# Numerical modelling of reflective multilayer-based X-ray optics


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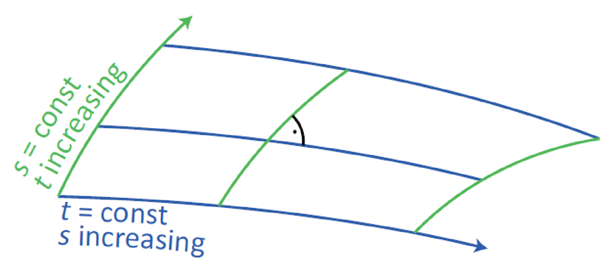
**Most of the scientific and technological progress relies on the development of characterisation techniques capable of investigating matter at very high spatial resolution and chemical sensitivity. With the advent of high-brightness coherent X-ray sources, techniques based on X-rays are particularly attractive if one can manufacture flawless optics, i.e. optics capable of either propagating a perfect wavefront from the source to the sample without degradation or correcting the wave front imperfections. Artificially stratified films deposited on a mirror surface are envisaged as promising candidates to this purpose.**


## TAKAGI-TAUPIN EQUATION FOR MULTILAYERS

**Extension of an existing model using Takagi-Taupin equations to model the X-ray propagation in multilayered structures [1].**




**Most general case in the numerical model : curved geometry**

**Two basic assumptions and simplifications of the Takagi-Taupin theory :**

1. **Two-beam diffraction (incoming and outgoing) approximation allowing to build a wave field as a summation of two spherical waves.**

$$\psi(\vec{r}) = P_1 e^{ikr_1} + P_2 e^{-ikr_2}$$

2. **The layered structure is periodic and its electric susceptibility can be reduced to its first order Fourier series expansion:**

$$\chi = \chi_0 + \sum_{h\neq 0} \chi_h e^{i\tilde{h}t} \approx \chi_0 + \chi_{\bar{1}} e^{-i\tilde{h}t} + \chi_1 e^{i\tilde{h}t}$$

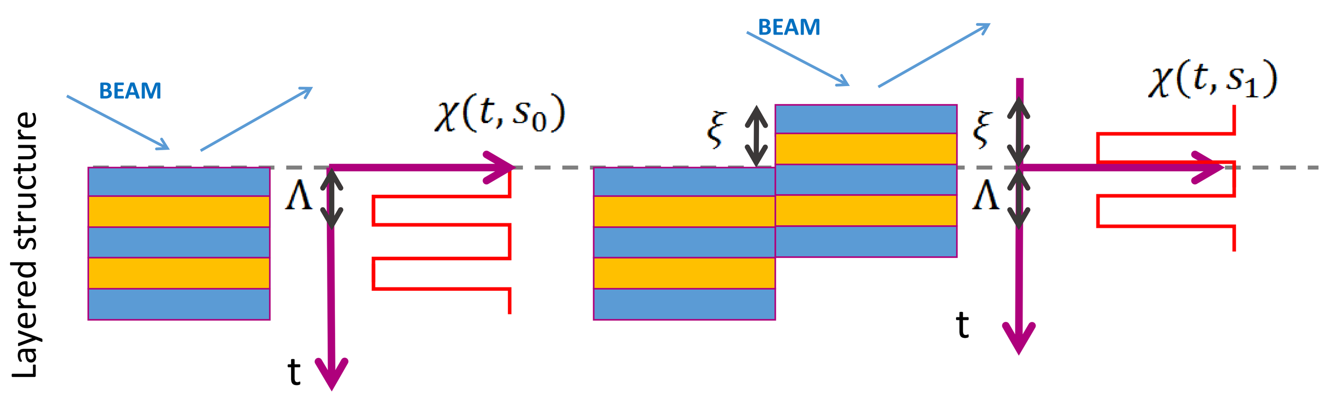
**Taking into account the above assumptions, the fundamental equation of scalar diffraction theory reads:**

$$\nabla^2\psi + k^2(1+\chi)\psi = 0$$

**From which two coupled first order partial differential equations can be derived :**

$$(\alpha^2\partial_s + \beta^2\partial_t)\psi_0 = i(u_0\psi_0 + u_1\psi_1)$$
$$(\alpha^2\partial_s - \beta^2\partial_t)\psi_1 = i(u_0\psi_1 + u_{\bar{1}}\psi_0)$$

- **Incoming wave :** $\psi_0$
- **Reflected wave :** $\psi_1$
- **Flat case :** $\alpha, \beta = cst$
- $u_h = k\chi_h/2$
- **Susceptibility Fourier series coefficients :** $\chi_0, \chi_1, \chi_{\bar{1}}$




$\tilde{h} = 2\pi/\Lambda$

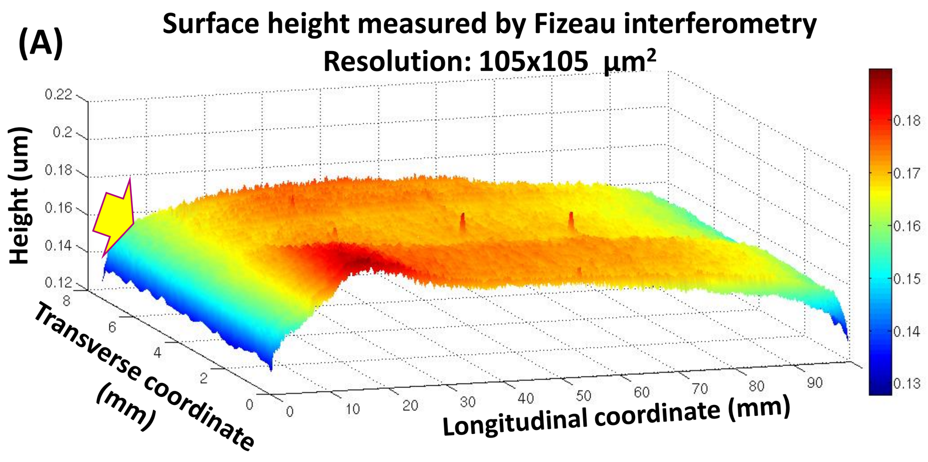
$\chi(t, s_n) = \chi_{0n} + \chi_{1n} e^{i\tilde{h}t} + \chi_{\bar{1}n} e^{-i\tilde{h}t}$

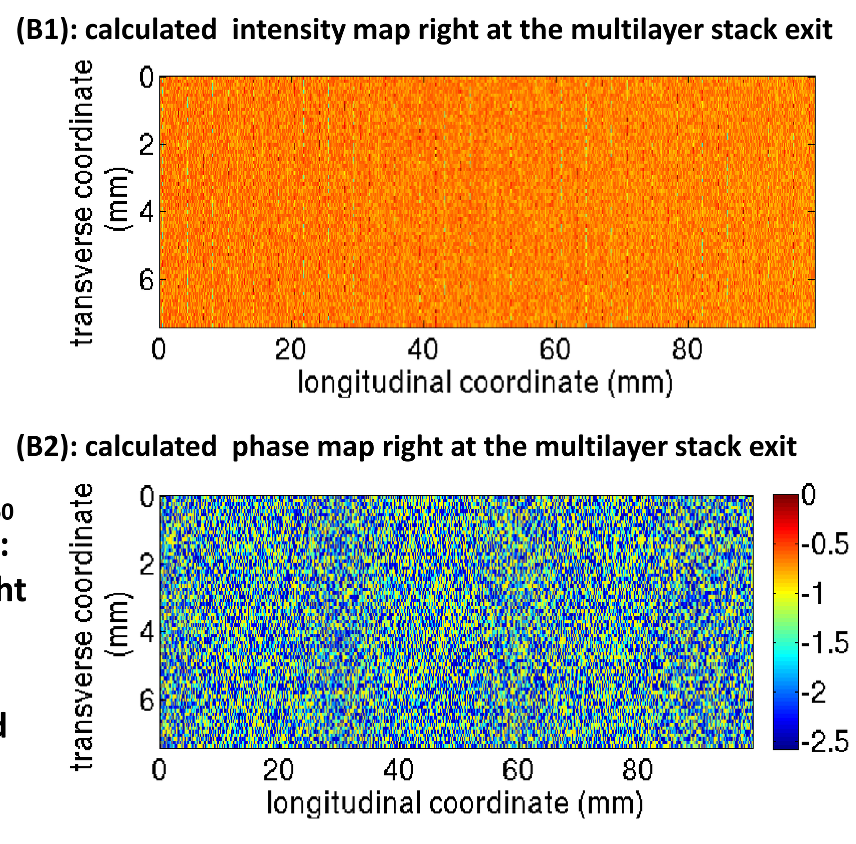
at $s_0$ : $\chi_0 = \langle\chi\rangle$, $\chi_{10} = \chi_1$, $\chi_{\bar{1}0} = \chi_{\bar{1}}$

at $s_1$ : $\chi_0 = \langle\chi\rangle$, $\chi_{11} = \chi_1 e^{i\tilde{h}\xi}$, $\chi_{\bar{1}1} = \chi_{\bar{1}} e^{-i\tilde{h}\xi}$

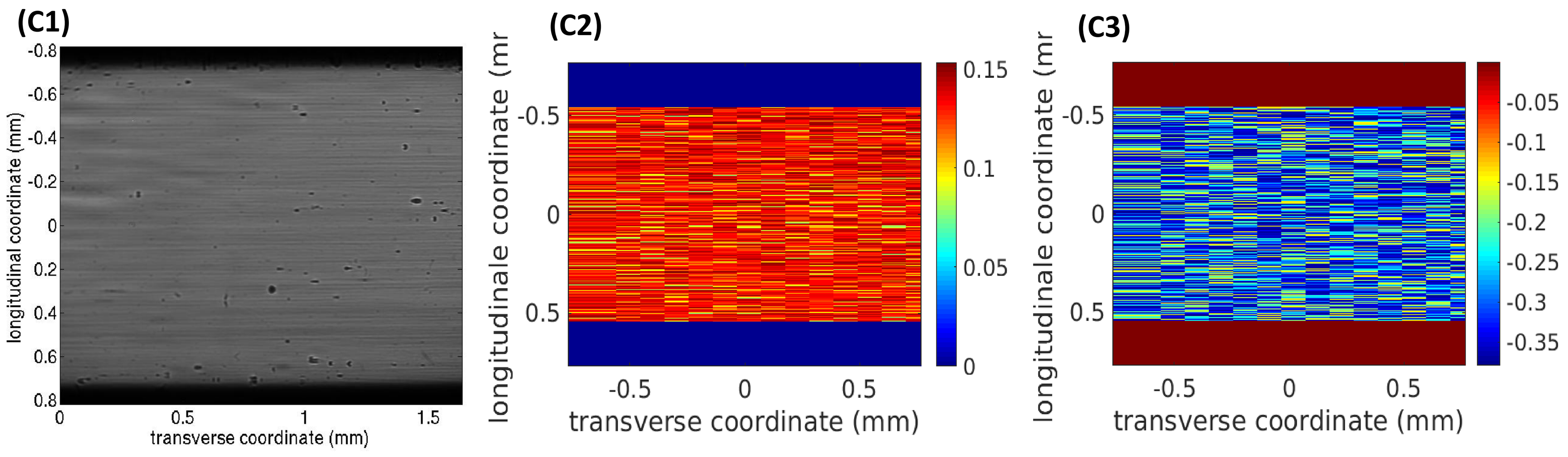
$s_n$ : $\Rightarrow \chi_{0n} = \langle\chi\rangle$, $\Rightarrow \chi_{1n} = \chi_1 e^{i\tilde{h}\xi_n}$, $\Rightarrow \chi_{\bar{1}n} = \chi_{\bar{1}} e^{-i\tilde{h}\xi_n}$

## COMPUTATION




**(A): Height deviation surface map of a 4 nm period $[W/B_4C]_{60}$ multilayer measured by Fizeau interferometry. (B1) and (B2): calculated intensity and phase map from metrology data right at the multilayer stack exit.**
**(C1): Image recorded after X-ray reflection on the multilayer (E = 15 keV, mirror-to-detector distance = 650 mm). (C2) and (C3): intensity and phase maps simulated on a virtual detector by paraxial propagation, respectively.**

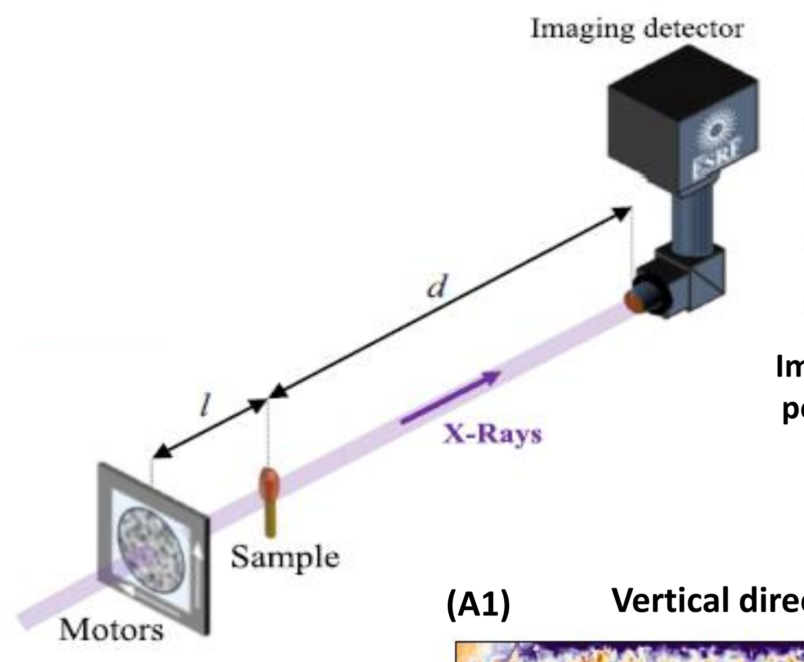



**The computation shows that multilayer mirrors can be considered as phase objects where absorption effects are negligible (cf. B1 & B2).**

**The current assumption is that "stripes" are mainly produced by interference effects from phase distortion propagation from the mirror to the detector.**

**In the Takagi-Taupin formalism, 2D height maps are computed as series of profiles. This allows the artificial reproduction of the experimentally observed stripes .**

## SPECKLE WAVEFRONT MEASUREMENTS



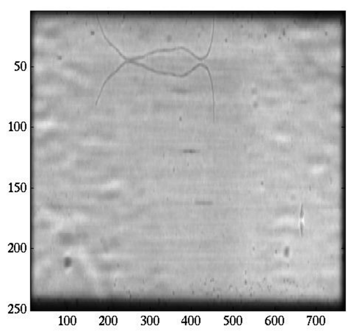
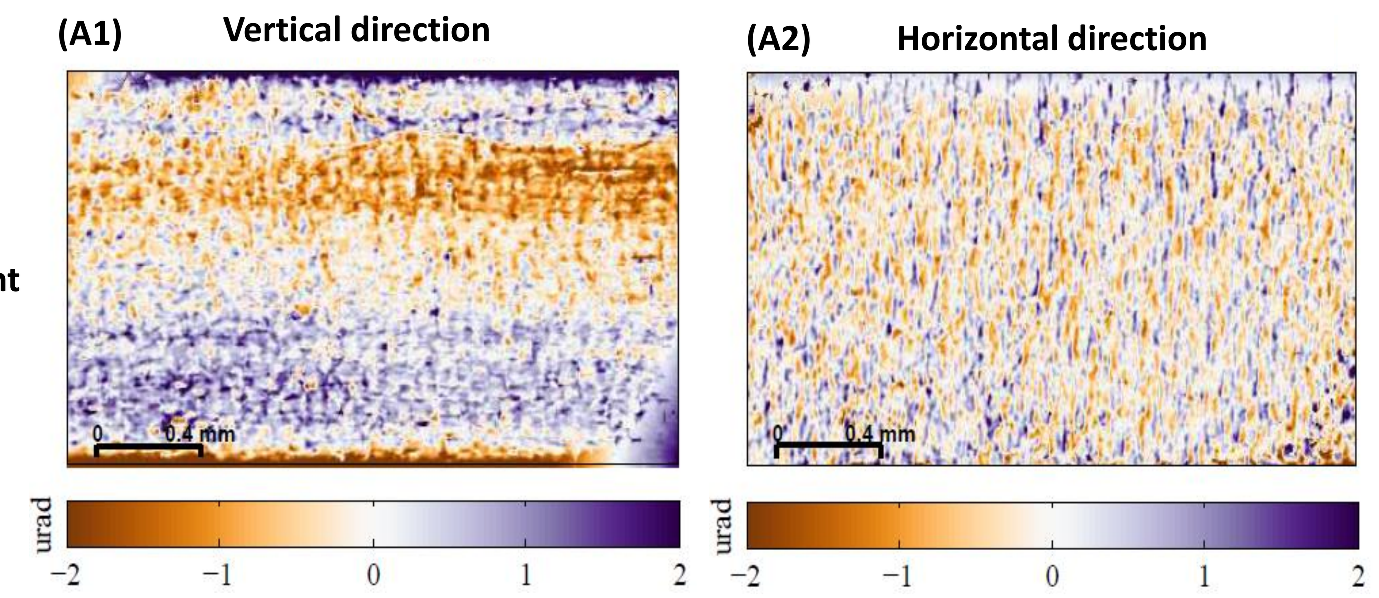
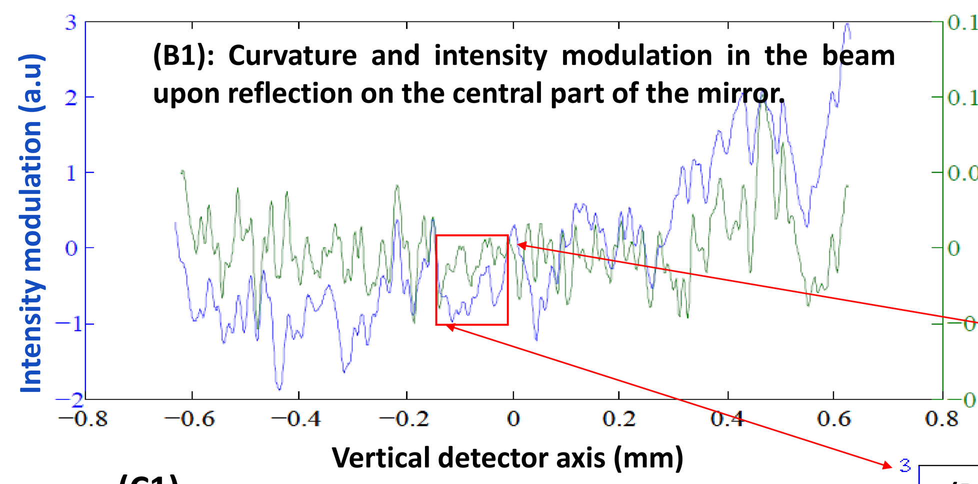



**Image obtained with a 4 nm period multilayer $[W/B_4C]_{60}$**

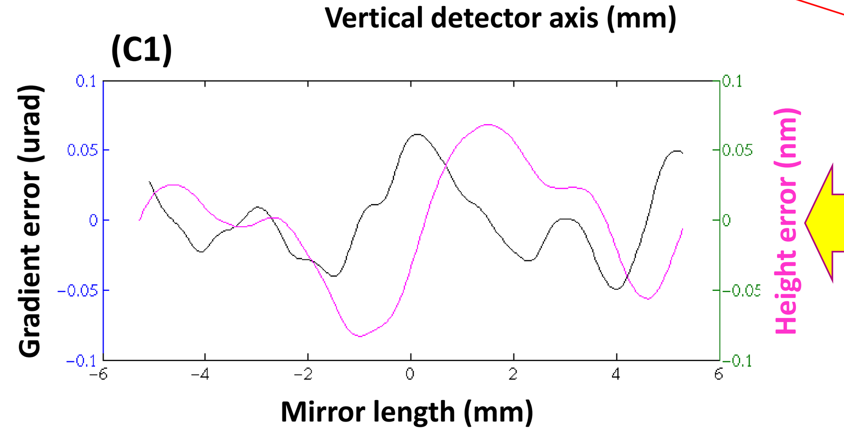
**SPECKLE wavefront measurement using a FReLoN CCD camera [2] (pixel size = 5.8 x 5.8 µm²)**
**Multilayer-detector distance: 990 mm**
**Multilayer-membrane distance: 450 mm**

**2D Differential wavefront gradient error**




**Good correlation between intensity modulation and wavefront curvature.**



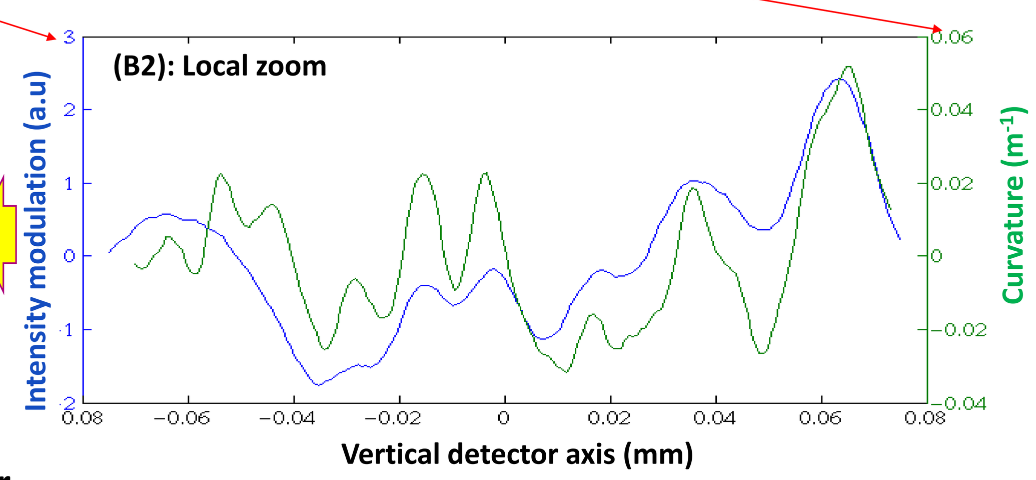
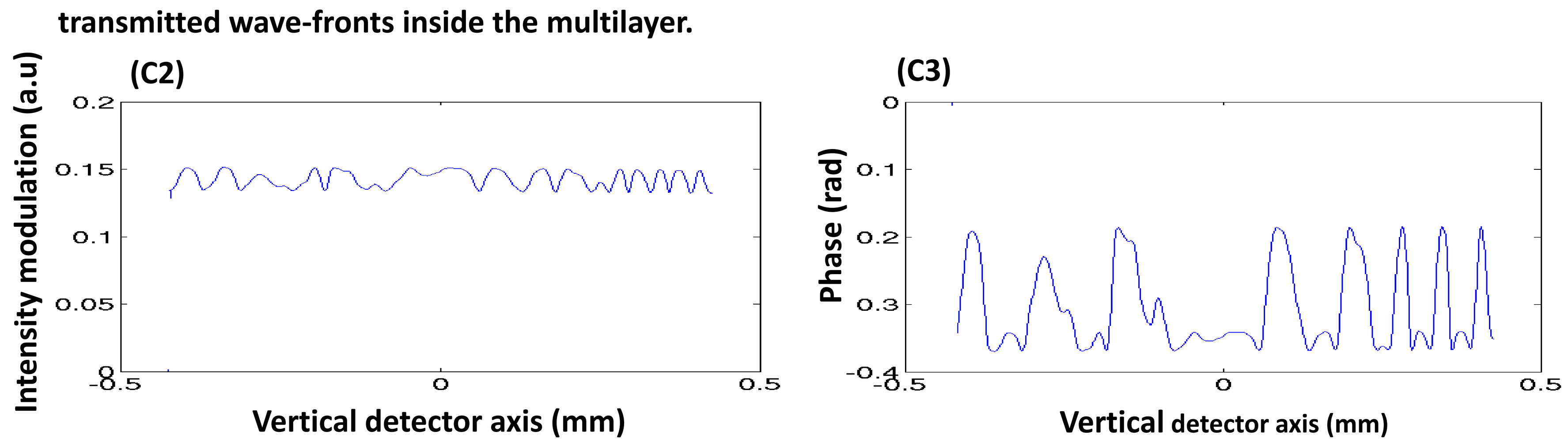
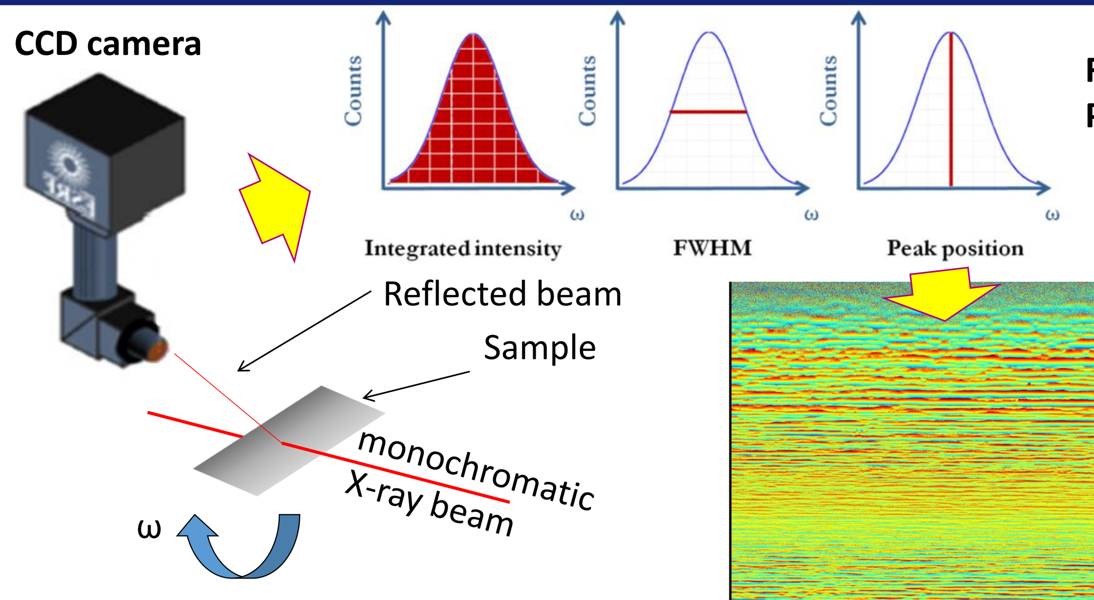




**Figure (C1): local height deviation of the mirror recovered from the curvature measurement.**

**Intensity modulation (C2) and phase profile (C3) obtained from simulation of X-ray reflection on the mirror height profile using the Tagaki-Taupin equations for calculating the diffracted and transmitted wave-fronts inside the multilayer.**

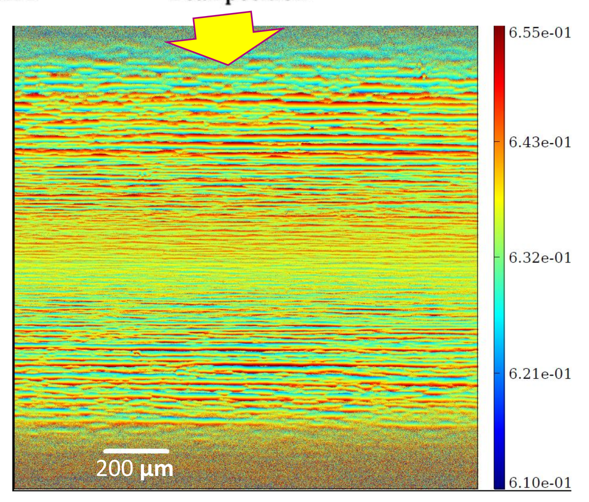



## ROCKING CURVE IMAGING : preliminary results




**Field of view: 1.5 mm x 1.5 mm**
**Pixel size: 0.75µm**

**The sample is rotated ('rocked') around the Bragg diffraction angle (here 600 images collected over a range of 0.06 deg)**




**Mapping of the peak position obtained using Rocking Curve Imaging.**
**The variation of peak position may be associated to surface and layer imperfections.**

## Perspectives

- **Future works will include:**
- **Comparison of simulations with speckle based measurements, least square estimate wavefront retrieval [4].**
- **New model taking into consideration information obtained from online speckle-based metrology and rocking curve imaging.**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