

# **Mirror Reflectivity in XFEL cavity**

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# Contents

1. Reflection Formula
2. Simulation
3. Inclusion of interaction with gain
4. Conclusion

# 1. Reflection Formula

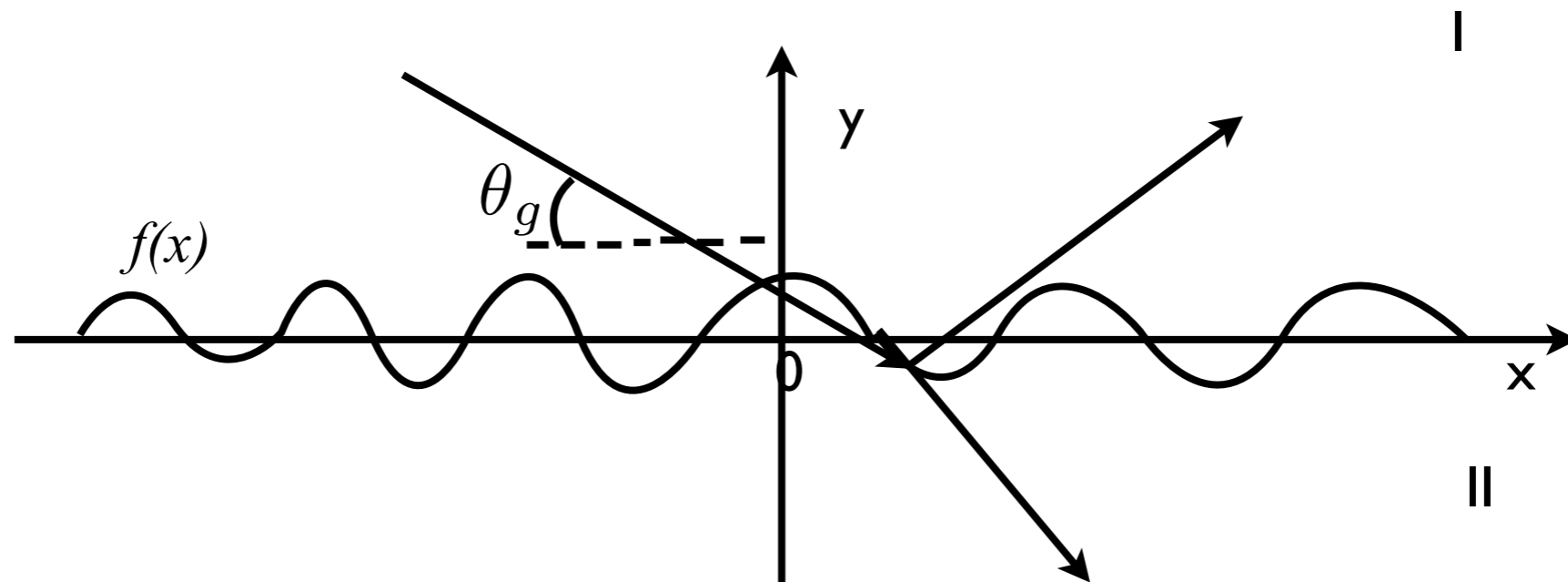
- well-known specular reflectivity formula

$$\mathcal{R} \approx r_0 e^{-2k^2 \theta_g^2 \sigma^2} \quad \frac{k_g}{k_I} \ll \theta \quad \text{Debye-Waller}$$

$$\mathcal{R} \approx r_0 e^{-2k^2 \theta_g \sqrt{n^2 - \cos^2 \theta_g} \sigma^2} \quad \frac{k_g}{k_I} \gg \theta \quad \text{Nevot-Croce}$$

## Helmholtz equation

$$\Delta u_I + k_1^2 u_I = 0, \quad k_1^2 = \omega^2 \epsilon_1 \mu_1 = \omega^2 n_1^2 / c^2 \quad \text{for } y > f(x)$$
$$\Delta u_{II} + k_2^2 u_{II} = 0, \quad k_2^2 = \omega^2 \epsilon_2 \mu_2 = \omega^2 n_2^2 / c^2 \quad \text{for } y < f(x)$$



## Boundary conditions

$$u_I(x, f(x)) = u_{II}(x, f(x))$$

$$\text{for } P \text{ polarization } \frac{\partial u_I}{\partial n}(x, f(x)) = \frac{\partial u_{II}}{\partial n}(x, f(x))$$

$$\text{for } S \text{ polarization } \epsilon_1 \frac{\partial u_I}{\partial n}(x, f(x)) = \epsilon_2 \frac{\partial u_{II}}{\partial n}(x, f(x))$$

## The general solution to Helmholtz equation

$$u_I(x, y) = \int_{-\infty}^{\infty} d\alpha (a_\alpha e^{i\alpha x + i\beta y} + a'_\alpha e^{i\alpha x - i\beta y}), \quad \beta_\alpha = \sqrt{k_1^2 - \alpha^2}$$

$$u_{II}(x, y) = \int_{-\infty}^{\infty} d\alpha (b_\alpha e^{i\alpha x + i\beta' y} + b'_\alpha e^{i\alpha x - i\beta' y}), \quad \beta'_\alpha = \sqrt{k_2^2 - \alpha^2}$$

Assuming  $|\beta_\alpha f(x)| \ll 1$ , we expand boundary condition to its second order, arriving at matrix equation.

$$A\mathcal{X} + A'\mathcal{Y} = B\mathcal{Z}$$

$$C\mathcal{X} + C'\mathcal{Y} = D\mathcal{Z}$$

For compact computation, we introduced matrix notation as

$$\mathcal{X}_{\alpha'} = a_{\alpha'}, \mathcal{Y}_{\alpha} = a'_{\alpha}, \mathcal{Z}_{\alpha} = b_{\alpha}$$

$$\mathcal{A}_{\alpha, \alpha'} = \delta_{\alpha, \alpha'} + i\beta_{\alpha'} \tilde{f}_{\alpha' - \alpha} - \frac{1}{2} \beta_{\alpha'}^2 \tilde{f}_{\alpha' - \alpha}^2$$

$$\begin{aligned} \mathcal{C}_{\alpha, \alpha'} = & i\beta_{\alpha'} \delta_{\alpha, \alpha'} - \beta_{\alpha'}^2 \tilde{f}_{\alpha' - \alpha} - i\alpha' \tilde{f}'_{\alpha' - \alpha} \\ & - \frac{i}{2} \beta_{\alpha'}^3 \tilde{f}_{\alpha' - \alpha}^2 + \alpha' \beta_{\alpha'} (\tilde{f} \tilde{f}')_{\alpha' - \alpha} - \frac{i}{2} \beta_{\alpha'} (\tilde{f}')^2_{\alpha' - \alpha} \end{aligned}$$

$\mathcal{A}'\mathcal{B}, \mathcal{C}', \mathcal{D}$  are obtained from  $\mathcal{A}, \mathcal{C}$  by replacing  $\beta_{\alpha}$  with  $-\beta_{\alpha}, \beta'_{\alpha}$ , respectively.

Its formal solution is given as

$$\begin{aligned} \mathcal{Y} &= -(\mathcal{B}^{-1} \mathcal{A}' - \mathcal{D}^{-1} \mathcal{C}')^{-1} (\mathcal{B}^{-1} \mathcal{A} - \mathcal{D}^{-1} \mathcal{C}) \mathcal{X} \\ \mathcal{Z} &= (\mathcal{A}'^{-1} \mathcal{B} - \mathcal{C}'^{-1} \mathcal{D})^{-1} (\mathcal{A}'^{-1} \mathcal{A} - \mathcal{C}'^{-1} \mathcal{C}) \mathcal{X} \end{aligned}$$

Above matrices are evaluated to be

$$a'_{\alpha} = \int_{-\infty}^{\infty} d\alpha' a_{\alpha'} \frac{(\beta'_{\alpha} - \beta_{\alpha})}{(\beta'_{\alpha} + \beta_{\alpha})} [\delta_{\alpha\alpha'} + 2i\beta_{\alpha'} \tilde{f}_{\alpha'-\alpha} - \beta_{\alpha'} \{ (\beta'_{\alpha} + \beta'_{\alpha'}) \tilde{f}^2_{\alpha'-\alpha} + 2(\beta_{\alpha''} - \beta'_{\alpha''}) \tilde{f}_{\alpha''-\alpha} \tilde{f}_{\alpha'-\alpha''} \}]$$

(1)  $\frac{k_g}{k_I} \ll \theta$ , specular reflectivity reduces to Debye-Waller

$$\beta'_{\alpha+\kappa} \approx \beta'_{\alpha}, \quad \beta_{\alpha+\kappa} \approx \beta_{\alpha} \rightarrow \mathcal{R} \approx r_0 e^{-2k^2 \theta_g^2 \sigma^2}$$

(2)  $\frac{k_g}{k_I} \gg \theta$ , it reduces to Nevot-Croce

$$\beta_{\alpha+\kappa} \approx \beta'_{\alpha+\kappa} \rightarrow \mathcal{R} \approx r_0 e^{-2k^2 \theta_g \sqrt{n^2 - \cos^2 \theta_g} \sigma^2}$$

## 2. Simulation

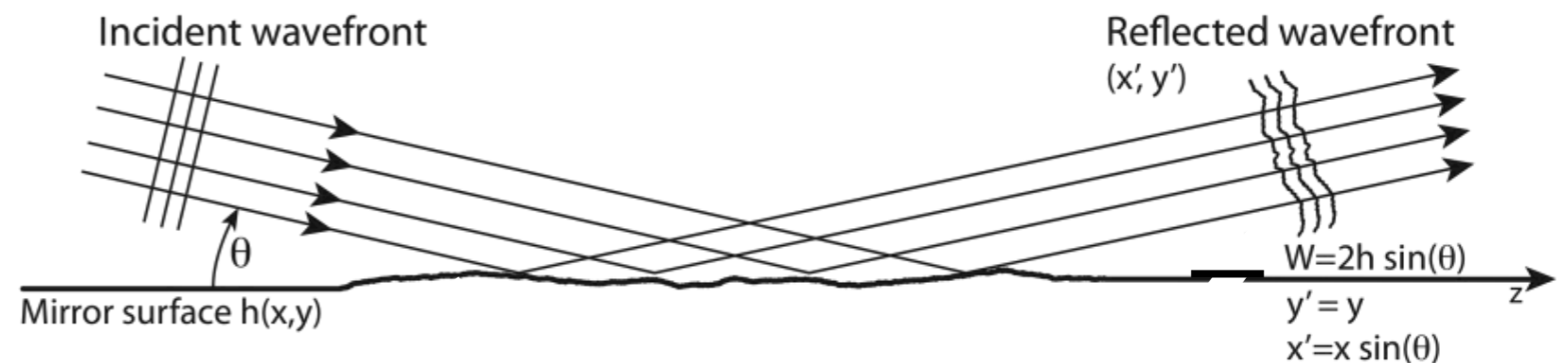
### Method

Propagation of  $E$  field through cavity is described by Fourier optics

- Vacuum Propagation**

$$\tilde{E}(\vec{k}_\perp; z'') = \tilde{E}(\vec{k}_\perp; z) e^{ik(z''-z) - \frac{i(z''-z)}{2k} k_\perp^2}$$

wave vector
distance
- Mirror Transform** Path difference  $W$  leads to phase difference of X-ray.



$$E_{out}(\vec{x}; z) = r_0 A(x/\theta_g, y) e^{-2ik\theta_g h(x/\theta_g, y) - \frac{ik}{2f} x^2} E_{in}(\vec{x}; z)$$

aperture
grazing angle

Fresnel reflectivity
focal length

# Mode Deformation

Power  $P$  at some point after mirror:

$$P(\vec{x}'_{\perp}; z') = \frac{1}{\lambda^4 (z' - z'')^2 (z'' - z)^2} \int \int \int \int d^2 x''_{\perp} d^2 x_{\perp} d^2 X''_{\perp} d^2 X_{\perp} \\ E^*(\vec{X}_{\perp}; z) E(\vec{x}_{\perp}; z) e^{i\frac{k}{2} \mathcal{A}(x''_{\perp}{}^2 - X''_{\perp}{}^2)} e^{-ik\mathcal{C} \cdot x''_{\perp} + ik\mathcal{C}' \cdot X''_{\perp} - 2ik\theta_g (h(x'') - h(X''))} \\ e^{i\frac{k}{2(z'' - z)} (x_{\perp}^2 - X_{\perp}^2)}$$

$$\text{where } \mathcal{A} = \frac{1}{(z' - z'')} + \frac{1}{(z'' - z)} - \frac{1}{f}, \quad \mathcal{C} = \frac{x'_{\perp}}{z' - z''} + \frac{x_{\perp}}{z'' - z} \\ \mathcal{C}' = \frac{x'_{\perp}}{z' - z''} + \frac{X_{\perp}}{z'' - z}$$

Random height errors are statistically described by Gaussian distribution function.

$$w(h_1, h_2, \dots, h_N; s_1, s_2, \dots, s_n) = \frac{\sqrt{\det(\Gamma)} e^{-\frac{1}{2} \sum_{ij} \Gamma_{ij} h_i h_j}}{(\sqrt{2\pi})^n}$$



$$\text{where } \Gamma^{-1} = \begin{bmatrix} \sigma^2 & \sigma^2 g(s_1 - s_2) & \cdots & \sigma^2 g(s_1 - s_n) \\ \sigma^2 g(s_1 - s_2) & \sigma^2 & \cdots & \sigma^2 g(s_2 - s_n) \\ \cdots & \cdots & \cdots & \cdots \\ \sigma^2 g(s_1 - s_n) & \sigma^2 g(s_2 - s_n) & \cdots & \sigma^2 \end{bmatrix}$$

$$\sigma^2 = \langle h^2 \rangle, \quad g(x_2 - x_1) = \frac{1}{\sigma^2} \langle h(x_1)h(x_2) \rangle$$

*rms*

correlation function

Expanding for small  $h$  and ensemble averaging over mirror samples

$$\left\langle \frac{1}{\xi^2} \int_{s''}^{s''+\xi} \int_{x''}^{x''+\xi} d\tau' d\tau'' e^{-2ik\theta_g(h(\tau')-h(\tau'+\tau''))} \right\rangle$$

$$= 1 - 2k^2\theta_g^2\sigma^2(1 - g(s'')) = 1 - k^2\theta_g^2 \int d\kappa H(\kappa) \sin^2 \kappa s''$$

$$\text{Power Spectral Density } H(\kappa) = \frac{1}{T} \tilde{h}^*(\kappa) \tilde{h}(\kappa)$$

sample length

Inserting Hermite-Gauss modes for input  $E$  field, we obtain perturbation series

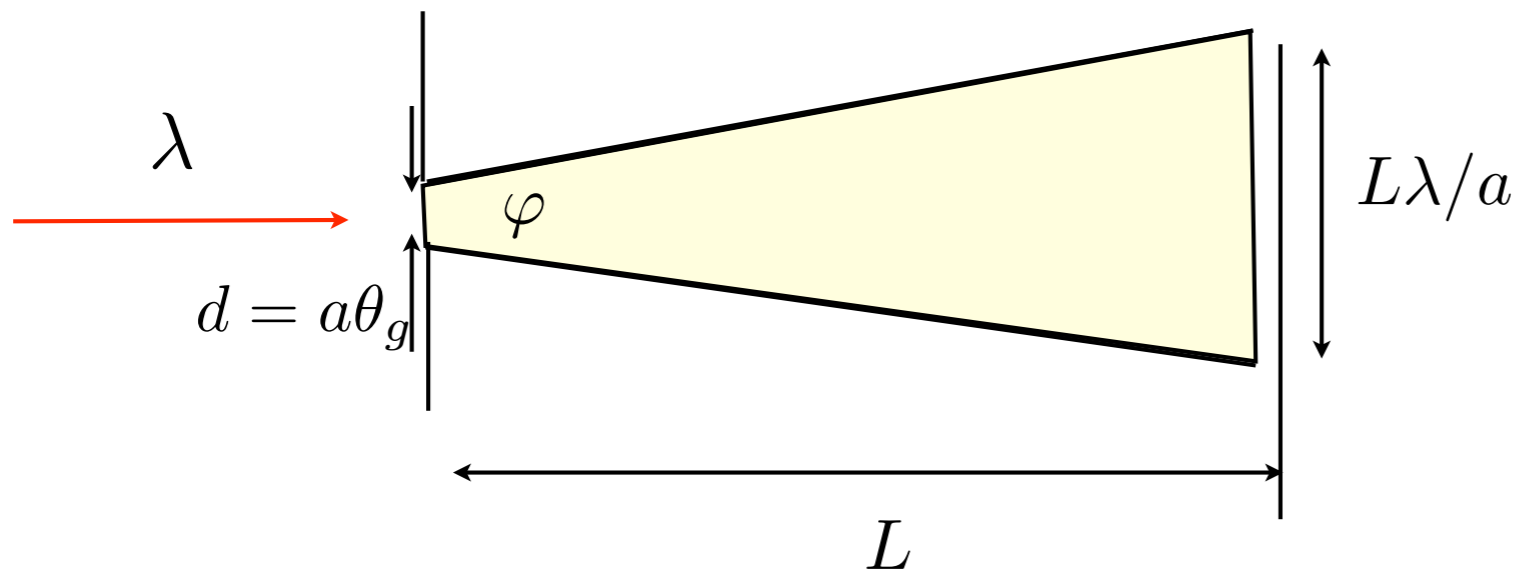
$$P_0(x'; z) = \Theta e^{-2\text{Re}[\mathcal{G}]x'^2}$$

$$\text{Re}[\mathcal{G}] = \frac{kz_R}{2L^2} \frac{1}{\left(1 + \frac{l}{L} - \frac{l}{f}\right)^2 + z_R^2 \left(\frac{1}{L} - \frac{1}{f}\right)^2}$$

$$P_2(x'; z') = \frac{k^2 \theta_g^2}{4} \int d\kappa H(\kappa) \Theta \left[ e^{-2\text{Re}\mathcal{G}(x'_\perp + (z' - z'') \frac{2\kappa}{k})^2} + e^{-2\text{Re}\mathcal{G}(x'_\perp - (z' - z'') \frac{2\kappa}{k})^2} - 2e^{-2\text{Re}\mathcal{G}x'_\perp{}^2} \right]$$

Diffraction of mode on the bump

$$\frac{\lambda(z' - z'')}{\lambda_g} = \frac{(z' - z'')\kappa}{k}$$



# Strehl ratio

$$\mathcal{R} = \frac{P(0)}{P_0(0)} = 1 - \frac{k^2 \theta_g^2}{2} \int d\kappa H(\kappa) \left(1 - e^{-8 \operatorname{Re} \mathcal{G} (z' - z'')^2 \frac{\kappa^2}{k^2}}\right)$$

Coherence length  $W^2 = \frac{8}{k^2} (z' - z'')^2 \operatorname{Re}[\mathcal{G}] \approx 7.53 \times 10^{-5} \text{ m}$

$$\mathcal{R} \approx 1 - \frac{k^2 \theta_g^2}{2} \left( \int_{1/l_m}^{1/W} d\kappa H(\kappa) W^2 \kappa^2 + \int_{1/W}^{1/\lambda} d\kappa H(\kappa) \right) \approx 1 - \frac{k^2 \theta_g^2}{2} W^2 \mu - \frac{k^2 \theta_g^2}{2} \sigma^2$$

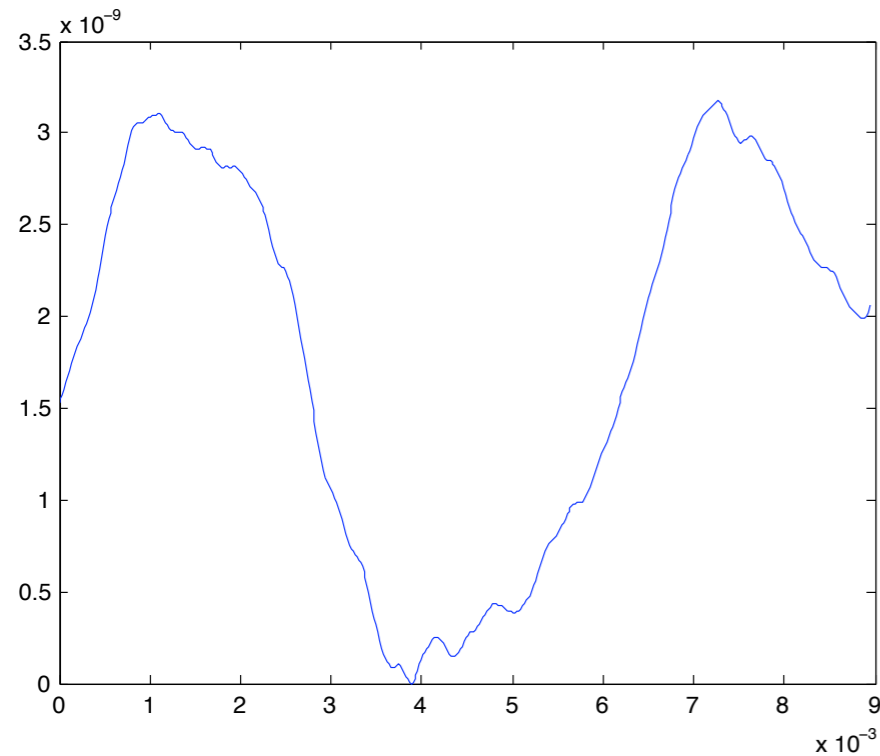
$$\mu = \int_{1/l_m}^{1/W} d\kappa H(\kappa) \kappa^2, \quad \sigma^2 = \int_{1/W}^{1/\lambda} d\kappa H(\kappa)$$

slope of figure error

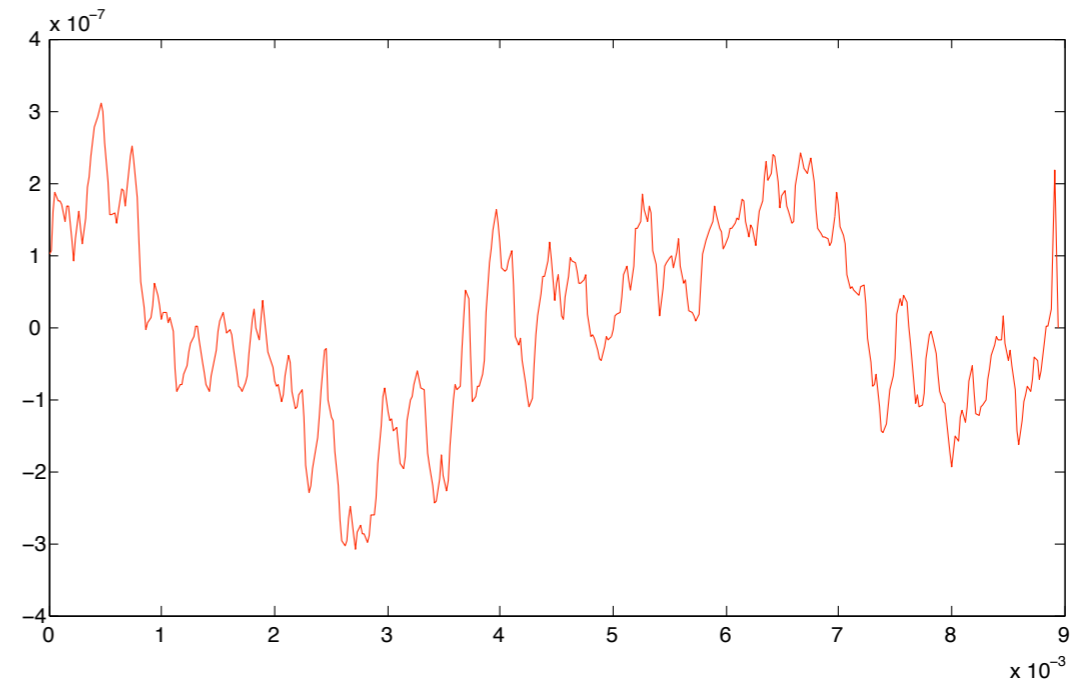
rms of finish error

# Mirror( $SiO_2$ ) PETRA-III, BESSY

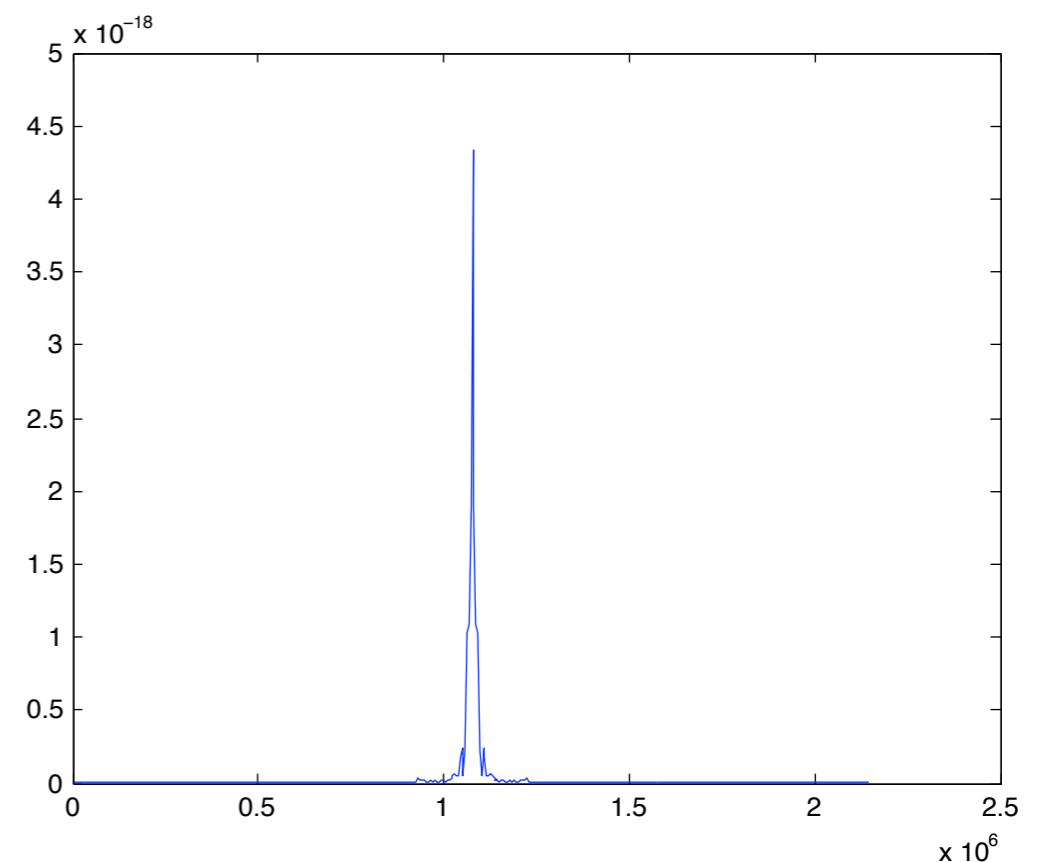
height profile



slope error



PSD(Power Spectral Density)



rms height  $1.0439 \times 10^{-9} \text{ m}$

refractive index

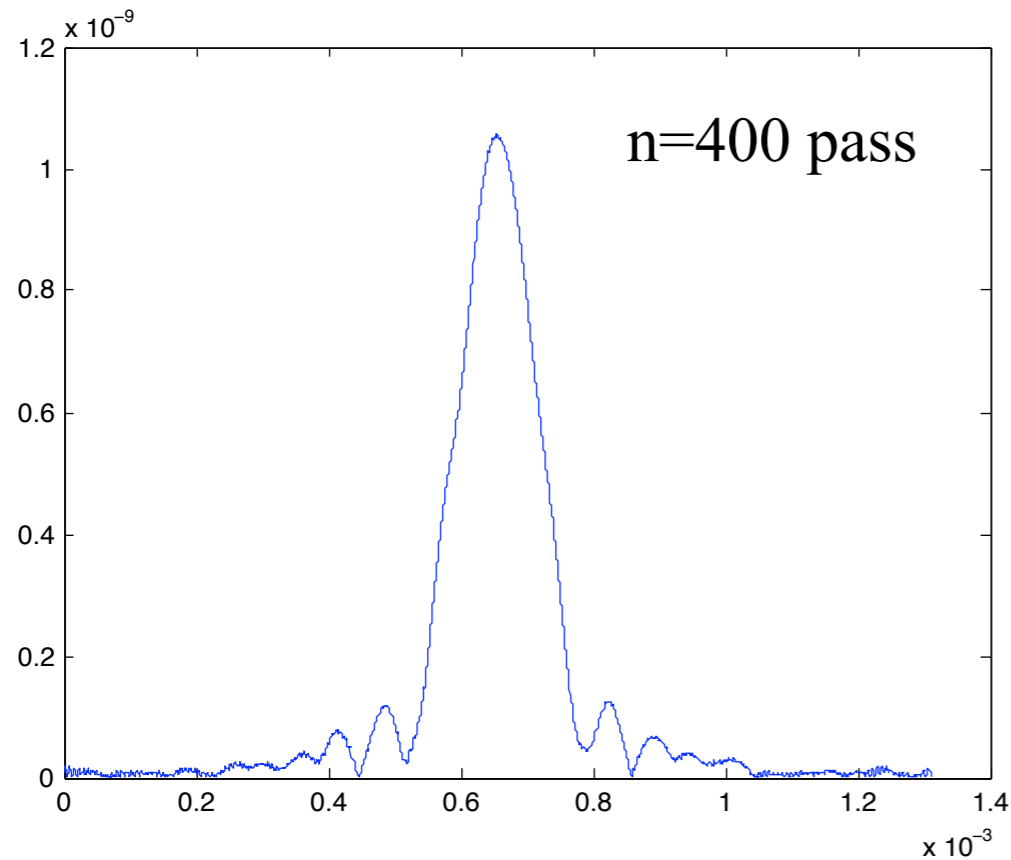
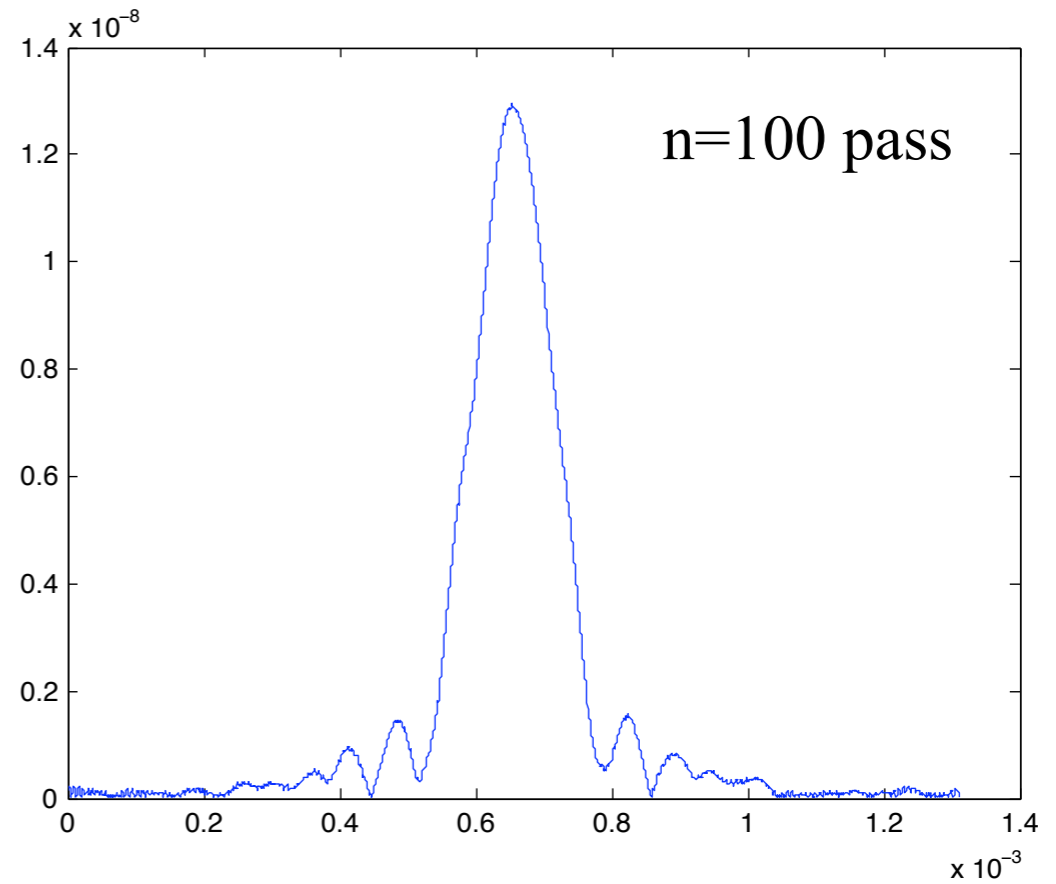
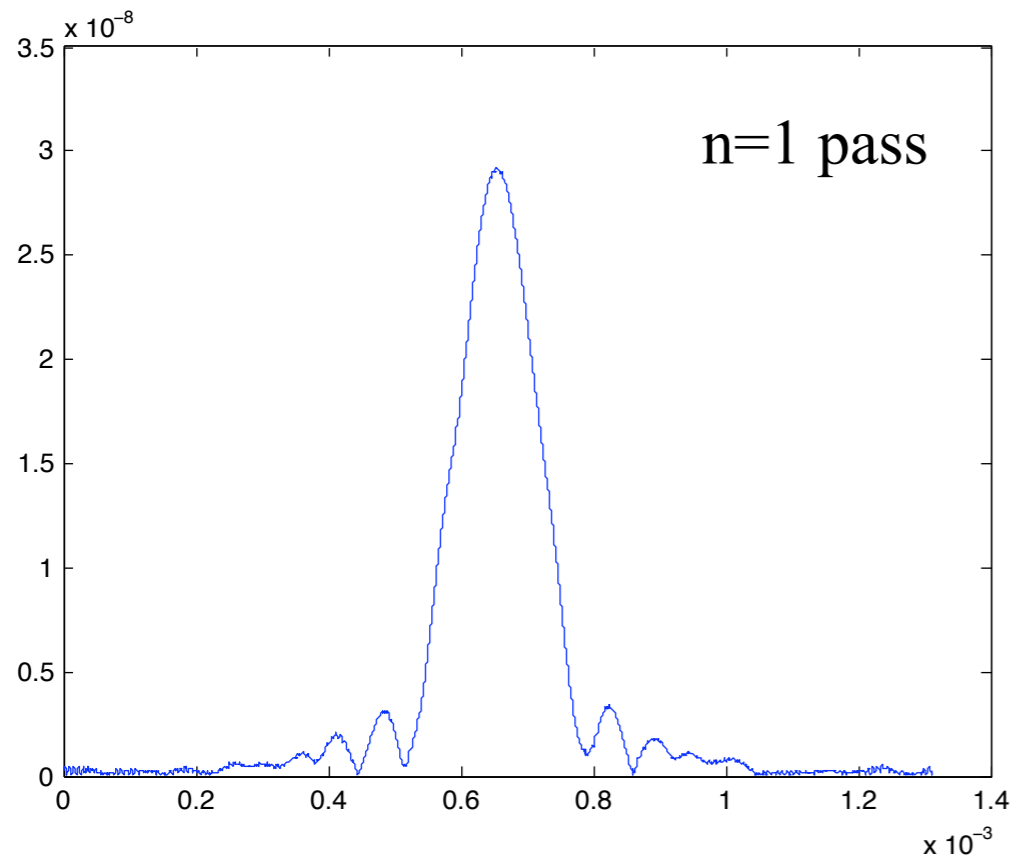
$$n = 1 - 3.17 \times 10^{-6} - (1.87 \times 10^{-8})i$$

aperture size 0.24m

rms slope error  $1.3003 \times 10^{-7}$

# Simulation Results

- Evolution of  $E$  field



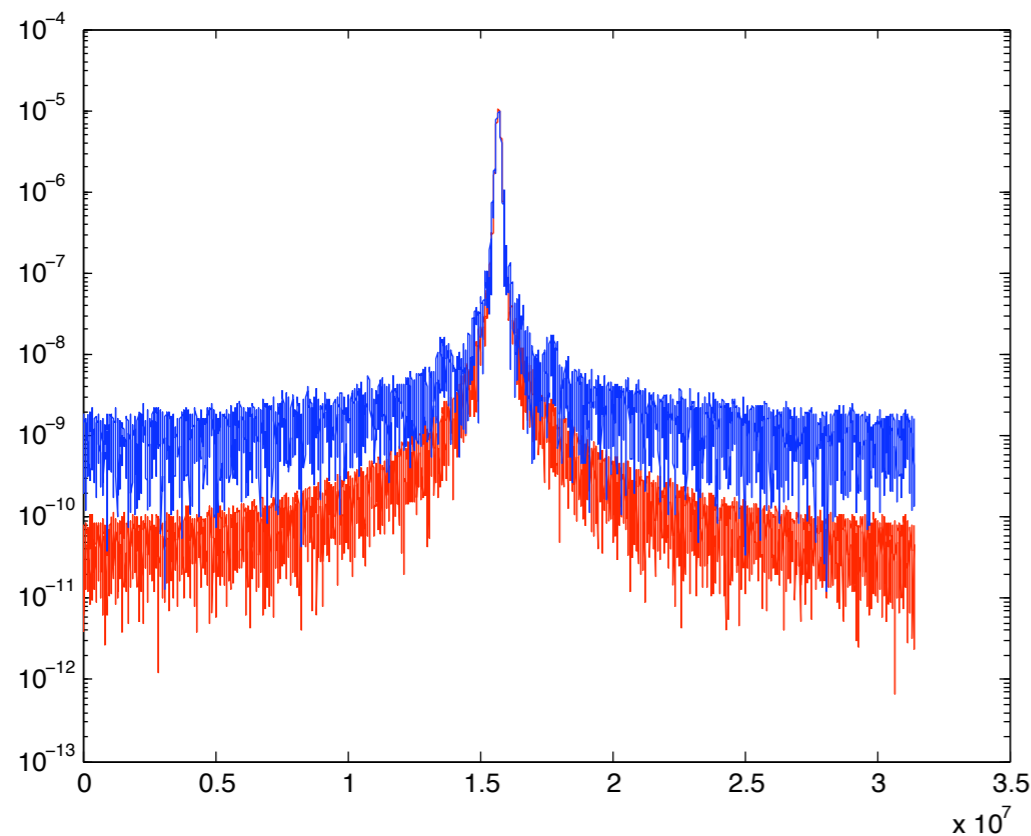
Power loss due to finite mirror size

Power loss was compensated by

gain  $g \sim 0.013$

$\rightarrow \alpha \sim 0.987$

# Peakpower reduction by Debye-Waller factor



Fourier transform of E-field

$$R_{theory} = |r_0|^2 e^{-\frac{k^2 \theta_g^2}{2} W^2 \mu - \frac{k^2 \theta_g^2}{2} \sigma^2} \approx 0.996$$

$$R_{simulation} = 0.997$$

## 3.2 The Effects of Gain

In small signal regime, radiation is amplified through FEL interaction

$$A_\nu(\phi; Z) = A_\nu(\phi; z_0) e^{(i\Delta\nu k_u + \frac{ik}{2}\phi^2)(Z-z_0)} \\ + \frac{g_n h_n}{\lambda^2} \int_{z_0}^Z \cdots \int_{z_0}^z d\phi' dz' d\eta d\dot{x} dx dz A_\nu(\phi'; z_0) e^{-(i\Delta\nu k_u + \frac{ik}{2}\phi^2)(z-z_0)} \\ \times e^{-i \int_{z_0}^z ds \xi_\nu(s)} e^{-i \int_{z_0}^{z'} ds \xi'_\nu(s)} e^{ik(\phi-\phi')x} \partial_\eta \bar{F}(\eta, x, \dot{x}; z_0)$$

$$\xi_\nu(z) = (\Delta\nu - 2\eta\nu)k_u + \frac{k}{2}(\phi - \dot{x})^2, \xi'_\nu(z) = (\Delta\nu - 2\eta\nu)k_u + \frac{k}{2}(\phi' - \dot{x})^2$$

We insert equation of motions for no focusing case

$$e^{-i \int_{z_0}^z ds \xi_\nu(s)} = e^{-i(z-z_0)[(\Delta\nu - 2\eta\nu)k_u + \frac{k}{2}(\phi - \dot{x})^2]} \\ e^{i \int_{z_0}^{z'} ds' \xi'_\nu(s')} = e^{i(z'-z_0)[(\Delta\nu - 2\eta\nu)k_u + \frac{k}{2}(\phi' - \dot{x})^2]}$$

We assume Gaussian distribution for electron beam

$$\bar{F}(\eta, x, \dot{x}) = \frac{1}{\sqrt{2\pi\sigma_\eta^2}} \frac{1}{2\pi\sigma_x^2} \frac{1}{2\pi\sigma_p^2} e^{-\frac{\eta^2}{2\sigma_\eta^2}} e^{-\frac{\dot{x}^2}{2\sigma_p^2}} e^{-\frac{x^2}{2\sigma_x^2}}$$

We analyze gain process in terms of cavity eigenmode (Hermite-Gaussian)

$$A'(\phi') = \int d\phi K(\phi', \phi) A(\phi)$$

$$c_n = G_{nm} d_m$$

$$c_n = \int d\phi' G_n^*(\phi') A'(\phi'), \quad d_m = \int d\phi G_m^*(\phi) A(\phi)$$

$$K_{nm} = \int d\phi' d\phi G_n^*(\phi') K(\phi', \phi) G_m(\phi)$$



After series of integration, final answer is

$$c_N = \frac{\mathcal{N}}{2^{N+M} N! M!} d_M \int_{z_0}^Z \int_{z_0}^z dz dz' \frac{(z - z')}{1 + i\sigma_p^2 k(z - z')} e^{-2\nu^2 k_u^2 \sigma_\eta^2 (z' - z)^2 + i(z' - z)\Delta\nu k_u}$$

$$\times \left[ \sum_{n,m} P_n P_m \sum_{a,b} C_{n,2a} C_{m,2b} \left(-\frac{2}{\kappa}\right)^{a+b} \left(\frac{iwk}{\sqrt{2}\kappa}\right)^{n-2a} \left(-\frac{iwk}{\sqrt{2}\kappa}\right)^{m-2b} \prod_{q=1}^a \prod_{q'=1}^b \left(\frac{1}{2} - q\right) \left(\frac{1}{2} - q'\right) \right. \\ \left. \times \sum_t C_{n-2a,2t} (-K)^{n-2a-2t} \left(-\frac{1}{B}\right)^{t'} \left(-\frac{1}{A}\right)^t \frac{1}{\sqrt{AB}} \prod_{p'=1}^{t'} \left(\frac{1}{2} - p'\right) \prod_{p=1}^t \left(\frac{1}{2} - p\right) \right]^2$$

$$\text{where } \mathcal{N} = -i4\pi^3 w^2 \nu k_u \frac{g_n h_n}{\lambda^4}, \quad 2t' = n - 2a - 2t + m - 2b$$

$$A = \left( \frac{\sigma_x^2 k^2}{2} - \frac{ikL}{2} + \frac{ik}{2}(z - z_0) + \frac{k^2 \sigma_p^2 (z - z_0)^2}{2(1 + ik\sigma_p^2(z - z'))} + \frac{w^2 k^2}{4} \right)$$

$$K = -\frac{\left( \sigma_x^2 k^2 + \frac{k^2 \sigma_p^2}{1 + ik\sigma_p^2(z - z')} (z' - z_0)(z - z_0) \right)}{2\left( \frac{\sigma_x^2 k^2}{2} - \frac{ikL}{2} + \frac{ik}{2}(z - z_0) + \frac{k^2 \sigma_p^2 (z - z_0)^2}{2(1 + ik\sigma_p^2(z - z'))} + \frac{w^2 k^2}{4} \right)}$$

$$B = -\frac{\left( \sigma_x^2 k^2 + \frac{k^2 \sigma_p^2}{1 + ik\sigma_p^2(z - z')} (z' - z_0)(z - z_0) \right)^2}{4\left( \frac{\sigma_x^2 k^2}{2} - \frac{ikL}{2} + \frac{ik}{2}(z - z_0) + \frac{k^2 \sigma_p^2 (z - z_0)^2}{2(1 + ik\sigma_p^2(z - z'))} + \frac{w^2 k^2}{4} \right)} \\ + \left( \frac{\sigma_x^2 k^2}{2} - \frac{ik}{2}(z' - z_0) + \frac{k^2 \sigma_p^2 (z' - z_0)^2}{2(1 + ik\sigma_p^2(z - z'))} + \frac{w^2 k^2}{4} \right)$$

In the limit of cold beam 1d, we reproduce gain formula

- when  $\sigma_p, \sigma_\eta \rightarrow 0, L/k \ll \Sigma_x^2 = \sigma_x^2 + \frac{w_0^2}{2}$

$$G_{00} \rightarrow -i2\sqrt{2}\pi\nu e^{i(\Delta\nu k_u - 2k)L} \frac{I}{I_A} \frac{K^2 [JJ]}{(1 + K^2/2)^{3/2}} \frac{N_u^3 \lambda^{3/2} \lambda_u^{1/2}}{\Sigma_x^2} \frac{\partial}{\partial x} \left( \frac{\sin^2 x}{x^2} \right)$$

where  $-2x = \Delta\nu k_u L$

# Beam parameters

## undulator parameters

$$\lambda_u = 1.76 \times 10^{-2} [m]$$

$$K = 1.51$$

$$N_u = 3000$$

$$I = 9.97 [A]$$

## radiation parameters

$$k_1 = 6.26 \times 10^{10} [m^{-1}]$$

$$\Delta\nu = 6.37 \times 10^{-4}$$

$$w_0 = 2.2 \times 10^{-5} [m]$$

## electron beam parameters

$$\gamma_0 = 1.37 \times 10^4$$

$$\sigma_x = 1.15 \times 10^{-5}$$

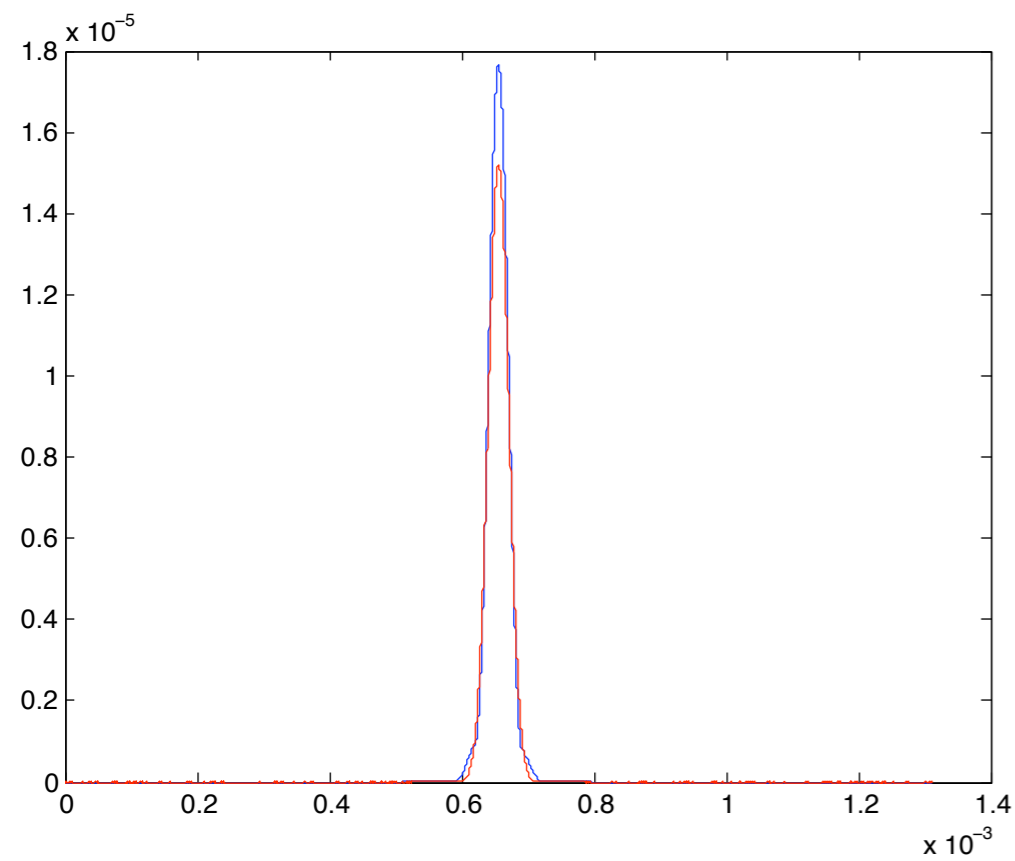
$$\sigma_p = 1.27 \times 10^{-6}$$

$$\sigma_\eta = 2 \times 10^{-4}$$

## Gain matrix

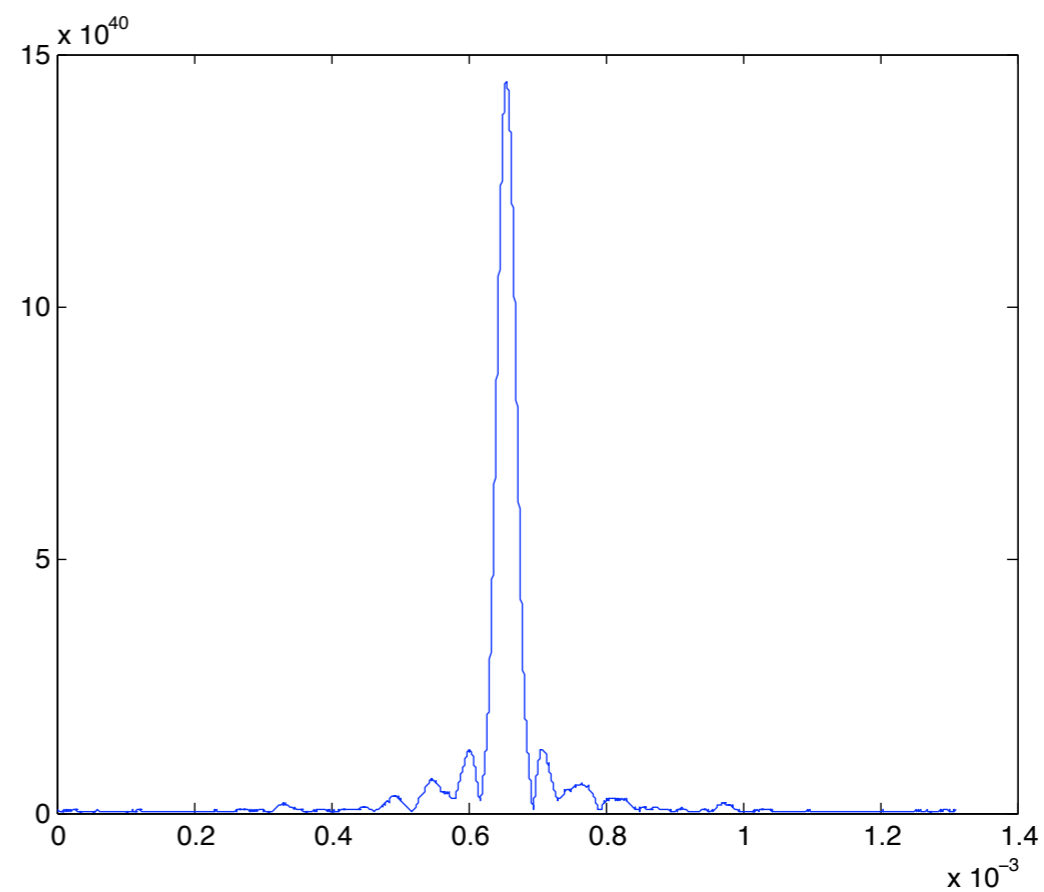
$$\begin{bmatrix} 0.1754 - 0.0721i & 0 & -0.0208 + 0.0192i & 0 & 0.0009 - 0.0009i \\ 0 & 0.0853 - 0.0567i & 0 & -0.0137 + 0.0179i & 0 \\ -0.0208 + 0.0192i & 0 & 0.0453 - 0.0528i & 0 & -0.0066 + 0.0160i \\ 0 & -0.0137 + 0.0179i & 0 & 0.0230 - 0.0474i & 0 \\ 0.0009 - 0.0009i & 0 & -0.0066 + 0.0160i & 0 & 0.0090 - 0.0409i \end{bmatrix}$$

# Simulation Result



n=1 pass  $E$  field at waist

$$g \sim 1.2669$$



n=400 pass  $E$  field at waist

## 4. Conclusion

- We derived reflection formula for mirror with surface errors
- We simulated the propagation mode in cavity and estimated power loss and gain