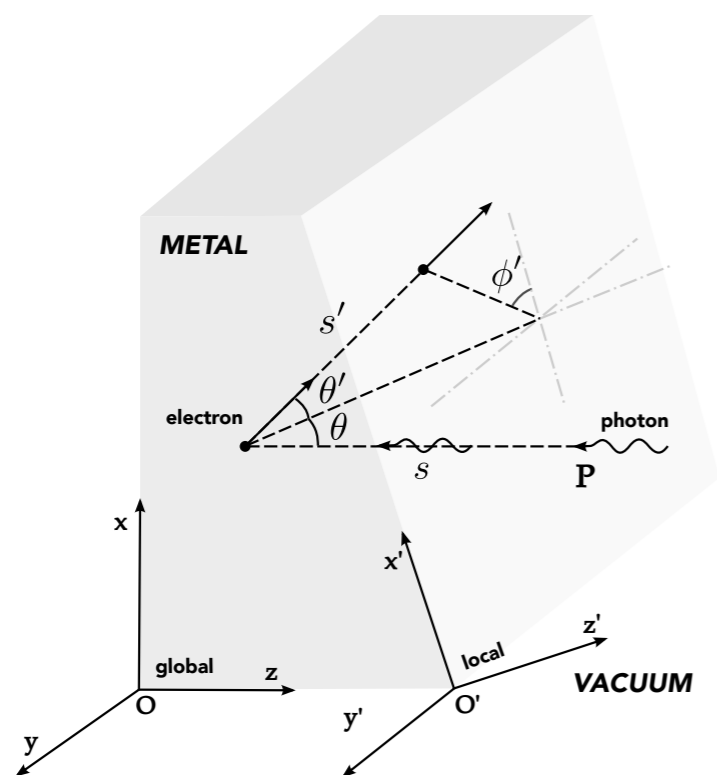
Difficulties in 3D case simulation

- Generate initial electron samples (**slope effect**)

Monte-Carlo Sampling

Generate $s \sim \text{Exp}(\lambda)$, $E \sim U(E_F - \hbar\omega, E_F)$, $\theta' \sim U(0, \pi/2)$, $\phi' \sim U(0, 2\pi)$, where $1/\lambda = 1/\lambda_{\text{opt}} + 1/\lambda_{\text{e-e}}$, then apply the filter condition $(E + \hbar\omega)\cos^2\theta' \geq \varphi_{\text{eff}}$.

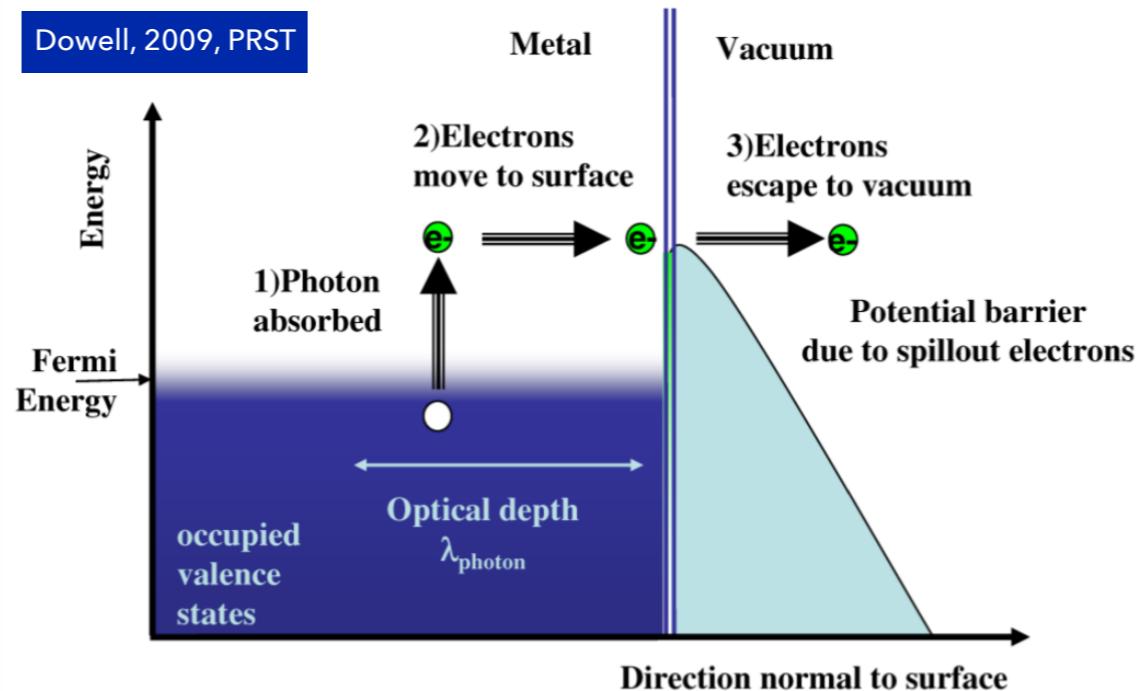
However the sampling efficiency is quite low ($\sim 1e-4$) because of the low QE of metals.



3-step Model

1. Absorption of the photon with energy $h\nu$
2. Migration including e-e scattering to the surface
3. Escape for electrons with kinematics above the barrier

Could sampling be applied by applying the Monte-Carlo method.



Motivation

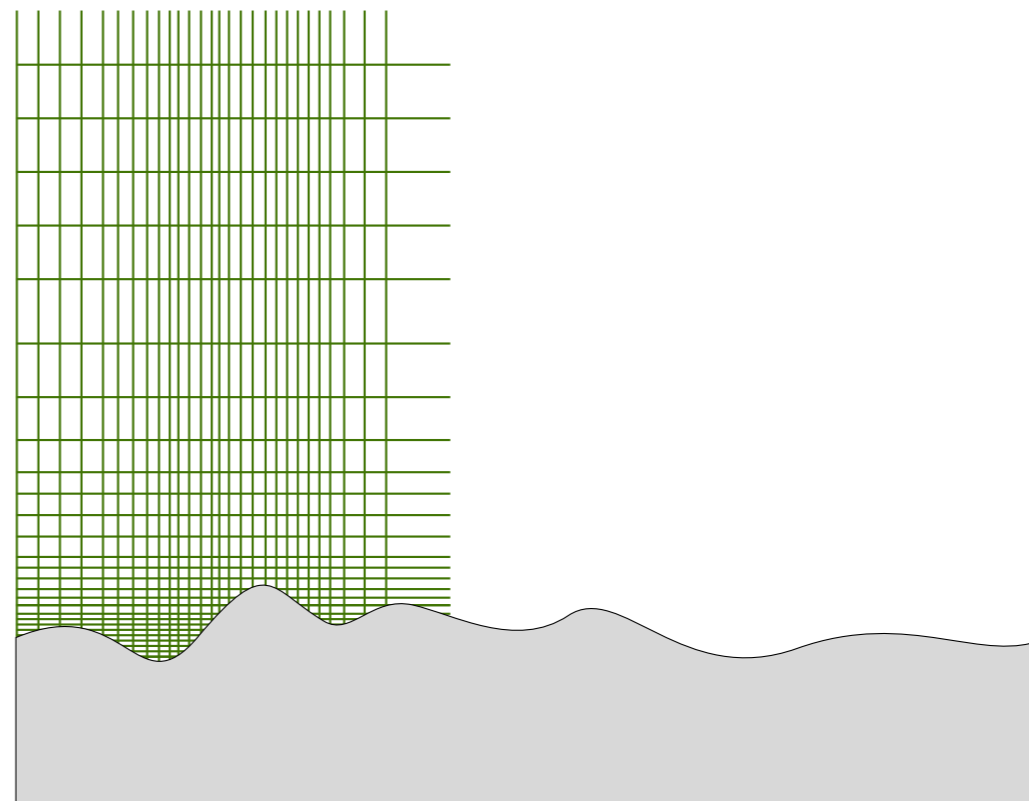
Difficulties in 3D case simulation

- Generate initial electron samples (**slope effect**)
- Simulation of the EM field near a real-life rough surface (**field effect**)

Meshing on the Rough Surface

The rms amplitude of the surface roughness is ~ 10 nm, the average rms wavelength is ~ 10 μm , and the size of the laser spot is ~ 1 mm. Meshing would be too memory-consuming.

Unrealistic to do this in EM field simulation code.



Motivation

How to deal with the difficulties in 3D case

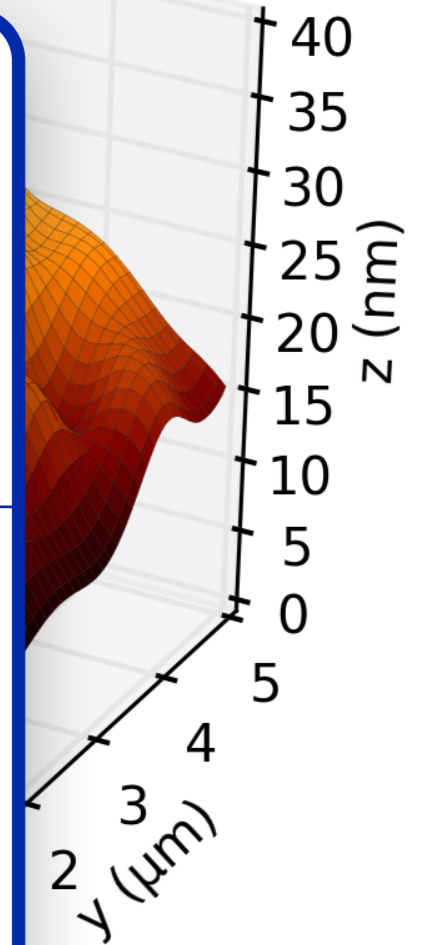
- Generate initial electron samples (slope effect)
- Simulation of near a real-life (field effect)

Utilize the Point Spread Function

By applying the Point Spread Function (PSF) of photocathode, one could reveal a simple rule for the electron distribution on the rough surface.

Thus the sampling efficiency could be significantly improved.

$$f_p(p_x, p_y, p_z) = \frac{C_p(\theta)p_z}{\sqrt{p_z^2 + p_m^2} \cdot \sqrt{p_x^2 + p_y^2 + p_z^2 + p_m^2}} \cdot H(p_z)H(p_M^2 - p_m^2 - p_x^2 - p_y^2 - p_z^2)$$
$$C_p(\theta) = \frac{1 - R(\theta)}{1 + \frac{\lambda_{\text{opt}}}{\lambda_{e-e}} \cos \theta} \cdot \frac{1}{4\pi m \hbar \omega}$$



Motivation

How to deal with the difficulties in 3D case

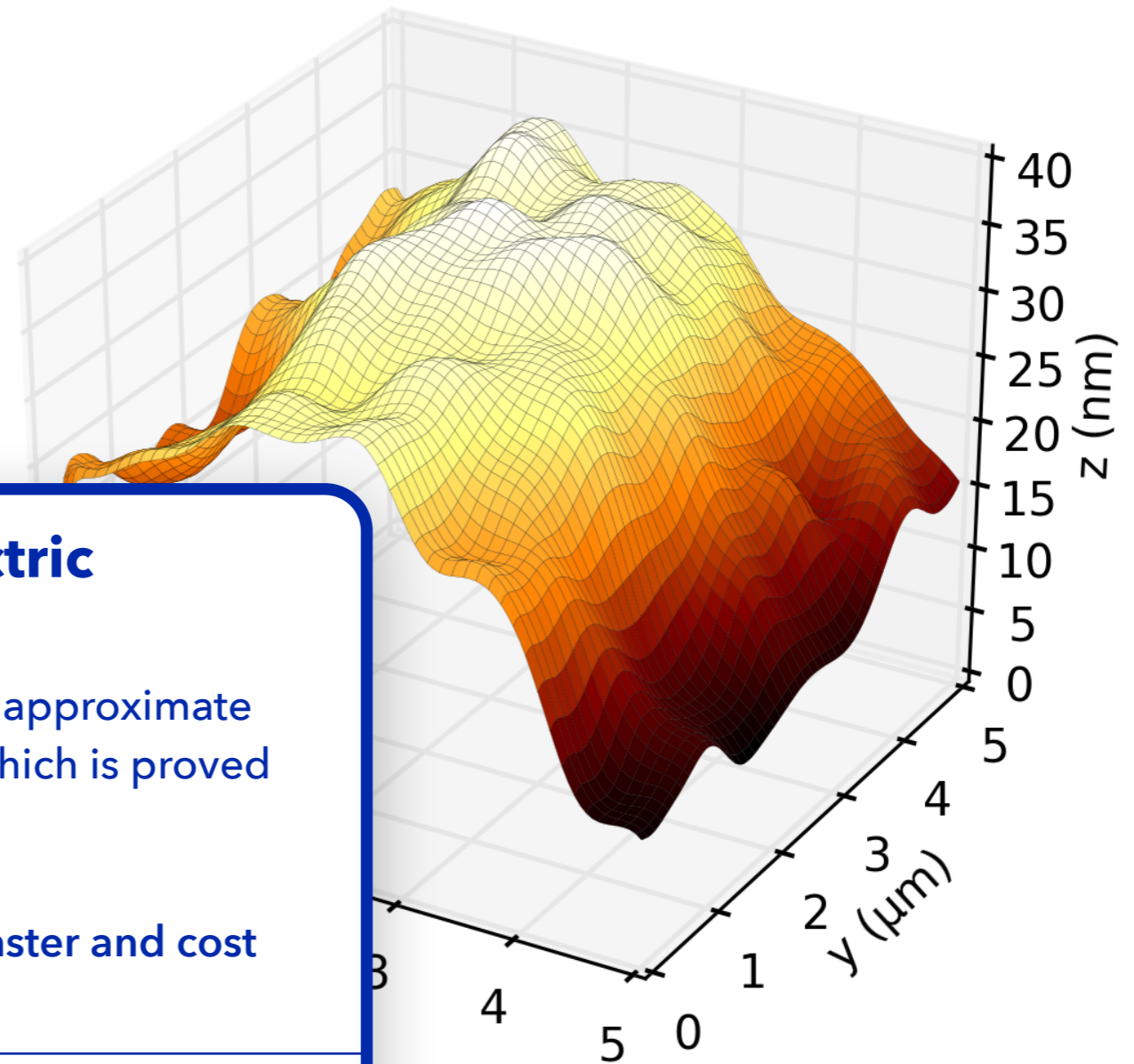
- Generate initial electron samples (**slope effect**)
- Simulation of the EM field near a real-life rough surface (**field effect**)

Approximate Formula for the Electric Potential

For gently undulating surface, there exist some approximate formula for the electric potential distribution, which is proved to be accurate enough for our case.

Therefore we could generate the fields much faster and cost much less memory.

$$\phi(x, y, z) = z - \int dk_x dk_y R(k_x, k_y) \cdot e^{j(k_x x + k_y y) - kz}$$



Modeling

The PSF of the flat surface

Point Spread Function

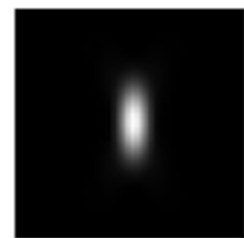
The response (image) is the convolution of the point spread function (PSF) and the source (object).



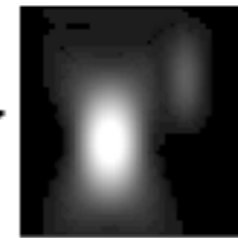
METAL VACUUM



Object



PSF



Image

$$D(x, y) = I(x, y) * f(x, y)$$

$$s \left(\frac{1}{\lambda_{\text{opt}}} + \frac{1}{\lambda_{\text{e-e}}} \right) + \frac{\hbar\omega - E_F}{4\pi} \sin \theta$$

p_y, p_z

$$\frac{\sqrt{x^2 + y^2}}{\lambda}$$

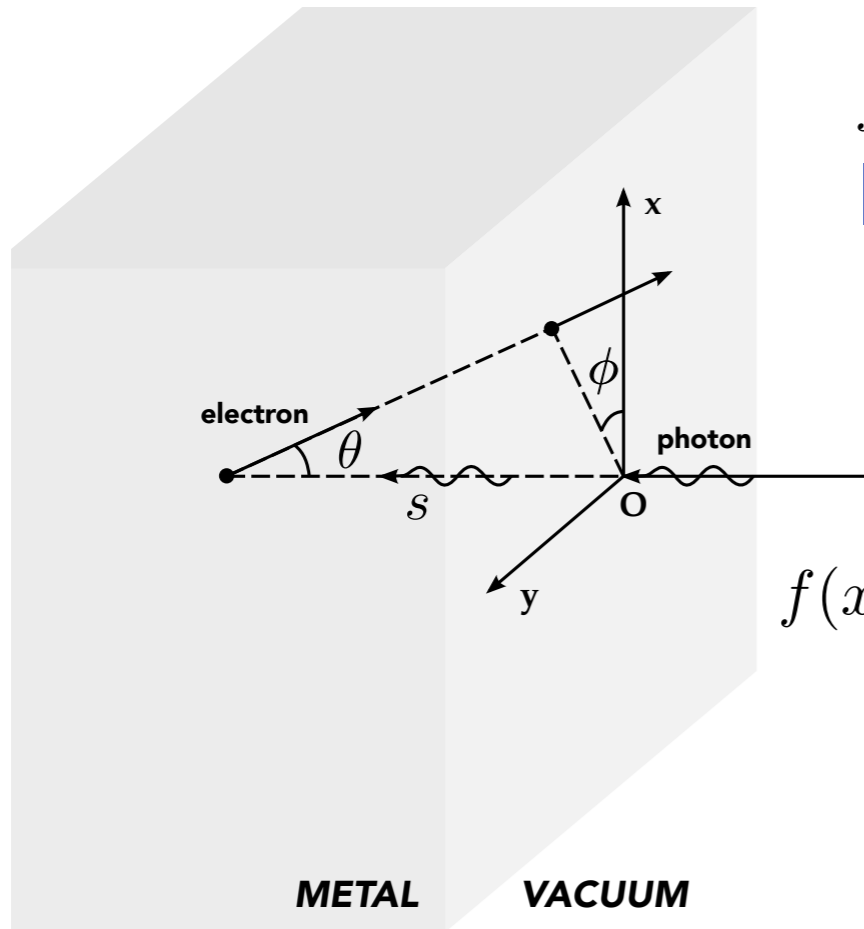
$$\delta(xp_y - yp_x)$$

p_m^2

$$p_M^2 - p_m^2 - p_x^2 - p_y^2 - p_z^2$$

Modeling

The PSF of the flat surface



$$f(s, \theta, \phi, E, \omega) = (1 - R) \frac{1}{\lambda_{\text{opt}}} \exp \left[-s \left(\frac{1}{\lambda_{\text{opt}}} + \frac{1}{\bar{\lambda}_{e-e}} \right) \right] \cdot \frac{H(E_F - E)H(E + \hbar\omega - E_F) \sin \theta}{\hbar\omega \cdot 4\pi}$$

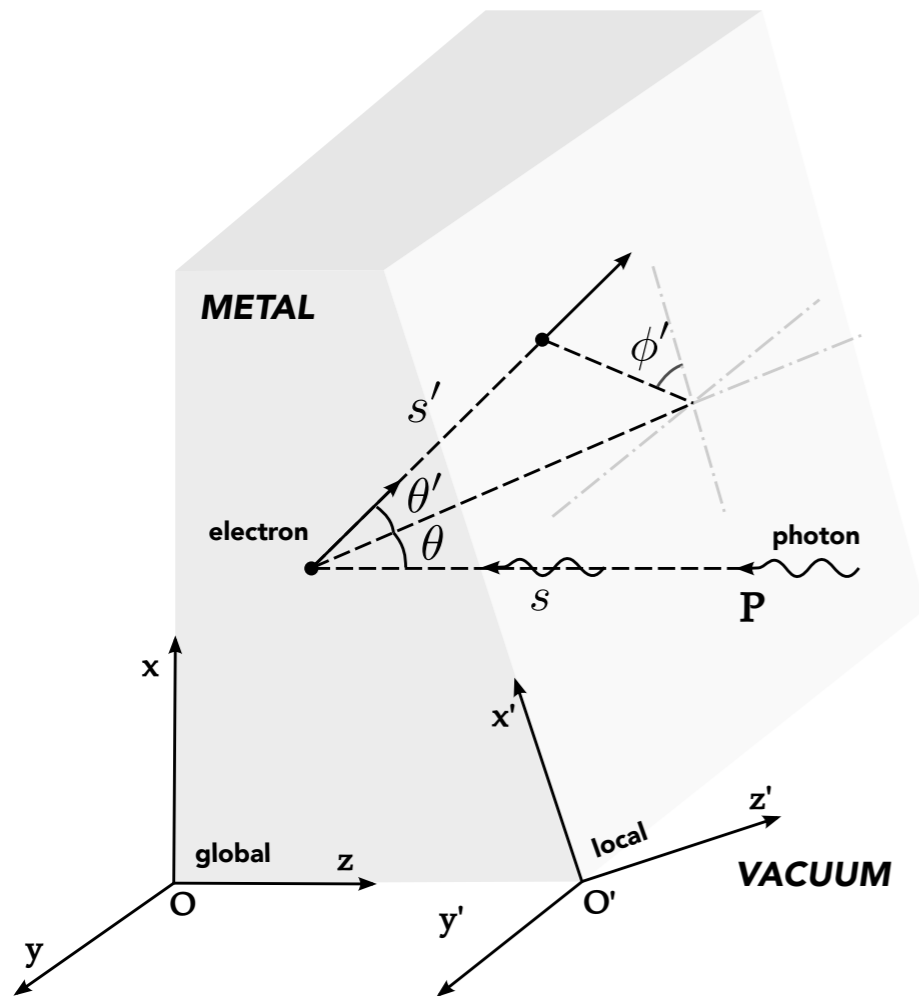
Dowell, 2009, PRST

Transform $(s, \theta, \phi, E, \omega)$ to (x, y, p_x, p_y, p_z)

$$f(x, y, p_x, p_y, p_z) = C \exp \left[-\frac{\sqrt{p_z^2 + p_m^2}}{\sqrt{p_x^2 + p_y^2}} \cdot \frac{\sqrt{x^2 + y^2}}{\lambda} \right] \cdot \frac{p_z}{\sqrt{p_x^2 + p_y^2 + p_z^2 + p_m^2}} \cdot \delta(xp_y - yp_x) \cdot H(p_z)H(xp_x)H(p_M^2 - p_m^2 - p_x^2 - p_y^2 - p_z^2)$$

Modeling

The PSF of the rough surface

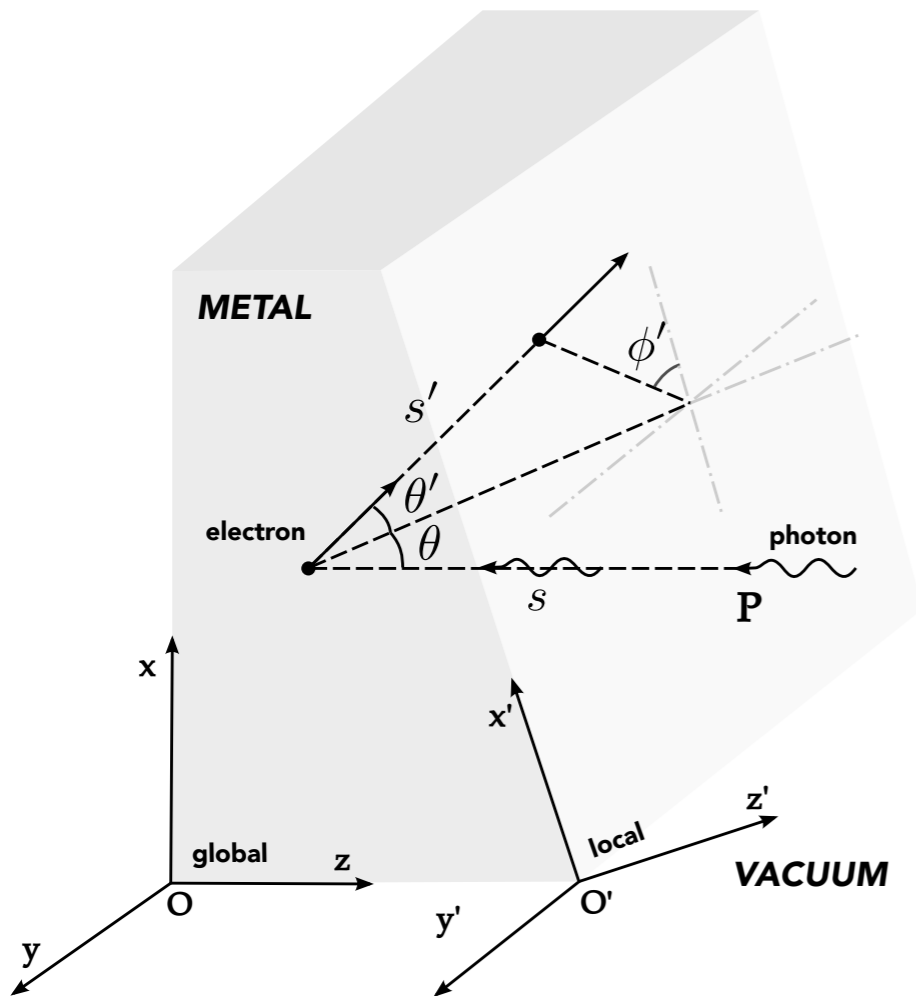


$$D|_{\mathbf{P}} = I(x, y) * f(x, y, p_x, p_y, p_z) \Big|_{x=x_0, y=y_0}$$

$$D|_{\mathbf{P}} \approx I(x_0, y_0) f_p(p_x, p_y, p_z)$$

Modeling

The PSF of the rough surface



$$D|_{\mathbf{P}} = I(x, y) * f(x, y, p_x, p_y, p_z) \Big|_{x=x_0, y=y_0}$$

$$D|_{\mathbf{P}} \approx I(x_0, y_0) f_p(p_x, p_y, p_z)$$

The Momentum PSF

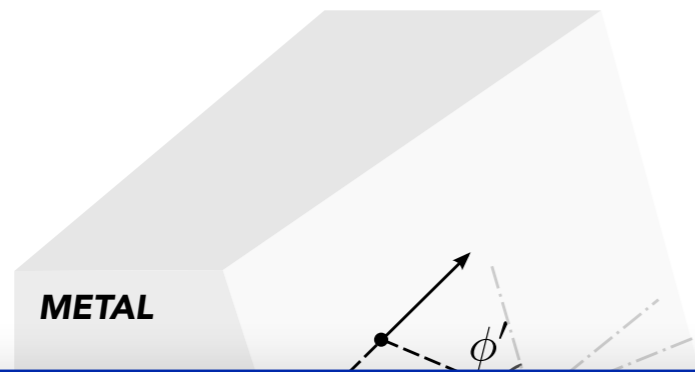
The momentum PSF is the integration of PSF over the real-space (x, y) .

$$f_p(p_x, p_y, p_z) = \frac{C_p(\theta)p_z}{\sqrt{p_z^2 + p_m^2} \cdot \sqrt{p_x^2 + p_y^2 + p_z^2 + p_m^2}} \cdot H(p_z)H(p_M^2 - p_m^2 - p_x^2 - p_y^2 - p_z^2)$$

$$C_p(\theta) = \frac{1 - R(\theta)}{1 + \frac{\lambda_{\text{opt}}}{\lambda_{e-e}} \cos \theta} \cdot \frac{1}{4\pi m \hbar \omega}$$

Modeling

The PSF of the rough surface

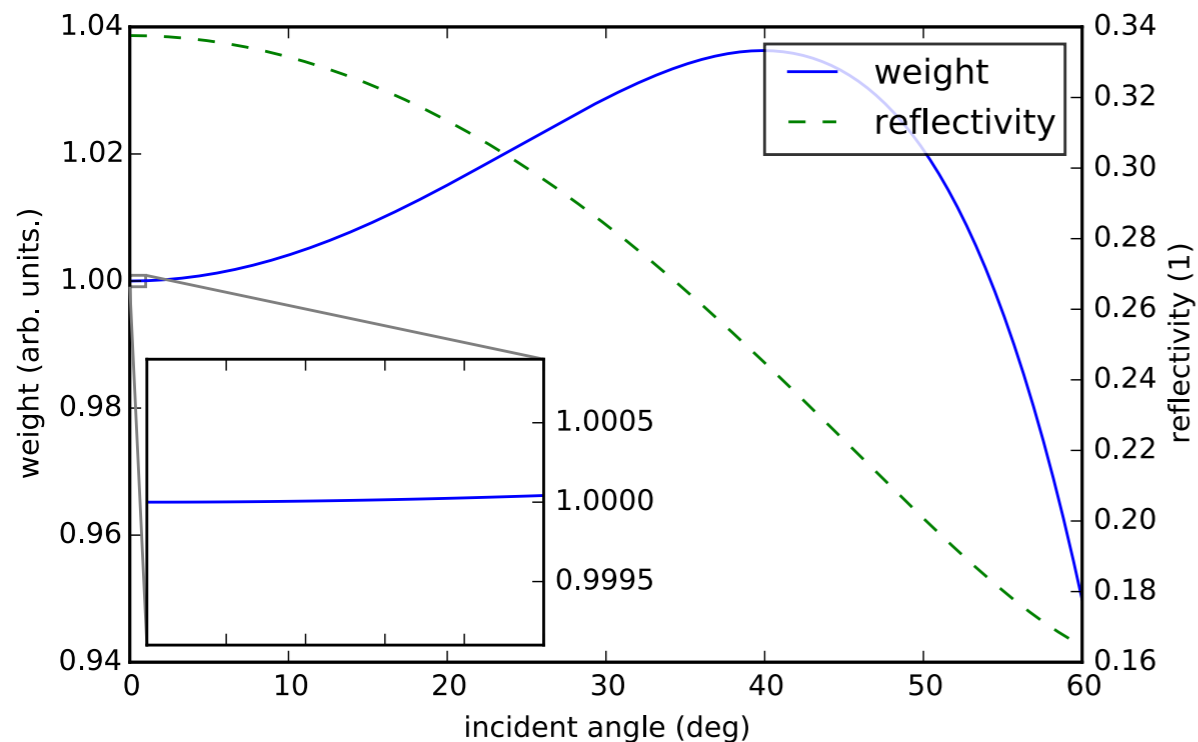


$$D|_{\mathbf{P}} = I(x, y) * f(x, y, p_x, p_y, p_z) \Big|_{x=x_0, y=y_0}$$

$$D|_{\mathbf{P}} \approx I(x_0, y_0) f_p(p_x, p_y, p_z)$$

The Effect of the Incident Angle

For a gently undulating surface, the effect of the incident angle could be neglected.



The Momentum PSF

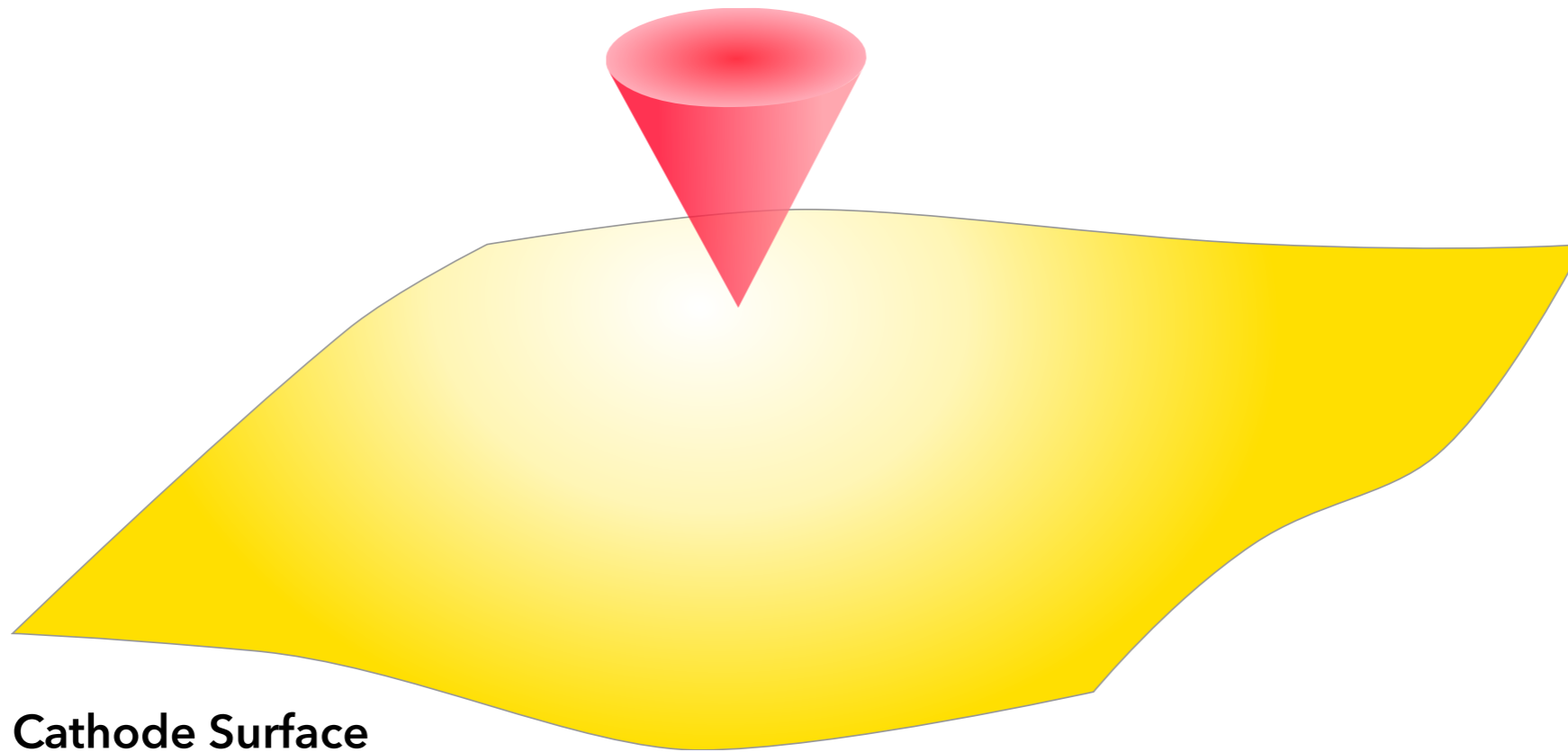
The momentum PSF is the integration of PSF over real-space (x, y) .

$$D(p_x, p_y, p_z) = \frac{C_p(\theta) p_z}{\sqrt{p_z^2 + p_m^2} \cdot \sqrt{p_x^2 + p_y^2 + p_z^2 + p_m^2}} \cdot H(p_z) H(p_M^2 - p_m^2 - p_x^2 - p_y^2 - p_z^2)$$

$$C_p(\theta) = \frac{1 - R(\theta)}{1 + \frac{\lambda_{\text{opt}}}{\lambda_{e-e}} \cos \theta} \cdot \frac{1}{4\pi m \hbar \omega}$$

Modeling

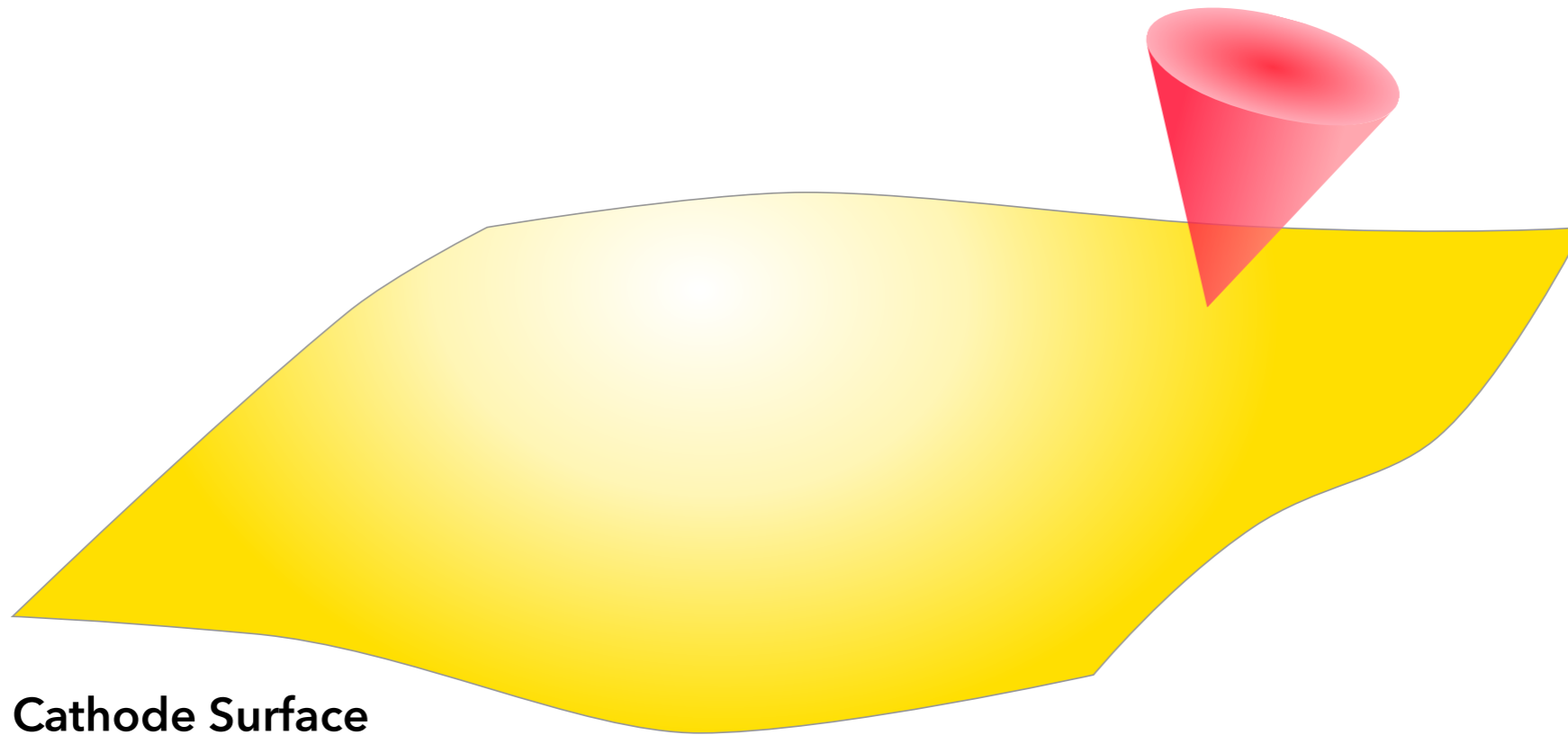
The slope effect on the rough surface



$$f_p(p_x, p_y, p_z) = \frac{C_{p0} \cdot p_z}{\sqrt{p_z^2 + p_m^2} \cdot \sqrt{p_x^2 + p_y^2 + p_z^2 + p_m^2}}$$

Modeling

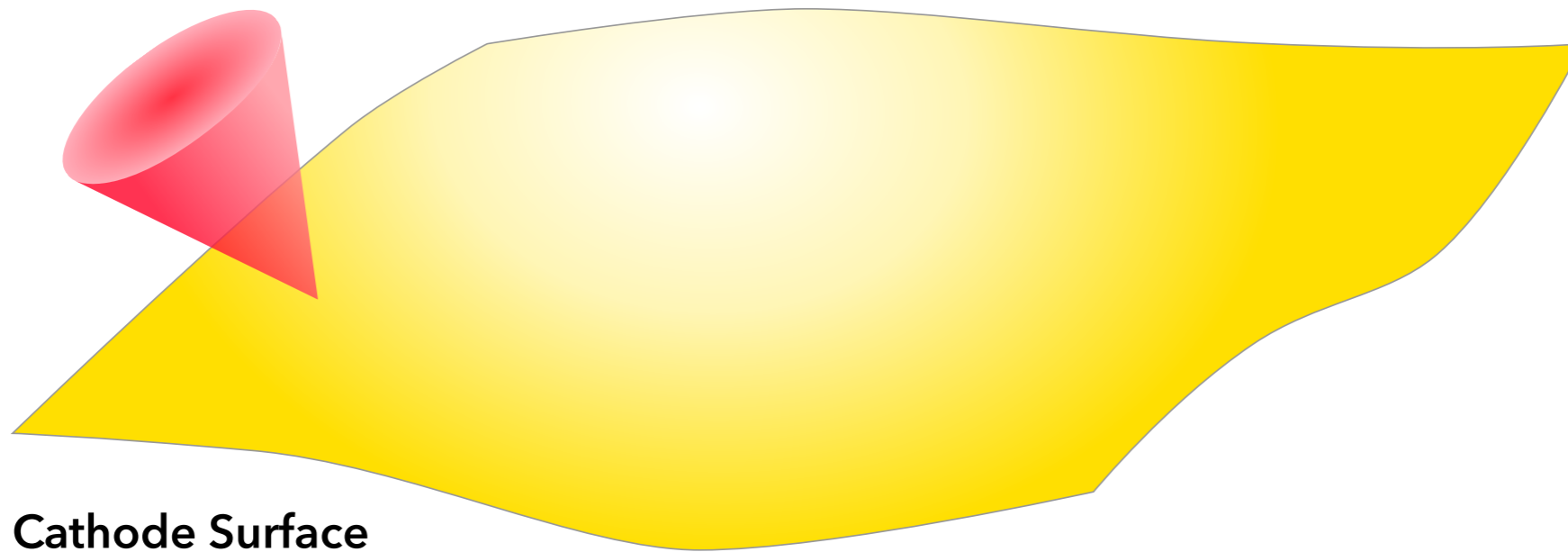
The slope effect on the rough surface



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Modeling

The slope effect on the rough surface



$$f_p(p_x, p_y, p_z) = \frac{C_{p0} \cdot p_z}{\sqrt{p_z^2 + p_m^2} \cdot \sqrt{p_x^2 + p_y^2 + p_z^2 + p_m^2}}$$

Modeling

The electric field distribution near the rough surface

$$\phi(x, y, z) = z + \int dk_x dk_y C(k_x, k_y) \cdot e^{j(k_x x + k_y y) - kz}$$

The Form of the Approximate Potential

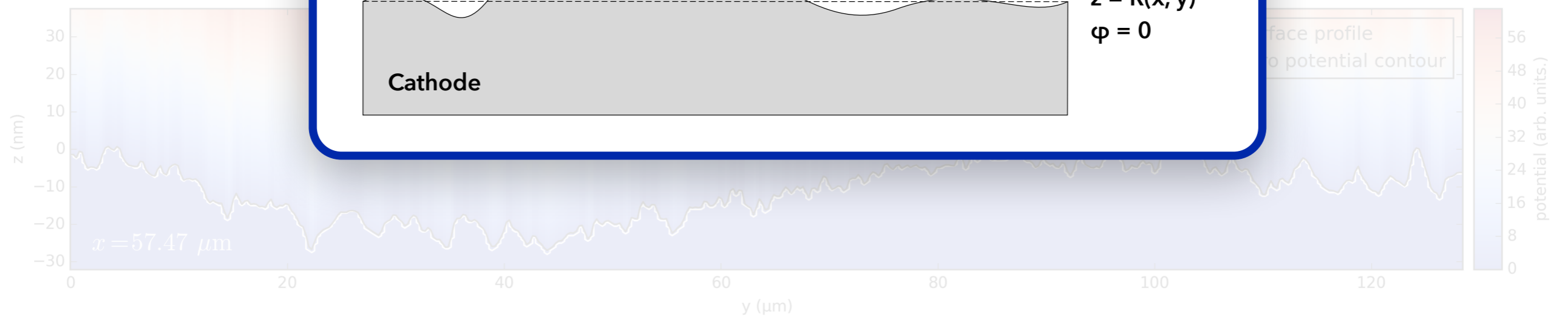
The form is set to satisfy the Laplace's equation and the B.C. for infinity.

----- $z = d \rightarrow +\infty$
 $\phi = d$

Vacuum $\Delta\phi = 0$

$z = R(x, y)$
 $\phi = 0$

Cathode



Modeling

The electric field distribution near the rough surface

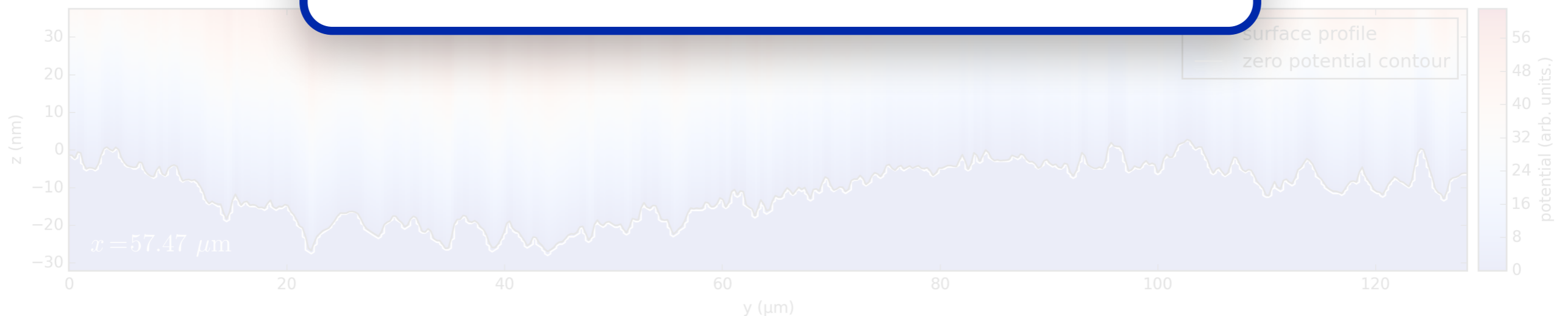
$$\phi(x, y, z) = z + \int dk_x dk_y C(k_x, k_y) \cdot e^{j(k_x x + k_y y) - kz}$$

$$\phi(x, y, z) = z - \int dk_x dk_y R(k_x, k_y) \cdot e^{j(k_x x + k_y y) - kz}$$

The B.C. at Surface

When $kR(x, y) \ll 1$, the B.C. at surface would lead to $C(k_x, k_y) = -R(k_x, k_y)$.

$$\begin{aligned} \phi(x, y, R(x, y)) &= R(x, y) + \int dk_x dk_y C(k_x, k_y) \cdot e^{j(k_x x + k_y y) - kR(x, y)} \\ &\approx R(x, y) + \int dk_x dk_y C(k_x, k_y) \cdot e^{j(k_x x + k_y y)} (1 - kR(x, y)) \\ &= \int dk_x dk_y (R(k_x, k_y) + C(k_x, k_y)) \cdot e^{j(k_x x + k_y y)} + O(1) \\ &= O(1) \quad \text{when } R(k_x, k_y) + C(k_x, k_y) = 0 \end{aligned}$$



Modeling

The electric field distribution near the rough surface

$$\phi(x, y, z) = z + \int dk_x dk_y C(k_x, k_y) \cdot e^{j(k_x x + k_y y) - kz}$$

$$\phi(x, y, z) = z -$$

The B.C. at Surf

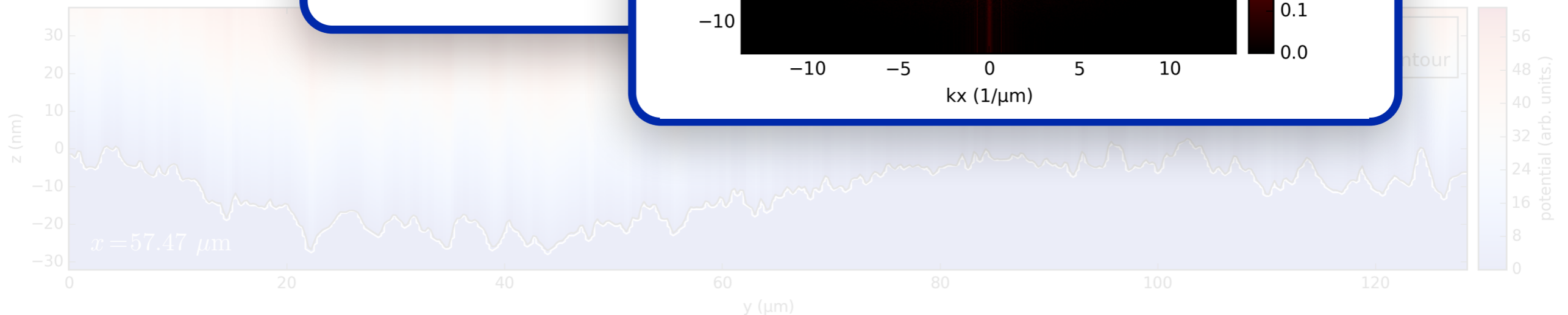
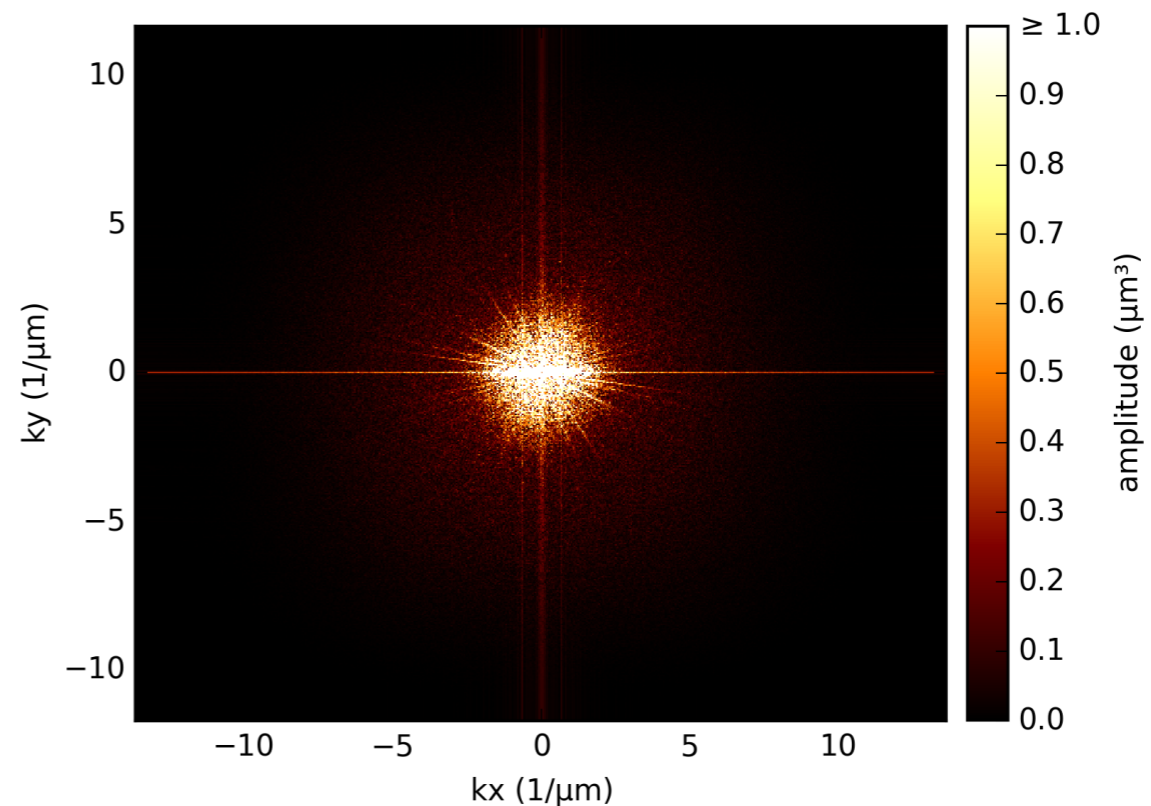
When $kR(x, y) \ll 1$,
 $C(k_x, k_y) = -R(k_x, k_y)$.

$$\begin{aligned} \phi(x, y, R(x, y)) &= R(x, y) \\ &\approx R(x, y) \\ &= \int dk_x \\ &= O(1) \end{aligned}$$

Gently Undulating Surface

A gently undulating surface should mean that:

$$\text{rms}(R) \cdot \text{rms}(k) \ll 1$$



Modeling

The electric field distribution near the rough surface

$$\phi(x, y, z) = z + \int dk_x dk_y C(k_x, k_y) \cdot e^{j(k_x x + k_y y) - kz}$$

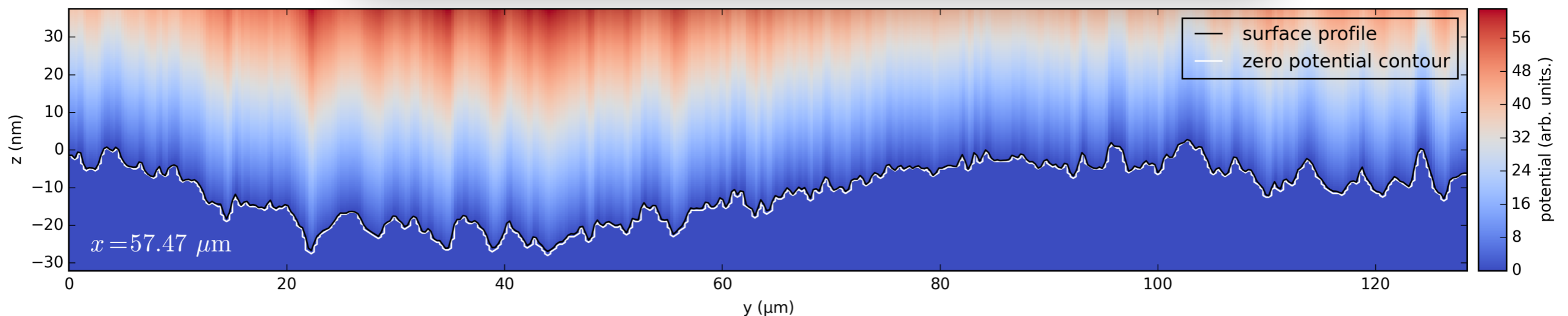
$$\phi(x, y, z) = z - \int dk_x dk_y R(k_x, k_y) \cdot e^{j(k_x x + k_y y) - kz}$$

Approximate Formula for the Electric Field

$$E_x = j \int dk_x dk_y \cdot k_x R(k_x, k_y) \cdot e^{j(k_x x + k_y y) - kz}$$

$$E_y = j \int dk_x dk_y \cdot k_y R(k_x, k_y) \cdot e^{j(k_x x + k_y y) - kz}$$

$$E_z = -1 - \int dk_x dk_y \cdot k R(k_x, k_y) \cdot e^{j(k_x x + k_y y) - kz}$$



Theory

3D arbitrary surface

Saturated Transverse Momentum

$$A = eE/m$$

$$\begin{aligned} p_\infty - p_0 &= m\sqrt{\frac{A}{2}} \cdot \int -\frac{E_x}{\sqrt{z}} dz \\ &= -jm\sqrt{\frac{\pi A}{2}} \cdot \int dk_x dk_y \frac{k_x}{\sqrt{k}} R(k_x, k_y) \cdot e^{j(k_x x + k_y y)} \end{aligned}$$

$$\varepsilon^2 = \langle x^2 \rangle \langle p_x^2 \rangle - \langle xp_x \rangle^2$$

Roughness Emittance on Arbitrary Gently Undulating Surface

$$\varepsilon_x^2 = \varepsilon_{D,x}^2 \left[1 - \langle \partial_x^2 R \rangle + \frac{\left\langle \left(p'_z \cdot \partial_x R + jm\sqrt{\frac{\pi A}{2}} \cdot \int dk_x dk_y \frac{k_x}{\sqrt{k}} R(k_x, k_y) \cdot e^{j(k_x x + k_y y)} \right)^2 \right\rangle}{\langle p_x'^2 \rangle} \right]$$

Simulation

The principles

- Initial electron beam sampling
- EM field generation
- Motion equation integration

Simulation

The principles

- Initial electron beam sampling

- EM f

Average Number of Attempts to Produce an Accepted Sample

- Moti

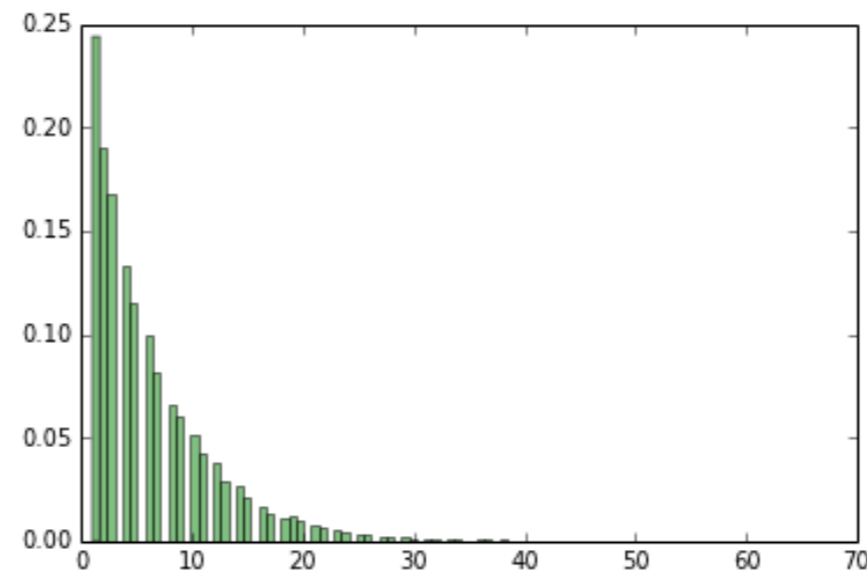
The samples generated by rejective method obey the geometry distribution.

$$N \sim G(p)$$

$$p_m = \sqrt{2m(E_F + \phi_{\text{eff}})}$$

$$p_M = \sqrt{2m(E_F + \hbar\omega)}$$

$$E(N) = \pi \left(1 + \frac{p_m}{p_M} \right) \approx 2\pi$$



Simulation

The principles

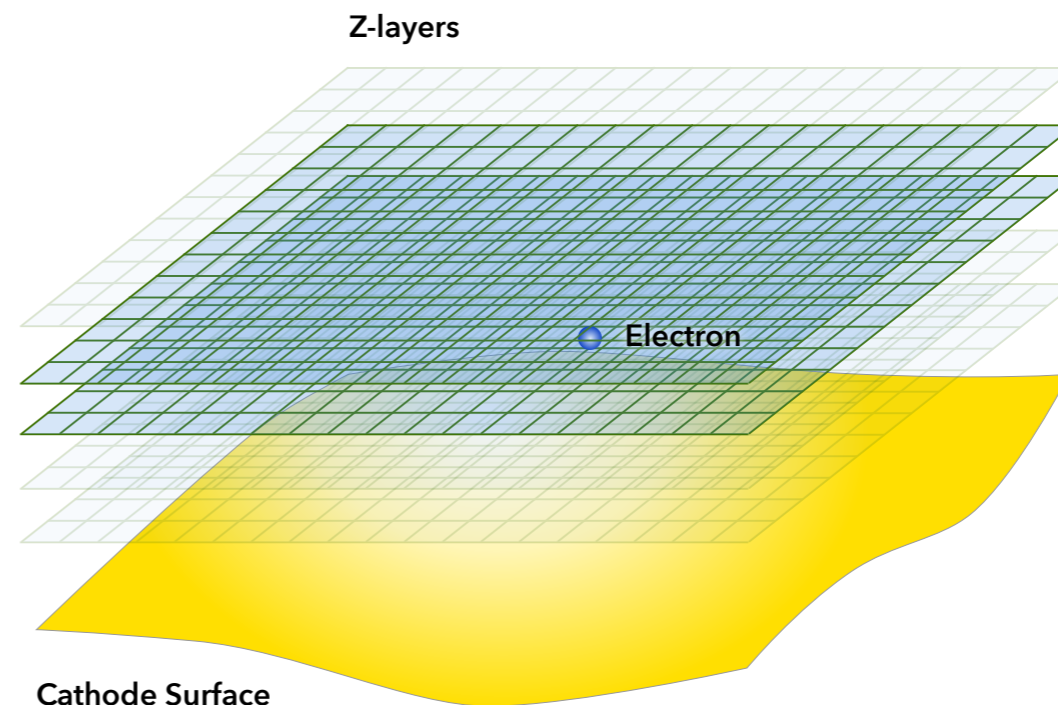
- Initial electron beam
- EM field generation
- Motion equation

Z-based Motion Equations

We choose the z-based motion equations because the E-field is calculated by z-layer, z-based motion could guarantee the accuracy.

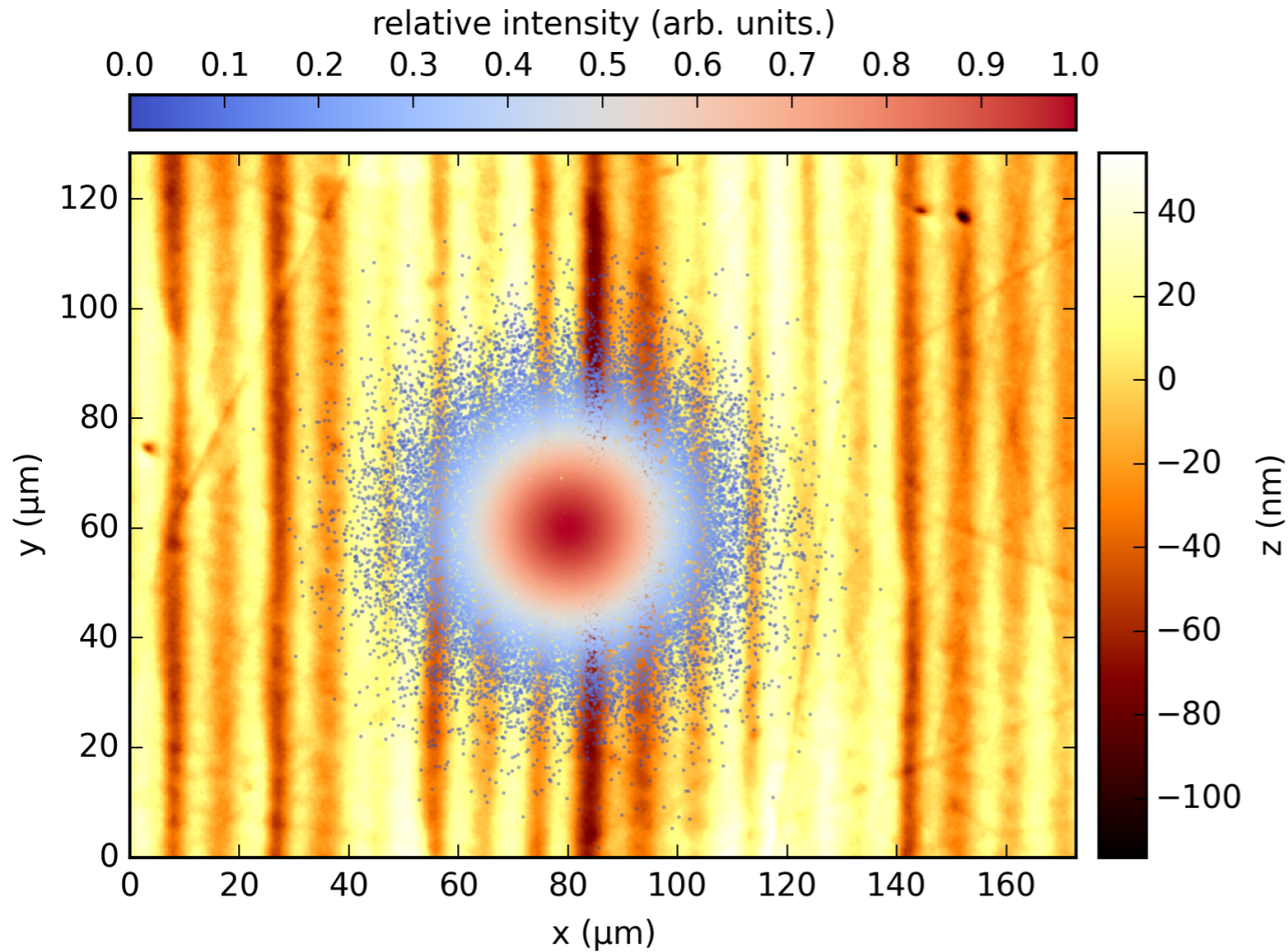
$$\frac{dp_x [\text{keV}/c]}{dz [\text{nm}]} = 511 \times 10^{-6} \cdot \frac{E_0 [\text{MV}/\text{m}]}{p_z [\text{keV}/c]} \cdot \hat{E}_x(x, y, z)$$

$$\frac{dx [\mu\text{m}]}{dz [\text{nm}]} = \frac{p_x [\text{keV}/c]}{p_z [\text{keV}/c]} \cdot 1 \times 10^{-3}$$



Simulation

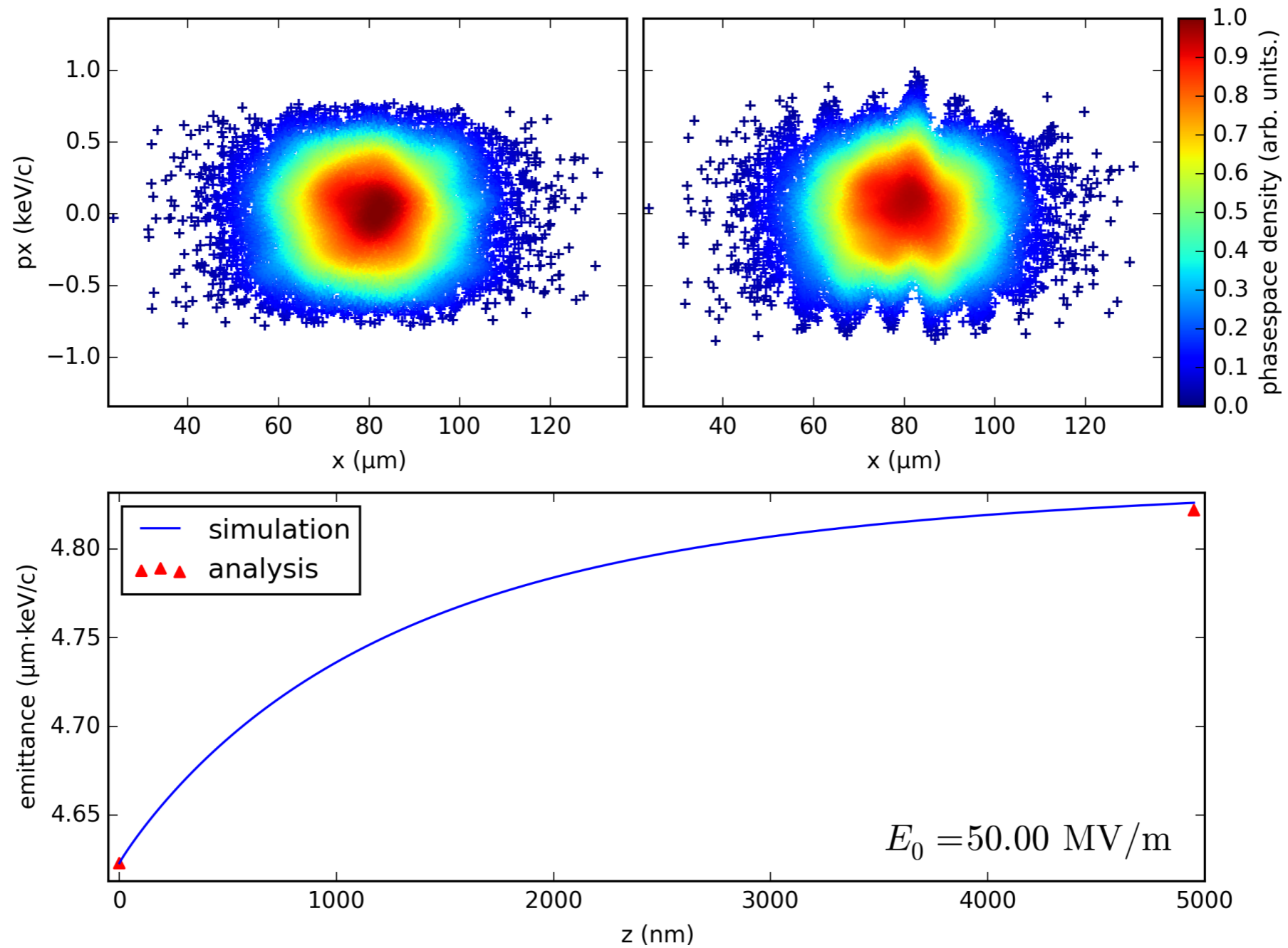
The simulation configuration



Parameter	Value	Unit	Description
λ_l	266.0	nm	laser wavelength
l-dist	uniform	-	laser transverse distribution
r_l	20.0	μm	laser transverse radius
x_l	80.0	μm	laser incident x center
y_l	60.0	μm	laser incident y center
mat	copper	-	material of the cathode
E_0	50.0	MV/m	effective electric field strength
ϕ_w	4.31	eV	work function
ϕ_{eff}	4.04	eV	effective work function
E_F	7.0	eV	Fermi energy
N	10000	-	number of particles
z_i	0	nm	simulation starting position
z_f	5000.0	nm	simulation ending position
dz	10.0	nm	simulation z step

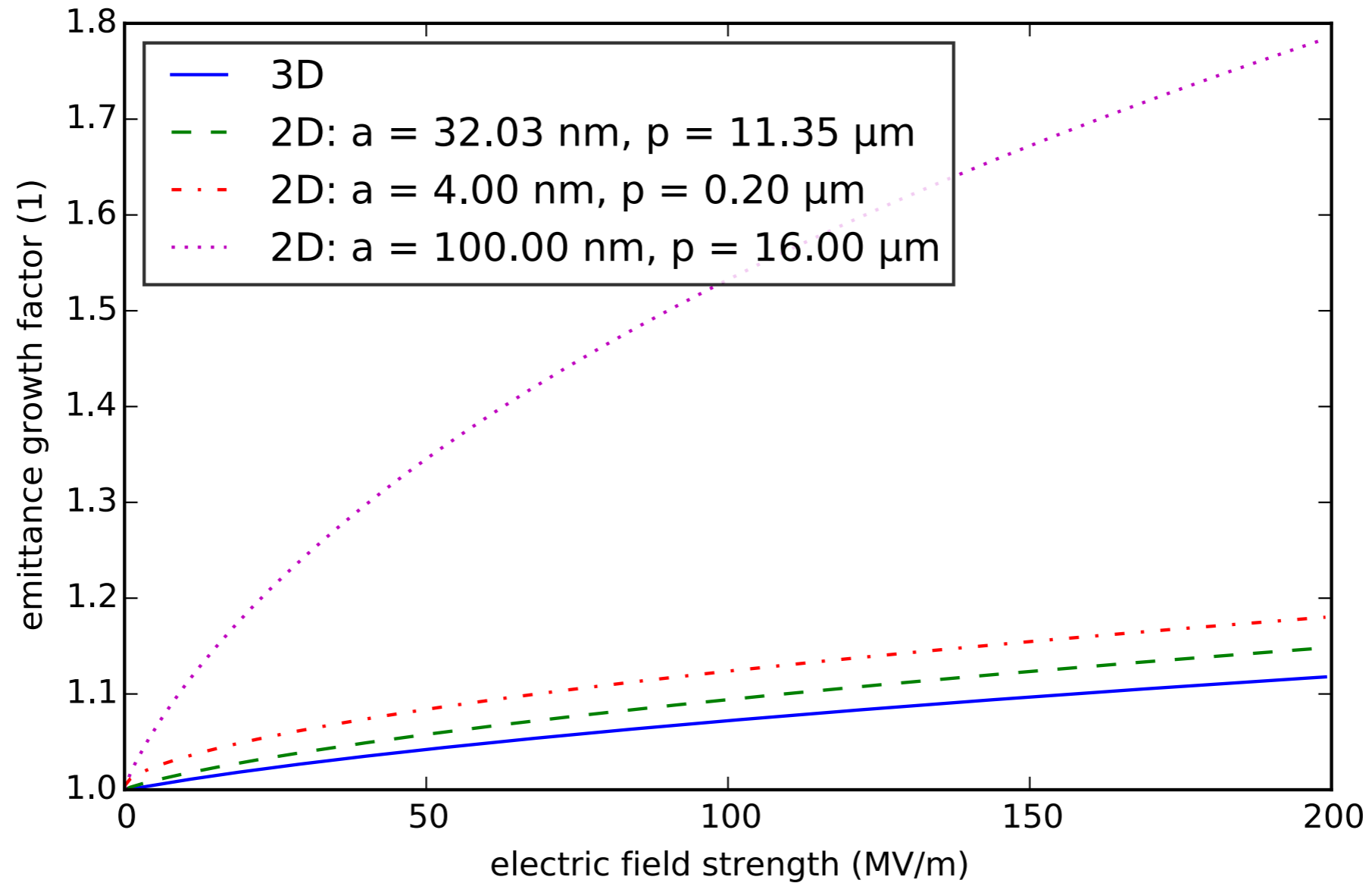
Simulation

The phase-space & emittance evolution



Simulation

Comparison between 2D and 3D result



$$\varepsilon_{n,x}^2 = \sigma_x^2 \cdot \left[\frac{\hbar\omega - \phi_{\text{eff}}}{3mc^2} + \frac{\pi e^2}{mc^2} \cdot \frac{R_q^2 E}{\lambda_q} \right]$$

Summary

Pros & Cons

- Reveal a simple rule for the initial phase-space distribution due to slope effect
- Predict the emittance growth / phase-space evolution based on the cathode morphology
- Show the roughness tolerance for a given emittance growth upper limit
- **NOT** include the **surface emission** effect
- **NOT** consider the possible **SPPs** (**S**urface **P**lasmon **P**olaritons) generation
- **NOT** consider the **microwave smoothing** effect
- **NOT** consider the **effective work function variation** due to the surface roughness

Thanks

Questions or Comments