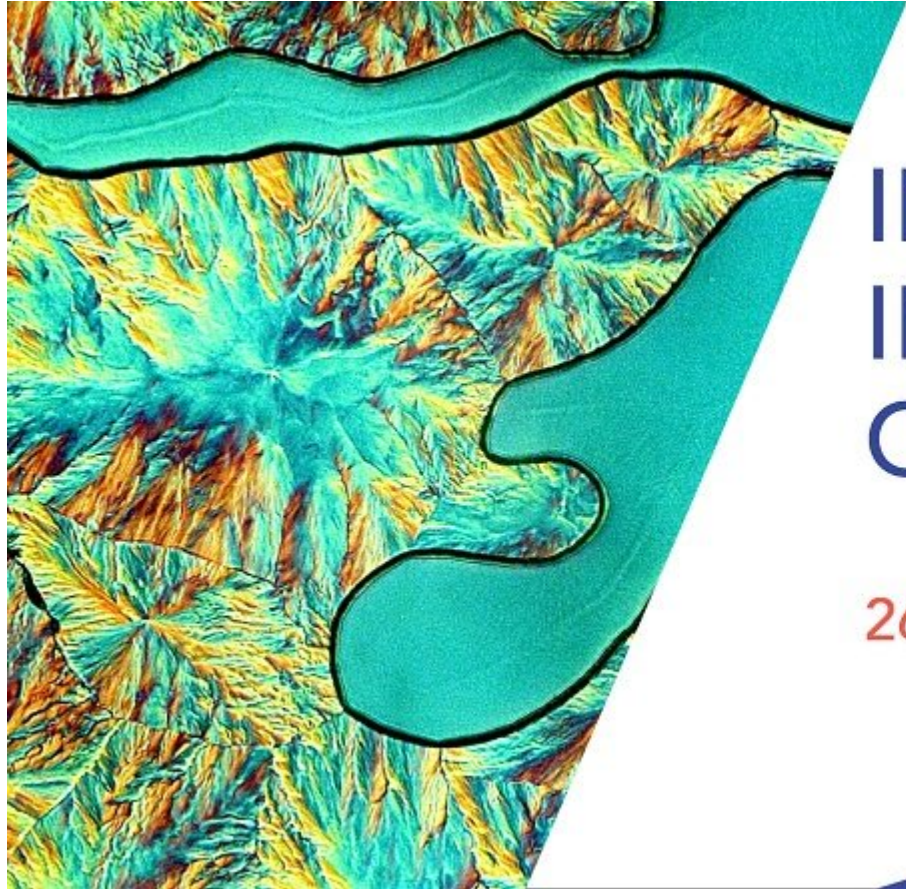




# Interface and Defect-induced Scattering in Optical Coatings

Jinlong Zhang, Tongji University

# The OSA Thin Films Technical Group Welcomes You!



## INTERFACE AND DEFECT- INDUCED SCATTERING IN OPTICAL COATINGS

26 May 2020 • 9:00 EDT

**OSA** Thin Films  
Technical Group

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# Our Technical Group at a Glance

## Our Focus

- Optical thin films and interference coatings from fundamentals to applications
- Serving a global community with thousand members like YOU

## Our Mission

- To connect people from academia, institutions and industries in the field
- To bridge the fundamentals, the know-hows and the new development
- To promote networking and career development through continuous learning

## Where To Find Us

- Technical Group Website: [www.osa.org/ThinFilmsTG](http://www.osa.org/ThinFilmsTG)
- LinkedIn: [www.linkedin.com/groups/4783616](https://www.linkedin.com/groups/4783616)
- Please let us know if you are interested in sharing your work or have ideas for our group activities

# Today's Webinar

## Interface and defect-induced scattering in optical coatings



### Dr. Jinlong Zhang

Institute of Precision Optical Engineering, Tongji University  
[jinlong@tongji.edu.cn](mailto:jinlong@tongji.edu.cn)

### Speaker's Short Bio:

Holds PhD in Optical Engineering from Zhejiang University  
10+ years in design, simulation and deposition for high quality optical coatings  
Extensive experience with developing nanostructure thin films



Thin Films  
Technical Group

# Interface and defect-induced scattering in optical coatings

**Jinlong Zhang, [jinlong@tongji.edu.cn](mailto:jinlong@tongji.edu.cn)**

**Institute of Precision Optical Engineering  
Key Laboratory of Advanced Micro-Structured Materials MOE**

**2020-05-26**

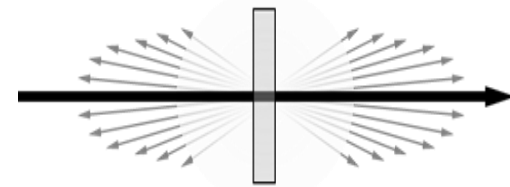
**01 Background**

**02 Recent progress of interface scattering**

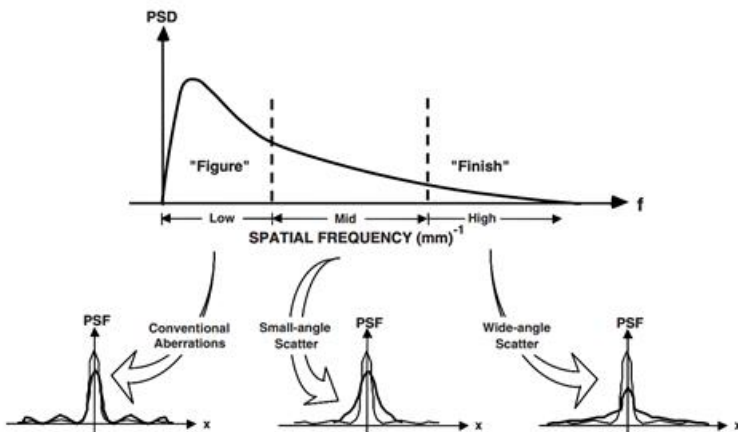
**03 Simulation, control of defect-induced scattering**

**04 Conclusion**

**Scattering light: Stray light that deviates from the mirror image due to structural defects in the film**



- Reducing the optical throughput
- Decreasing the image resolution by the narrow-angle scattering
- Decreasing the image contrast or signal-to-noise ratio by the wide-angle scattering
- Formation of ghost images, ...



$$PSF(\mathbf{r}) = PSF_{geom}(\mathbf{r}) * PSF_{scat}(\mathbf{r})$$

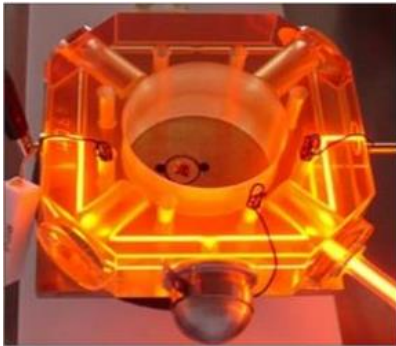
↓

$$\sim ARS(a_j r)$$

**Degradation the performance of optics**



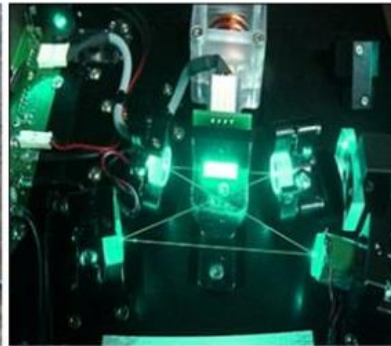
**Particularly critical for optics at short wavelengths, high resolution imaging, ultra-low loss laser optics, etc.**



laser gyroscope



gravitational wave  
detection



cavity ring-down  
spectroscopy



EUV mirror

- **Ultra-low loss laser coatings in the laser cavity mirrors need to control the scattering to ppm level**
- **Light scattering significantly enhanced due to the short wavelength**
- **The lock-in threshold of Laser Gyros is limited by scattering in the counterpropagating direction**

Scattering loss

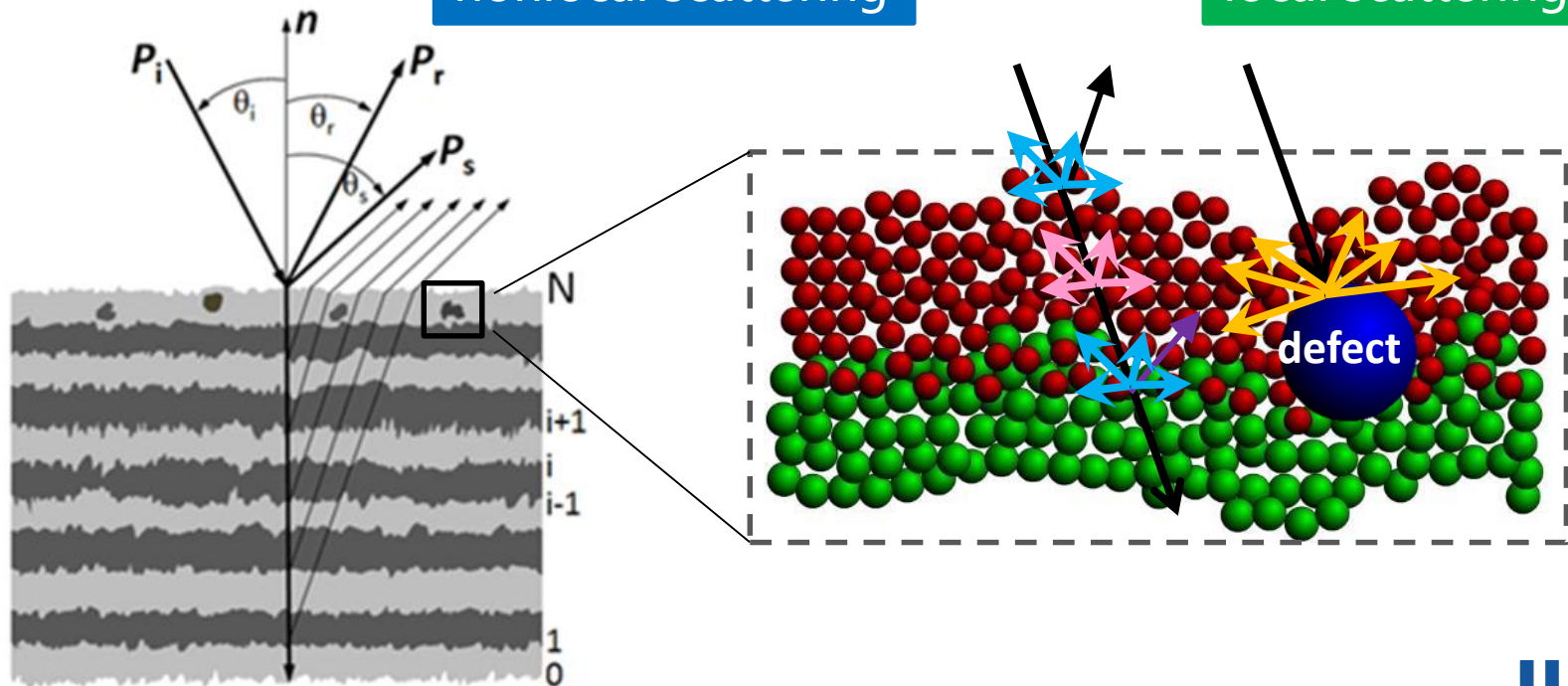
surface/interface roughness

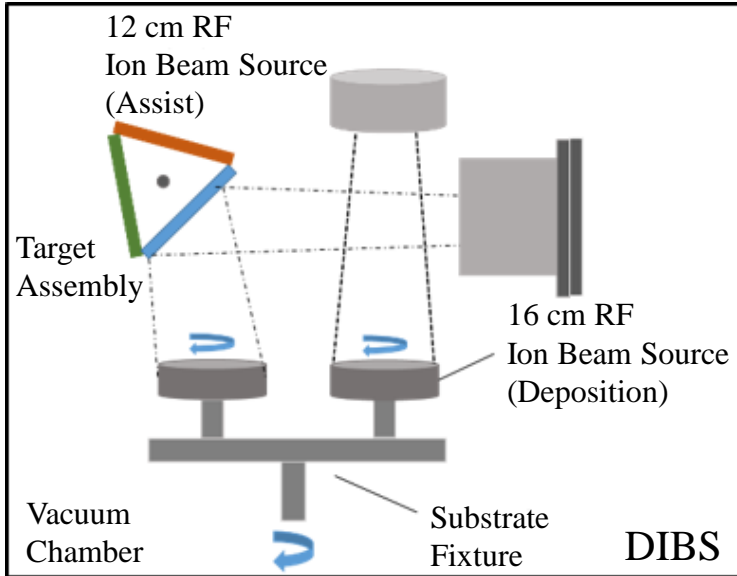
bulk inhomogeneity

local defects

nonlocal scattering

local scattering



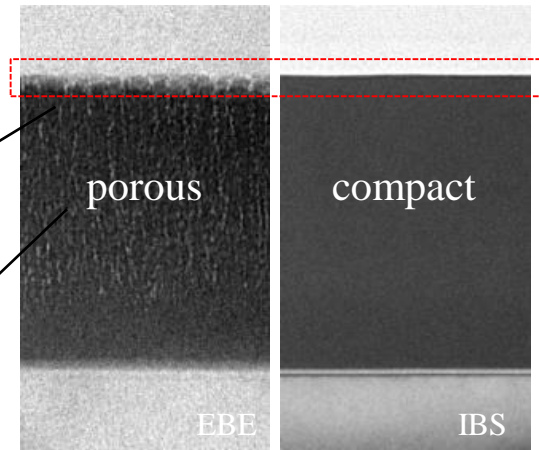


- smooth surface
- compact structure
- few defects from sputtering source

roughness-induced

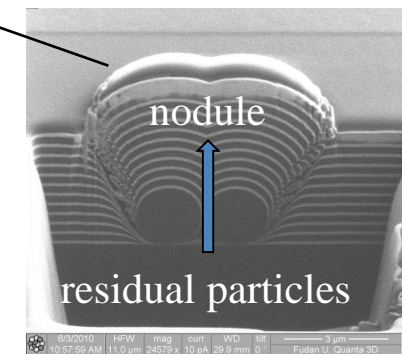
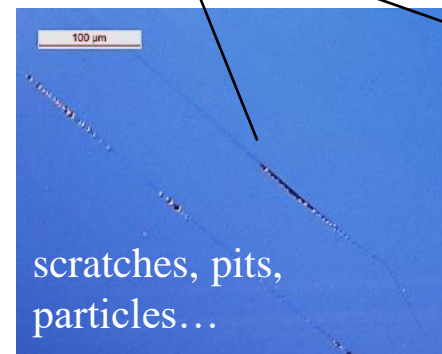
bulk inhomogeneity-induced

defect-induced scattering



advanced substrate processing/cleaning technology

**The best technical route:  $\text{SiO}_2/\text{Ta}_2\text{O}_5$  by IBS**



scratches, pits can be well controlled by super polishing

Year	Research Unit	$\lambda/\text{nm}$	$\sigma/\text{nm}$	$TIS_{\text{exp}}/\text{ppm}$
1999	RUS, POLYUS	632.8	0.35	50
2001	UK, BAE	632.8	0.1	6
2004	USA, REO	632.8	0.053	0.8
2004	USA, LIGO	1064	< 0.05	>> 0.5
2012	USA, IDEX	633	< 0.05	>> 0.5

$$TIS = 1 - \exp\left[-(4\pi\sigma \cos \theta_i / \lambda)^2\right] \approx (4\pi\sigma \cos \theta_i / \lambda)^2$$

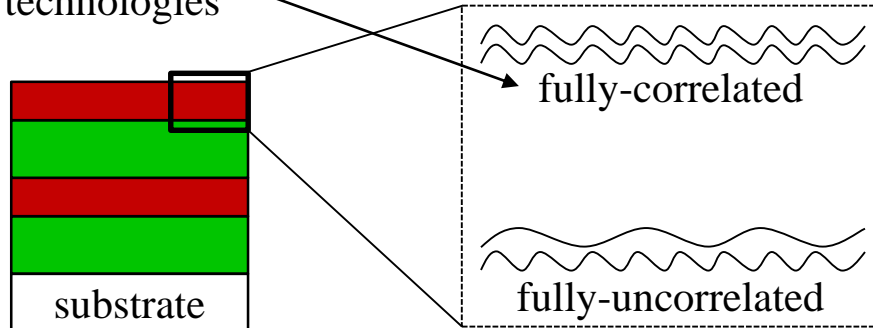
$$\sigma = \sqrt{2\pi \int_{\sin 2^\circ / \lambda}^{\sin 85^\circ / \lambda} PSD(\theta_s) d\theta_s} \quad \sim\text{ISO: 13696}$$

$TIS_{\text{exp}} \gg TIS_{\text{theor}}$ , interface scattering can not be neglected

$$ARS(\theta_s) \propto \sum_{i=0}^N \sum_{j=0}^N F_i F_j^* PSD_{ij}(f)$$

- reducing roughness
- reducing optical factor

state-of-the art deposition technologies



$$\rightarrow ARS(\theta_s) \propto \left| \sum_{j=0}^N F_j \right|^2 PSD(f)$$

$$F_j = (\varepsilon_j - \varepsilon_{j-1}) E(z_j, \theta_0) E(z_j, \theta_s)$$

- creating destructive interferences

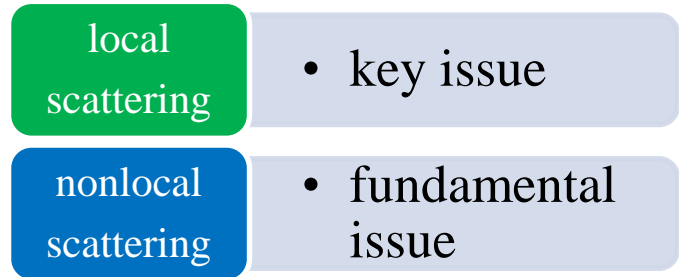
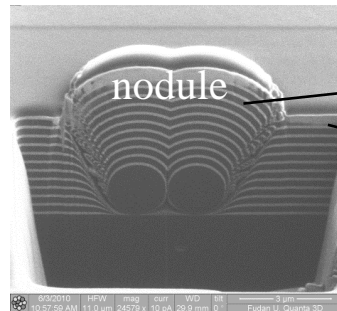
International round-robin experiment to test the International Organization for Standardization total-scattering draft standard

Lab	Sphere Type	Sphere Diameter (mm)	Range of Acceptance Angles (deg)	Angle of Incidence (deg)	Beam Diameter (mm)	Background Signal (ppm)	Relative Error (%)	Number of Points	Point Geometry
DMS	Coblentz	254	2.50-70.0	<2.0	2.5	5.0	2-3	3	Random
IOF	Coblentz	350	2.00-85.0	<1.0	0.3	<0.1	<10	201, 501, 1000	Line
JOP	Ulbricht	220	2.00-85.0	~0.2	1.0	1.4-4.0	<10	201	Line
LMTB	Ulbricht	150	2.90-70.0	<1.5	1.5	<5.0	<10	202	Line
LZH	Ulbricht	250	2.00-88.0	<3.0	0.4	<0.5	<10	300, 380, 1000	Line
NAWC	Coblentz	220	2.85-80.0	~0.5	1.0	20.0	~3	19	Circle
LINOS	Ulbricht	150	2.00-82.0	<1.5	1.5	<5.0	<10	50	Line
TOL	Ulbricht	250		~5.0	1.0	9.0		129	Line
TUD	Ulbricht	152	1.90-82.0	~2.0	1.0	2.0	<10	51	Line

significantly different results

characterization and control of the local scattering is the key issue

problem: measurement uncertainty



- key issue

- fundamental issue

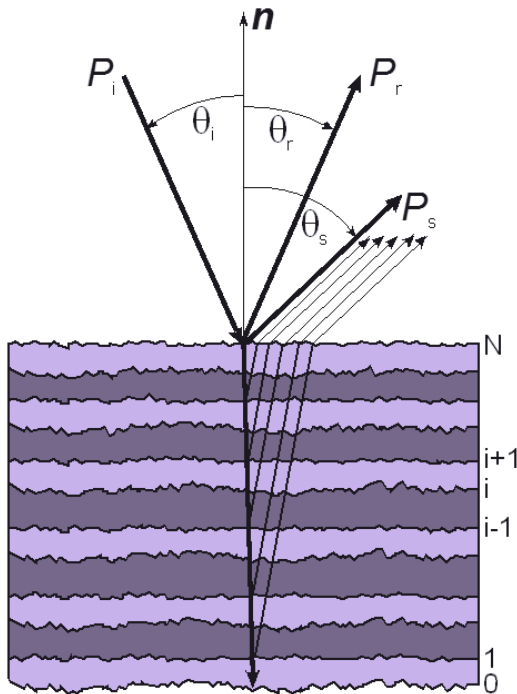
**residual defects are unavoidable**

**01 Background**

**02 Recent progress of interface scattering**

**03 Simulation, control of defect-induced scattering**

**04 Conclusion**



### Vector perturbation theory ( $\sigma \ll \lambda$ )

$$ARS(\theta_s) \propto \frac{1}{\lambda^4} \sum_{i=0}^N \sum_{j=0}^N \underbrace{F_i F_j^*}_{\text{Optical factors}} \underbrace{PSD_{ij}(f)}_{\text{Roughness factors}}$$

#### Optical factors

- Multilayer design
- Optical constants
- Polarization

#### Roughness factors

- PSDs of individual surfaces ( $i = j$ )
- Cross-correlation properties ( $i \neq j$ )

$$F_j = (\varepsilon_j - \varepsilon_{j-1}) E(z_j, \theta_0) E(z_j, \theta_s)$$

Coating design, Correlation of PSD

## Two approaches to control the interface scattering

## Relevant statistical surface characteristics:

- Surface height distribution function
- Surface autocovariance function

### Surface Power Spectral Density function

$$PSD(f_x, f_y) = \lim_{L \rightarrow \infty} \frac{1}{L^2} |FT\{h(x, y)\}|^2$$

surface spatial frequencies

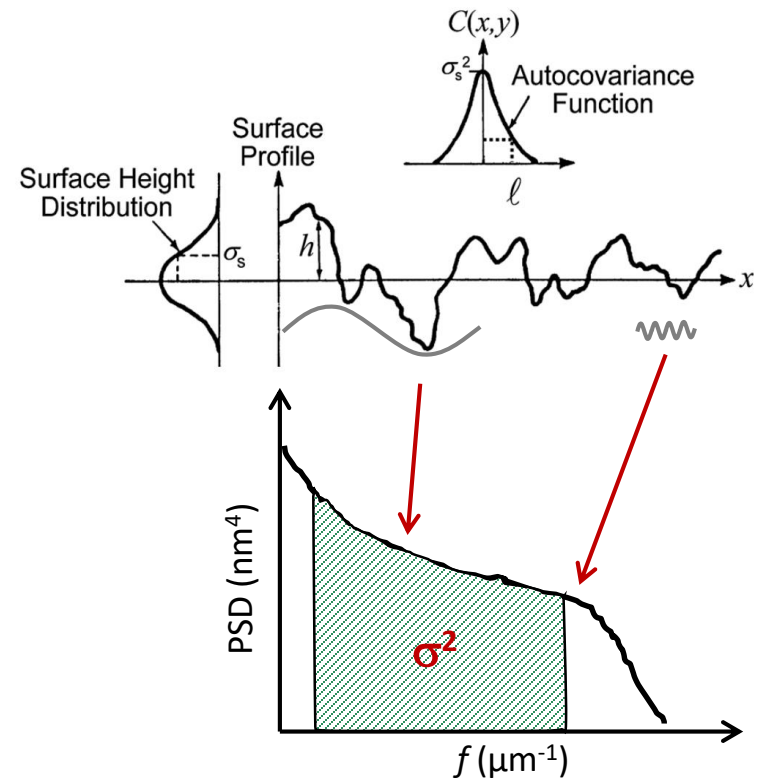
surface topography

- Power of different roughness components
- Fourier Transform of Autocovariance Function
- Isotropic roughness:  $PSD(f_x, f_y) \rightarrow PSD(f)$

### Rms roughness

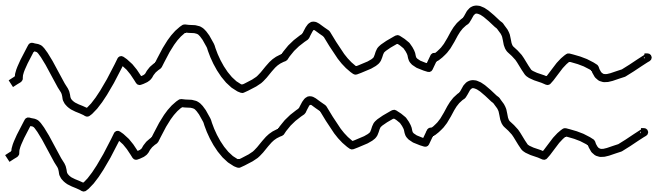
$$\sigma = \sqrt{2\pi \int_{f_{\min}}^{f_{\max}} PSD(f) f df}$$

- Standard deviation of surface topography
- Band-limited / relevant roughness



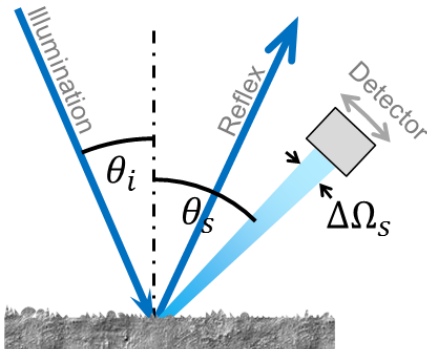


### Completely correlated interfaces model

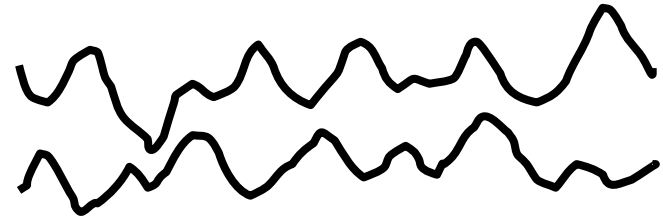


$$PSD_F = PSD_S = PSD_{SF}$$

$$ARS \propto \frac{1}{\lambda^4} \left| \sum_{j=0}^N F_j \right|^2 PSD(f)$$



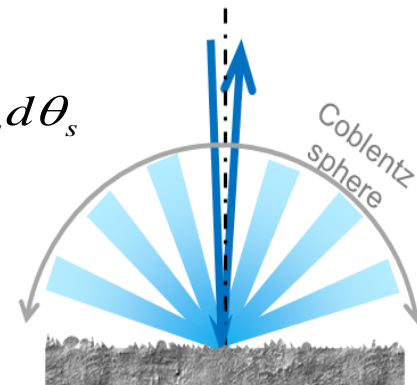
### Completely non-correlated interfaces model



$$PSD_{SF} = 0$$

$$ARS \propto \frac{1}{\lambda^4} \sum_{j=0}^N |F_j|^2 PSD(f)$$

$$TS_b = 2\pi \int_{2^\circ}^{85^\circ} ARS(\theta_s) \sin \theta_s d\theta_s$$



$$ARS(\theta_s) \propto \frac{1}{\lambda^4} \sum_{i=0}^N \sum_{j=0}^N F_i F_j^* PSD_{ij}(f)$$

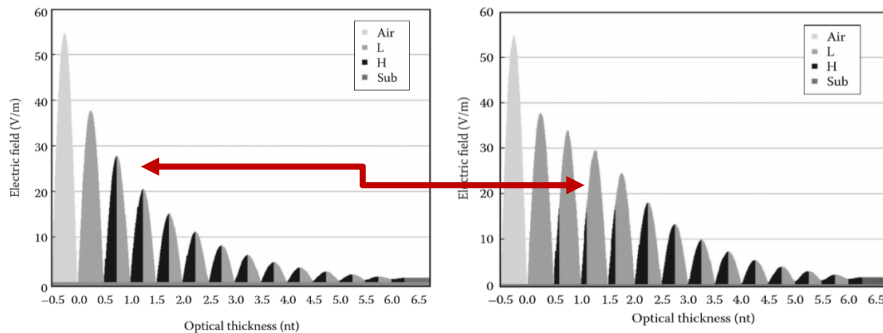
## Previous methods to adjust optical factors

Completely non-correlated  
interfaces model

To change the interface  
electric field

Completely correlated  
interfaces model

Eliminate  $F_i$  for a single layer  
with a particular thickness



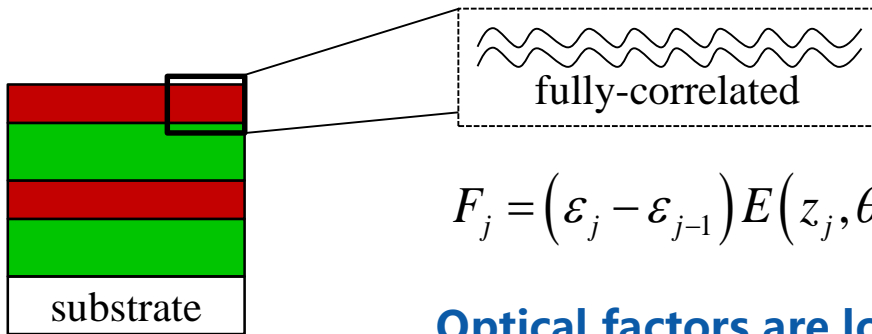
air - $n_0$	interface 0 - $\sigma_0$
material - $n$	interface 1 - $\sigma_1$
substrate - $n_s$	

optical thickness:  $ne = p\lambda$

complete cancellation of backscattering

1. Apfel J H. Optical coating design with reduced electric field intensity[J]. Applied optics, 1977, 16(7): 1880-1885.
2. C. Amra, G. Albrand, P. Roche, Theory and application of antiscattering single layers: antiscattering antireflection coatings, Appl. Opt. 25(16), 2695-2702 (1986).

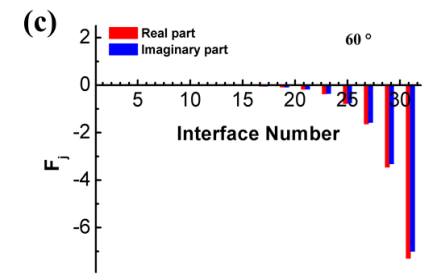
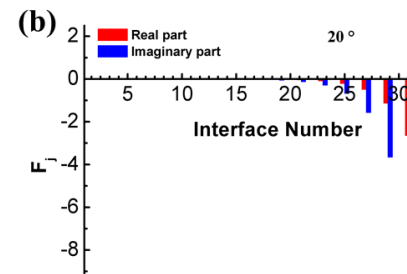
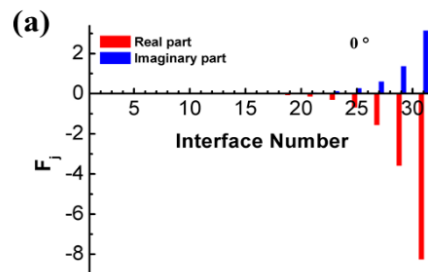
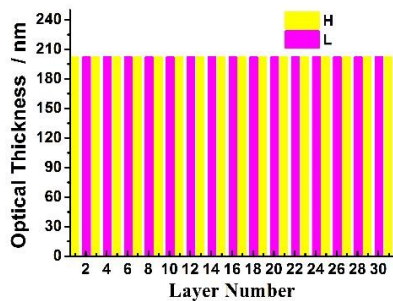
state-of-the art deposition technologies for low-loss coatings



$$ARS \propto \frac{1}{\lambda^4} \left| \sum_{j=0}^N F_j \right|^2 PSD(f)$$

$$F_j = (\epsilon_j - \epsilon_{j-1}) E(z_j, \theta_0) E(z_j, \theta_s)$$

Optical factors are located at the H on the L interfaces (odd numbers), they are complex and in the same phase

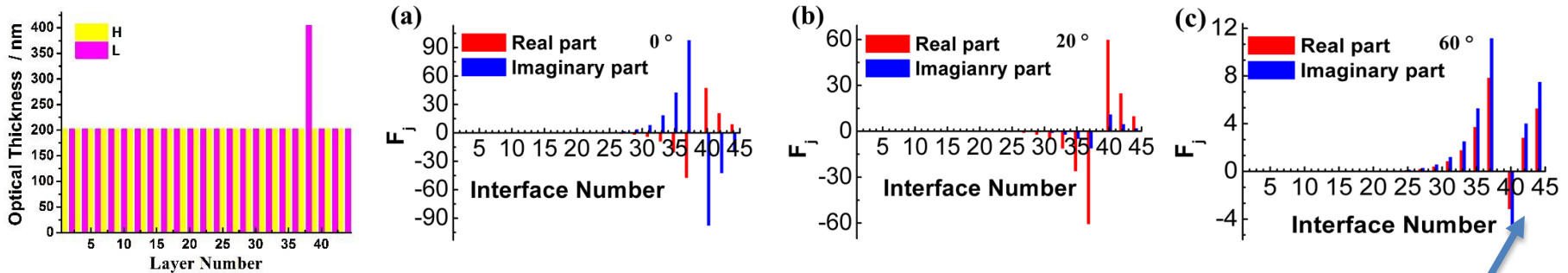


QWHR, s- incident, 800nm

Light scattered from various interfaces are constructive interference

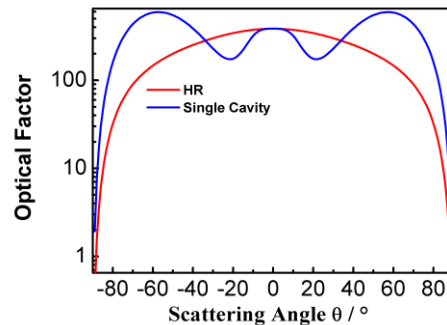
There is no solution of HR coating design to obtain destructive interferences of the scattering

Add FP structure in HR coating, not modify reflection  $F_j = (\varepsilon_j - \varepsilon_{j-1})E(z_j, \theta_0)E(z_j, \theta_s)$



$\varepsilon_j - \varepsilon_{j-1}$  exhibits opposite sign on both sides of the cavity, optical factors at the interfaces are in opposite phase

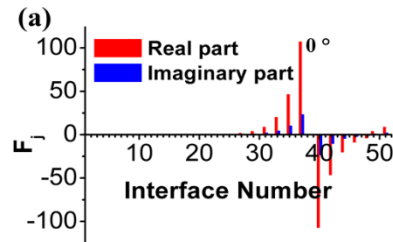
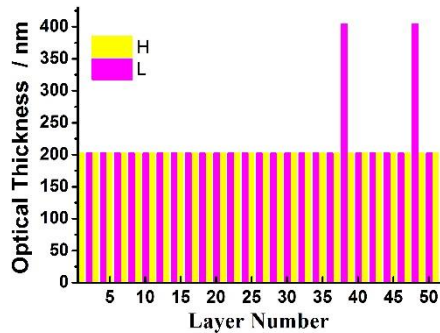
$$ARS \propto \frac{1}{\lambda^4} \left| \sum_{j=0}^N F_j \right|^2 PSD_{ij}(f)$$



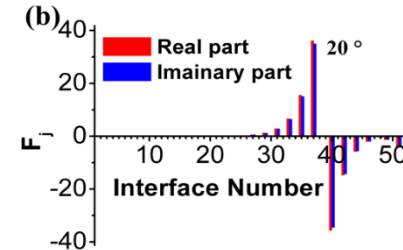
$F_j$  at top interfaces are in phase with that at inner interfaces due to the accumulation of the phase difference in large scattering angle

Reduce scattering in the near specular range from 10 to 35 degree, an increased value of the optical factors in large scattering angles

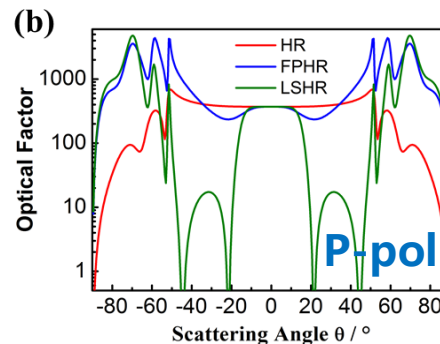
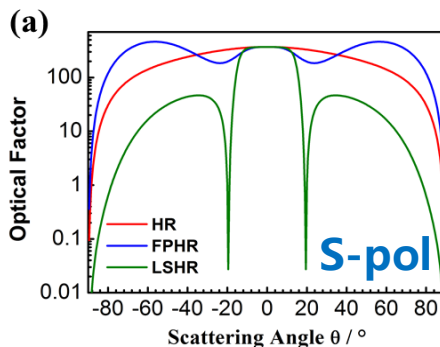
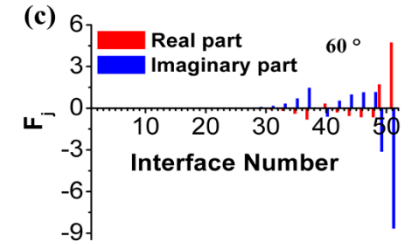
## A proper HR coating structure with two FP cavities



optical factors at interfaces have opposite phase



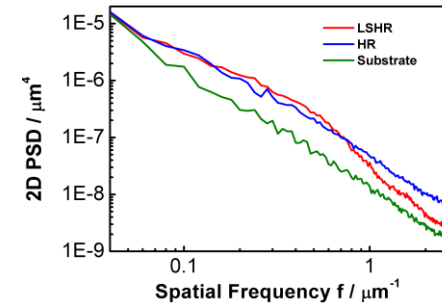
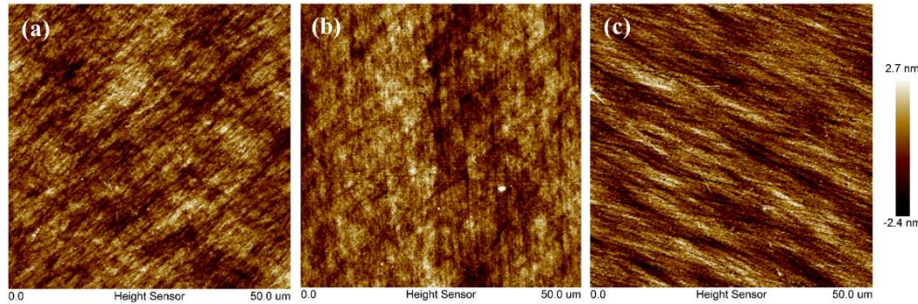
optical factors at the top two interfaces have opposite phase



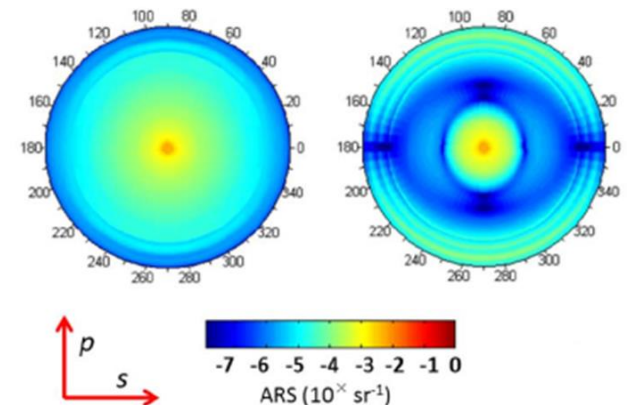
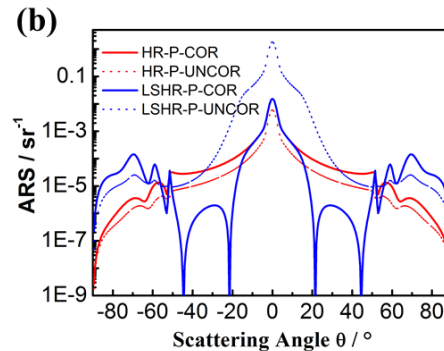
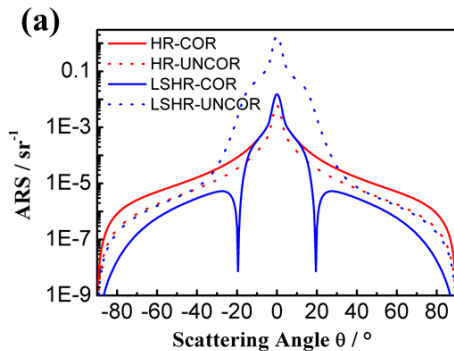
It is still possible to reduce the total scattering in the entire reflection hemisphere

**The destructive interference occurs in all directions for s-pol.**  
**The destructive interference does not occur in large scattering angles for p-pol.**

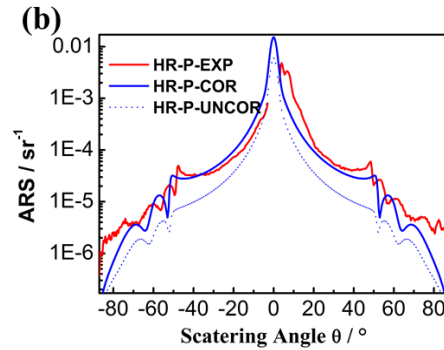
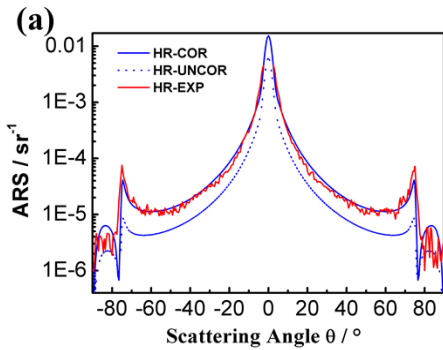
The QWHR and LSHR coatings were deposited by ion-assisted deposition



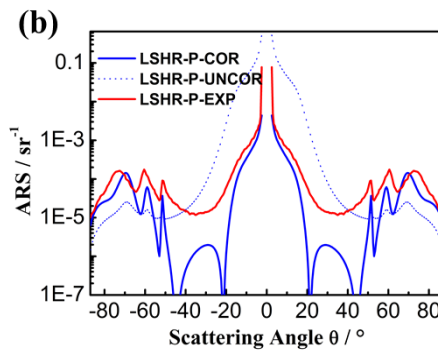
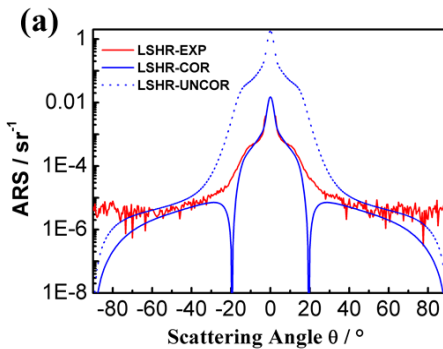
The PSD functions fitted with ABC model, The PSDs of both coatings are quite similar



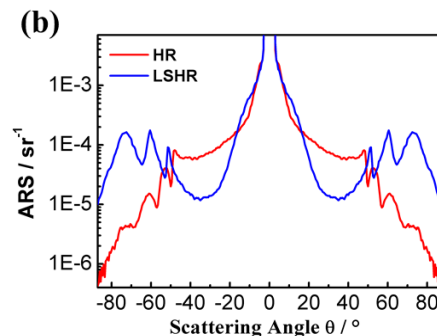
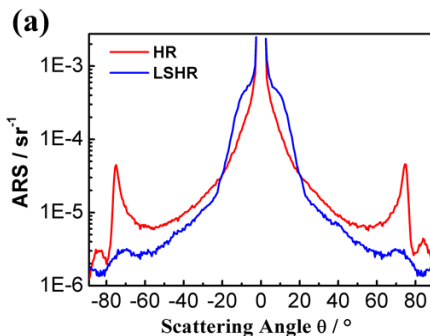
The destructive superposition of the optical factors results in the omnidirectional suppression of ARS for s-polarization



The experimental results show good correspondence to the theoretical, indicate high correlation of interface



An obvious deviation in the scattering angle between 10 and 30 degrees



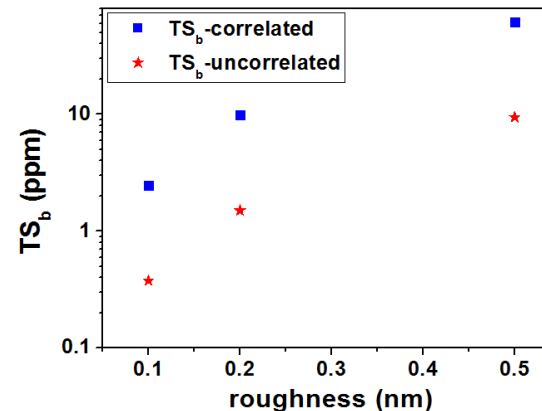
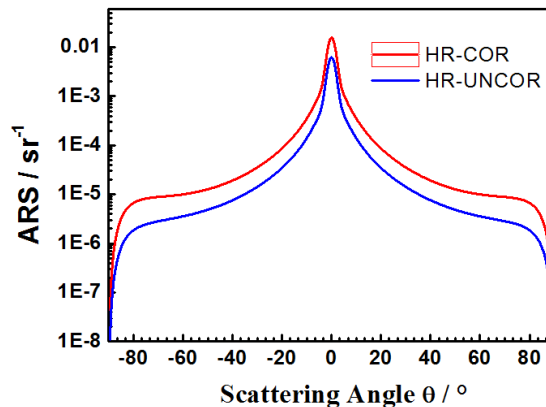
The TS for LSHR/QWHR is  $1.93E-4$ , and  $2.46E-4$  respectively  
Further control interface correlation

## Interface scattering

$$ARS(\theta_s) \propto \frac{1}{\lambda^4} \sum_{i=0}^N \sum_{j=0}^N F_i F_j^* \underbrace{PSD_{ij}(f)}$$

## Traditional means of optimizing PSD

- Reducing substrate roughness and Reducing surface roughness



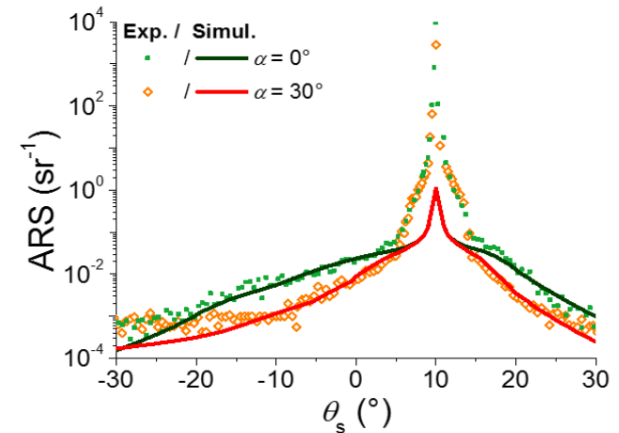
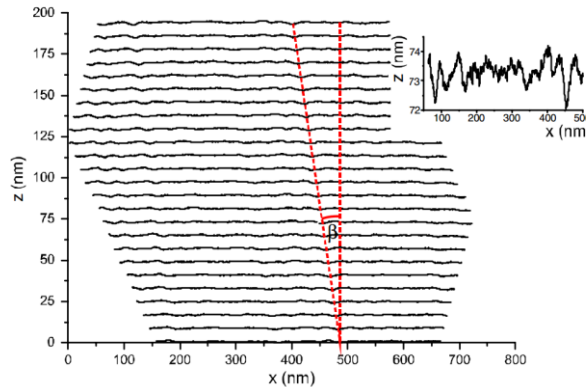
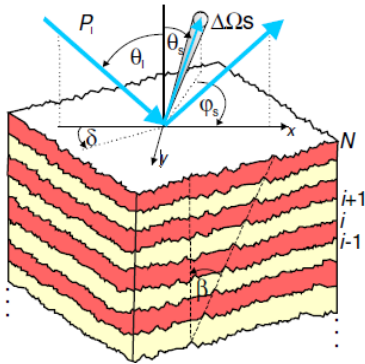
Scattering of QWHR is lower in the case of fully uncorrelated interfaces

The approach to optimize the correlation of interface roughness  $PSD_{ij}(f)$  to reduce interface scattering

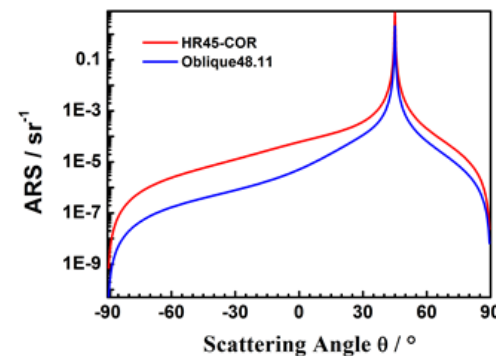


## Modulating $PSD_{ij}(f)$ by oblique multilayer deposition

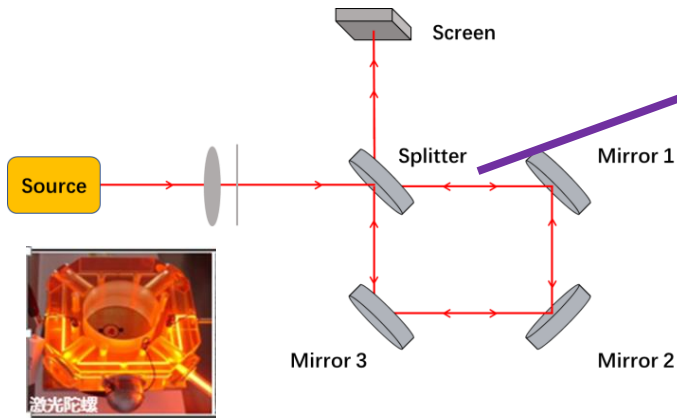
$$PSD_{ij,oblique}(f) = PSD_{ij,normal}(f) e^{-2\pi i \times f(z_i - z_j) \tan \beta \cos(\varphi_s + \delta)}$$



The total scattering loss is reduced by 28% with deposition angle of 30° in Mo/Si (HL)<sup>25</sup>,  $\lambda=13.5\text{nm}$

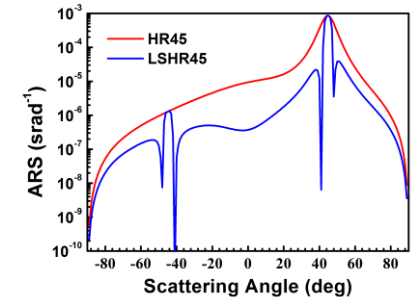


QWHR coating  
at 800nm



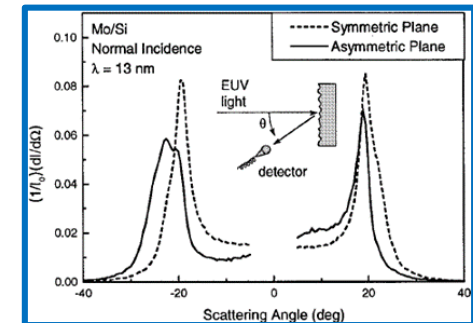
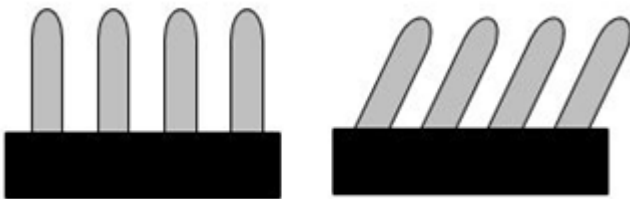
The lock-in threshold of Laser Gyros is limited by scattering in the counterpropagating direction

$$ARS(\theta_i, \pi, \theta_i) = \frac{k^4}{\pi^2} \cos^3 \theta_i \cdot |r(\theta_i)|^2 \cdot \text{PSD}(2k \sin \theta_i)$$



In the case of fully correlated roughness, the backscattering intensity could be only reduced through a decrease in the reflectivity

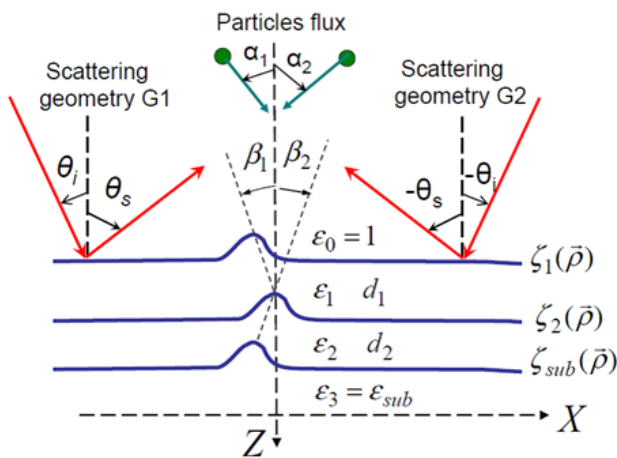
Oblique deposition make the scattering pattern asymmetric



Suppressed backscattering in towards the incident beam by oblique deposition

1. Gullikson E M, Stearns D G. Asymmetric extreme ultraviolet scattering from sputter-deposited multilayers[J]. Physical Review B, 1999, 59(20): 13273.

## A simplified model of a bi-layer by oblique deposition on a substrate



$$Z_2(\vec{\rho}) = Z_{sub}(\vec{\rho} + \vec{n}_x d_2 \tan \beta_2),$$

$$Z_1(\vec{\rho}) = Z_{sub}(\vec{\rho} + n_x d_2 \tan \beta_2 + n_x d_1 \tan \beta_1)$$

FT

$$Z_2^F(\vec{v}) = Z_{sub}^F(\vec{v}) e^{i\eta_2}, \quad Z_1^F(\vec{v}) = Z_{sub}^F(\vec{v}) e^{i(\eta_1 + \eta_2)},$$

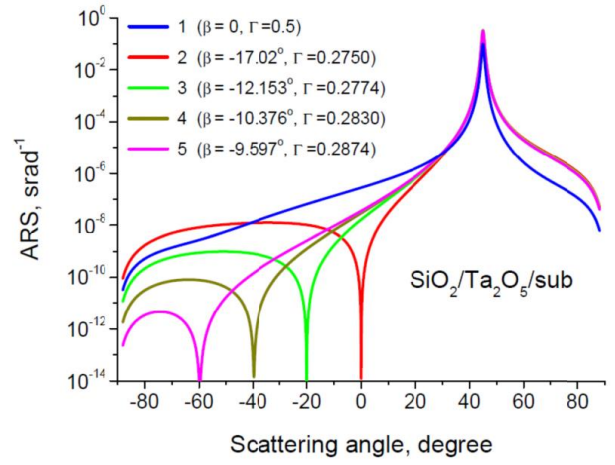
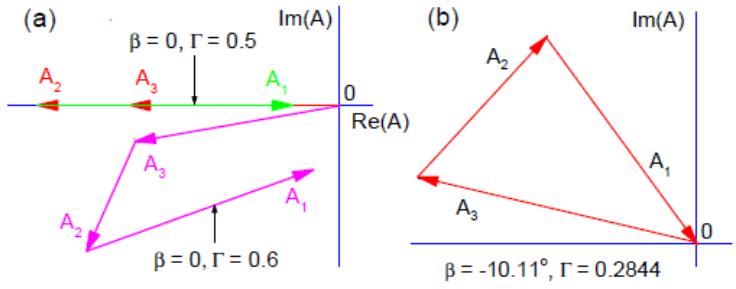
$$\eta_j \equiv -2\pi v_x d_j \tan \beta_j$$

$$ARS(\theta_s, \theta_i) \sim 1 + \underbrace{\frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_3 - \varepsilon_2} \cdot \frac{E_0(z_2, \theta_i) E_0(z_2, \theta_s)}{E_0(z_3, \theta_i) E_0(z_3, \theta_s)}}_{C \cdot \exp(i\gamma_2)} \cdot e^{i\eta_2} + \underbrace{\frac{\varepsilon_1 - \varepsilon_0}{\varepsilon_3 - \varepsilon_2} \cdot \frac{E_0(z_1, \theta_i) E_0(z_1, \theta_s)}{E_0(z_3, \theta_i) E_0(z_3, \theta_s)}}_{B \cdot \exp(i\gamma_{12})} \cdot e^{i(\eta_1 + \eta_2)}$$

The condition of total scattering suppression

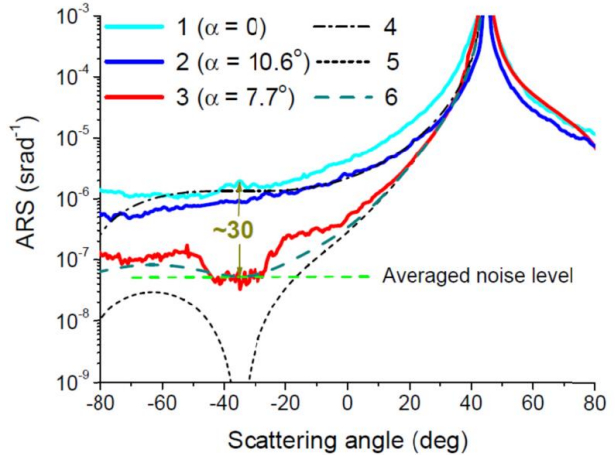
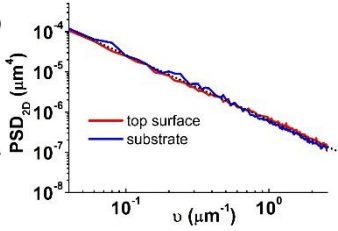
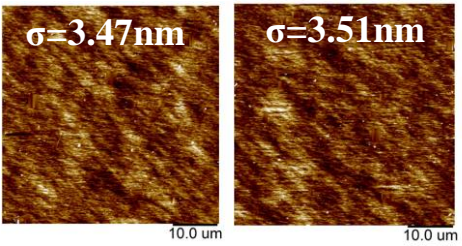
$$ARS = 1 + C e^{ic} + B e^{ib} = 0$$

$$ARS = 1 + Ce^{ic} + Be^{ib} = 0$$



Design bi-layers providing total scattering suppression at any desired scattering angle

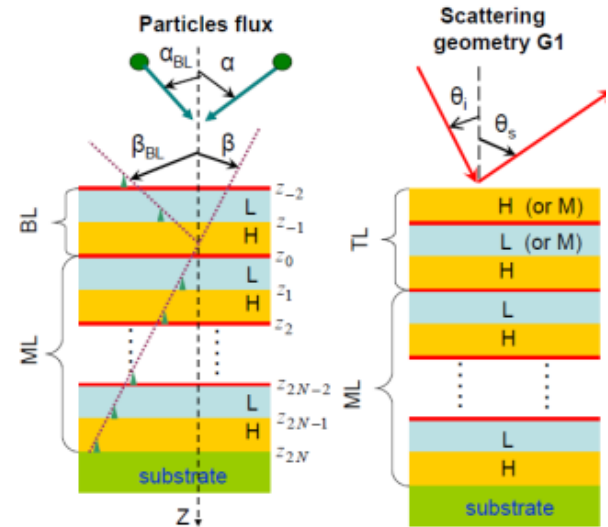
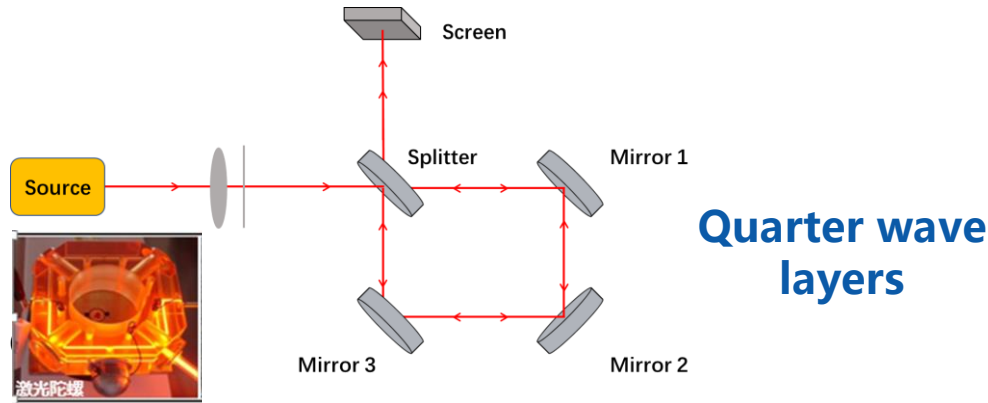
IBS to deposit the bi-layer



The growth angle is difficult to determine

The suppression of backscattering in the desired direction due to interference was experimentally observed

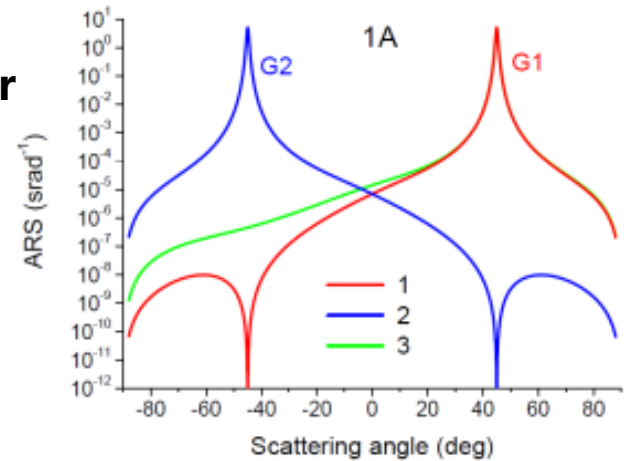
Suppresses scattering of HR coatings for both counter-propagating waves at once



The condition of the scattering suppression for bi-layer

$$A(\theta_i = -\theta_s = 45^\circ) = \frac{k^2}{4\pi} (1 - \epsilon_L) \cdot E_0^2(\theta_i) \cdot \frac{\kappa_H^2}{\kappa_L^2} \cdot \frac{e^{2i\eta_{BL}}}{1 - e^{-i\eta} \kappa_L^2 / \kappa_H^2} \cdot \zeta_{ML}^F(\vec{v})$$

$$\times \left[ \underbrace{1 - \frac{\epsilon_L - \sin^2 \theta_i}{\epsilon_H - \sin^2 \theta_i} \left( \frac{\epsilon_H - \epsilon_L}{\epsilon_L - 1} e^{-i\eta_{BL}} + e^{-i\eta} \right)}_F \right] = 0; \quad \kappa_{H,L} = \frac{2\pi}{\lambda} \sqrt{\epsilon_{H,L} - \sin^2 \theta_i}$$



The maximal field intensity is achieved on the mirror top resulting in increasing absorption and parasitic scattering from the contamination

**01 Background**

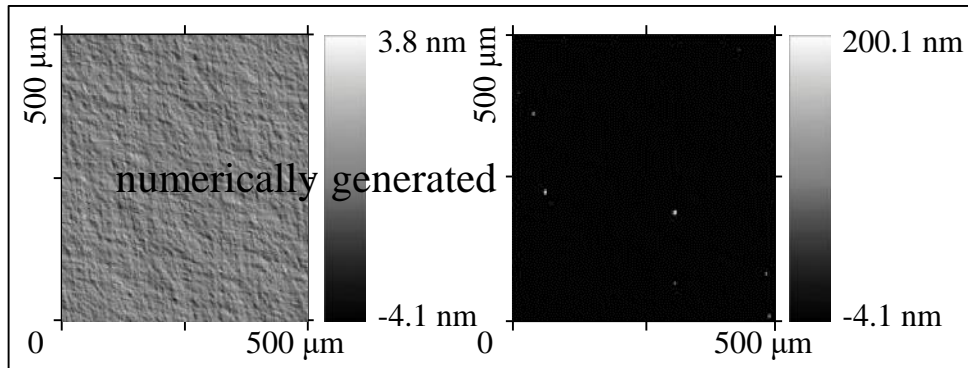
**02 Recent progress of interface scattering**

**03 Simulation, control of defect-induced scattering**

**04 Conclusion**

### simple shaped defect

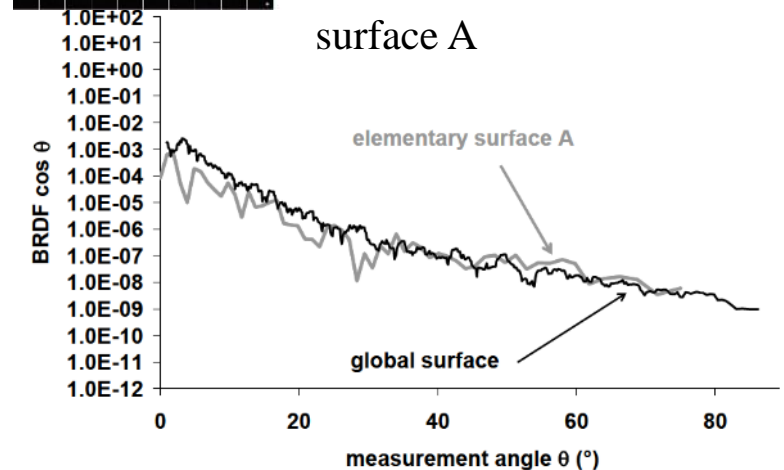
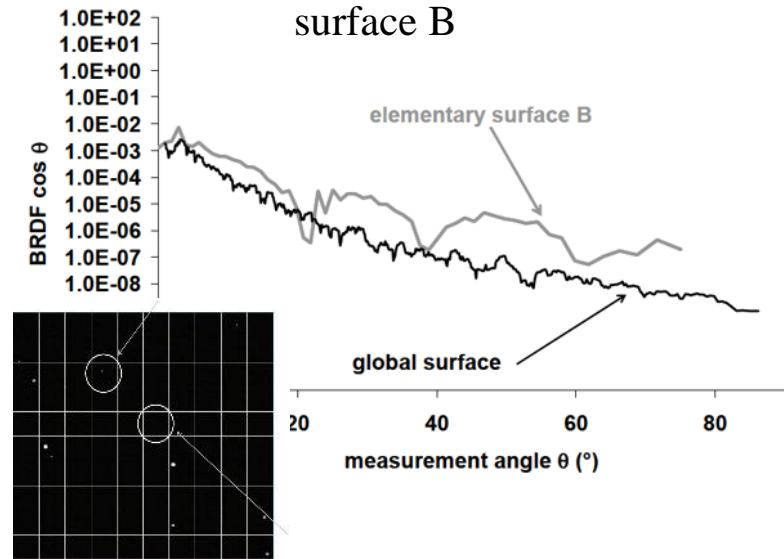
e.g., dome shaped defect on sub.



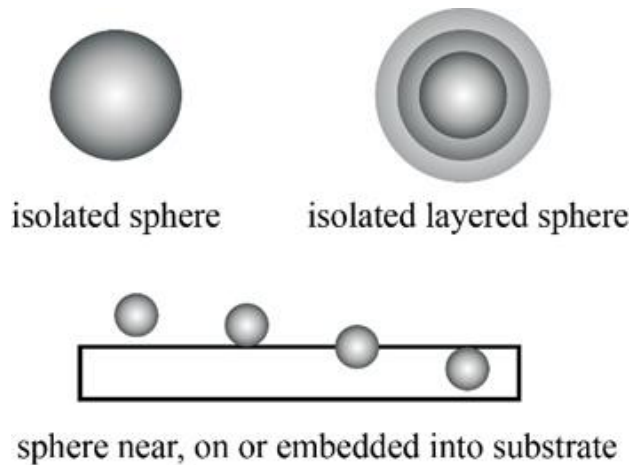
based on first-order perturbation

$$BRDF \cos \theta \propto \left[ \frac{J_1 \left( \frac{2\pi a}{\lambda} \sin \theta \right)}{\frac{2\pi a}{\lambda} \sin \theta} \right]^2$$

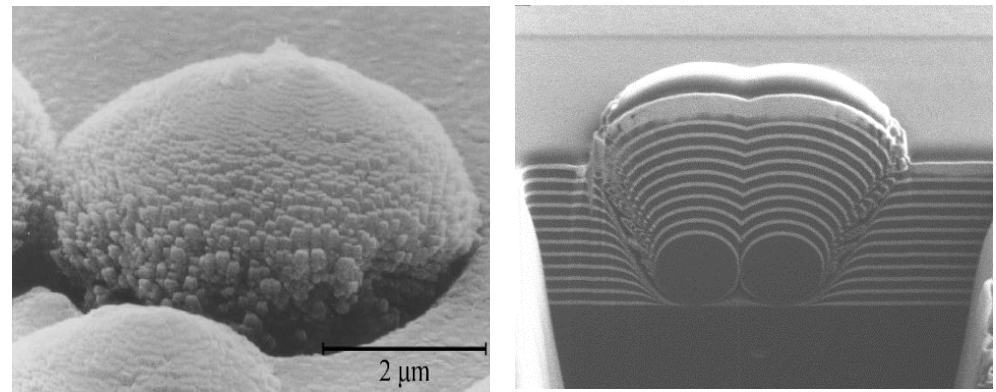
$$\sin \theta_m \approx \frac{Z_m}{\pi} \frac{\lambda}{2a}$$



## Simplified models in traditional analytical methods



## The actually complex-shaped nodular defects

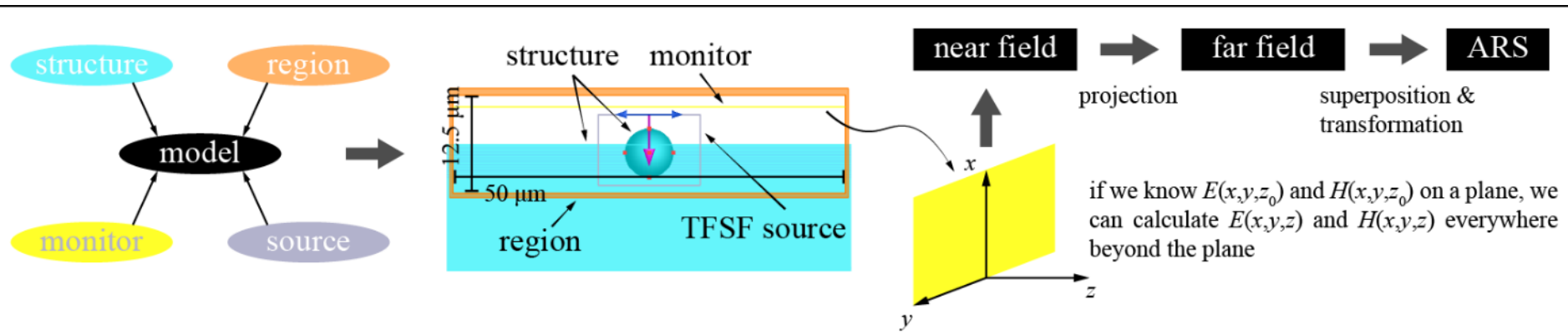


**FDTD method is widely used in solving the scattering problem of the structure on the order of illumination wavelength**

- 1、 A. Doicu, Y. Eremin, et al., *Opt. Com.* 159(4), 266-277 (1999)
- 2、 M J. Brett, R N. Tait, et al., *J. Mat. Sci.* 3(1), 64-70 (1992)



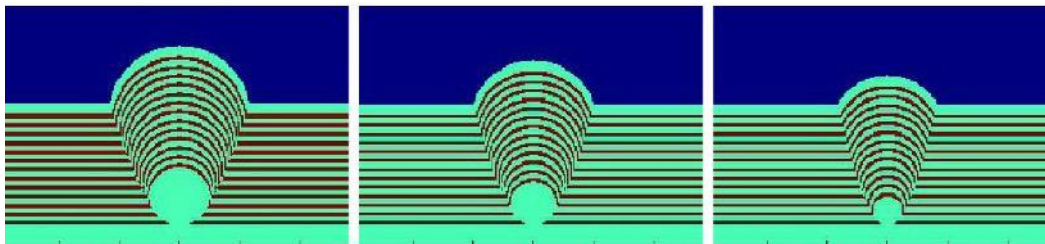
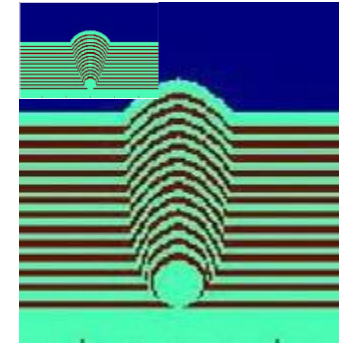
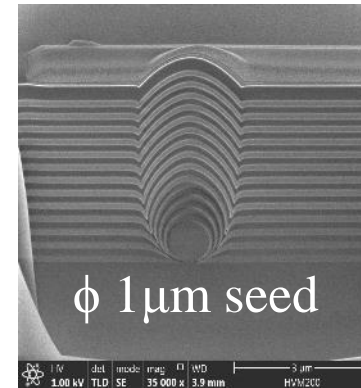
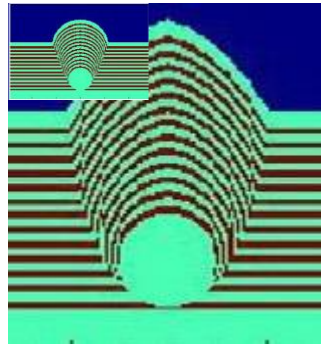
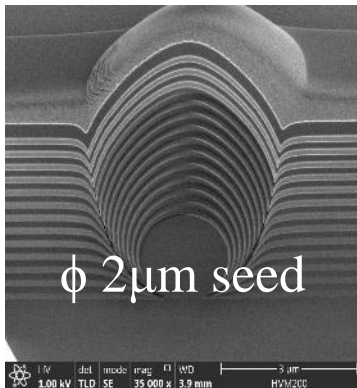
## FDTD simulation process



- region: PML boundary condition
- TFSF source:  $E=1 \text{ V}\cdot\text{m}^{-1}$ ,  $\lambda=1064 \text{ nm}$ , linear polarization, normal incidence

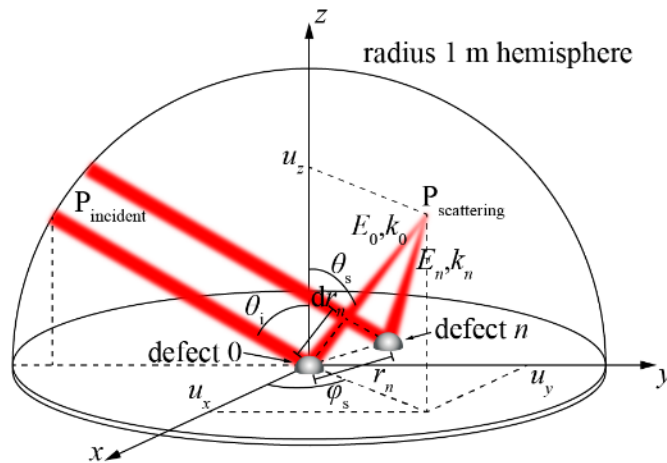
TFSF (total field scattered field) source separates the simulation region into two regions, the region inside TFSF box contains total field, the region outside contains only scattered field

## SEM cross-sectional micrographs

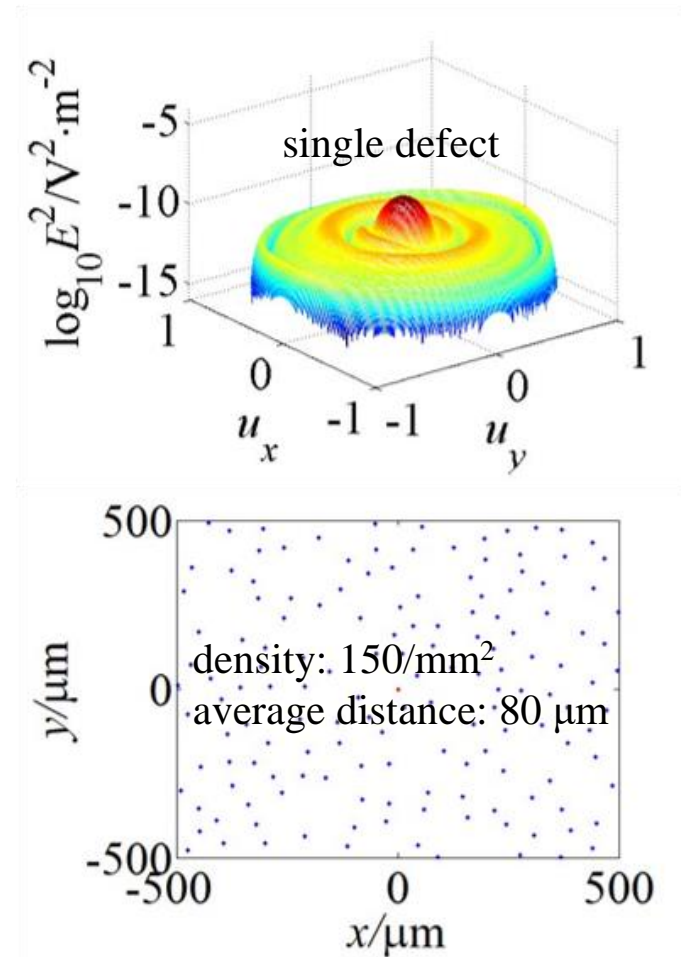
(d) 2.5dt - 2  $\mu\text{m}$ (e) 2.5dt - 1.5  $\mu\text{m}$ (f) 2.5dt - 1  $\mu\text{m}$ 

FS-fused silica substrate, H-Ta<sub>2</sub>O<sub>5</sub>,  
L-SiO<sub>2</sub>, FS|(HL)<sup>13</sup>L|Air @ 1064nm

the real shapes are exactly different from the 2.5dt models

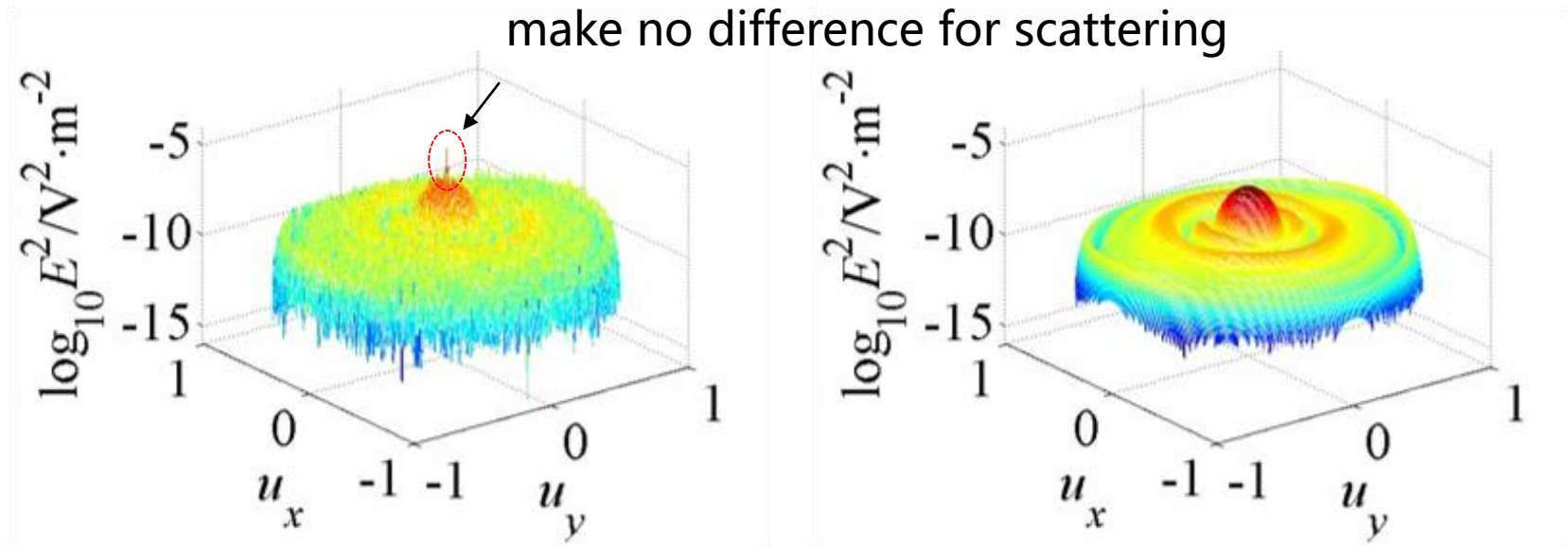


$$\begin{cases} E_{\text{amplitude}}^2 = \left( \sum E_0 e^{ik_0 \cdot dr_n} \right) \cdot \left( \sum E_0 e^{ik_0 \cdot dr_n} \right)^* \\ E_{\text{intensity}}^2 = nE_0^2 \end{cases}$$

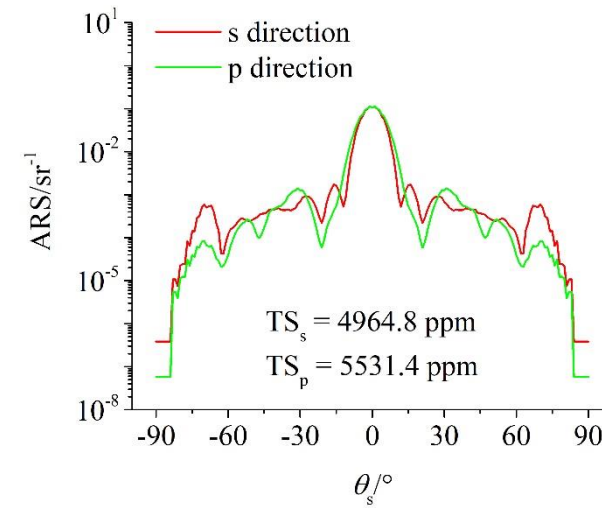
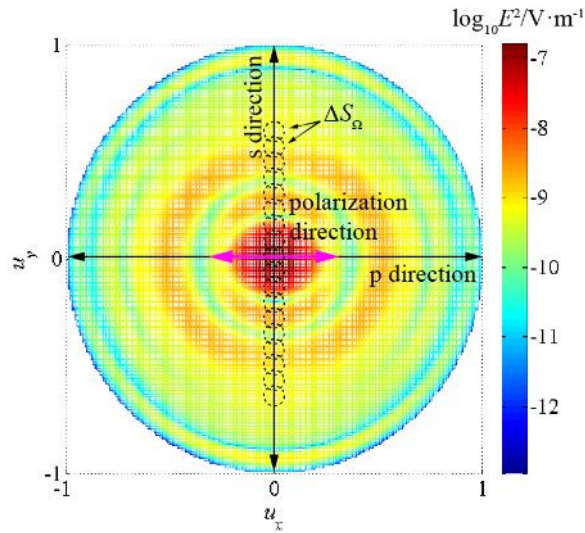


amplitude superposition

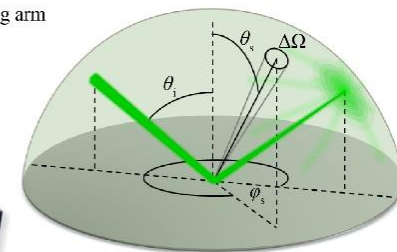
intensity superposition



when the average distance  $\gg$  defect size, except for the enormous burrs and a coherent enhancement at the center, the rough outlines of the amplitude and intensity superposition are same

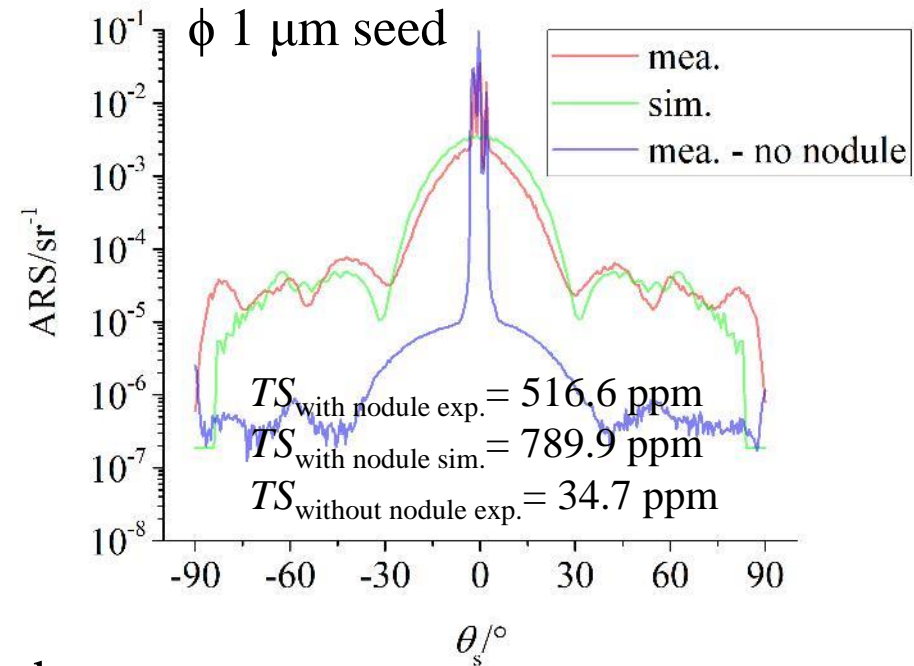
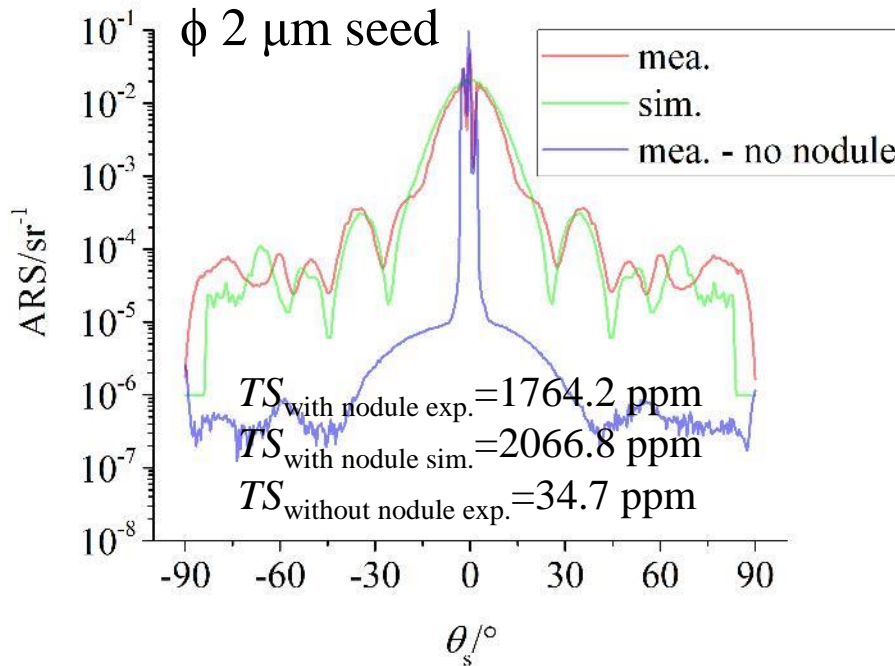


$$ARS = \frac{dP_s}{P_i d\Omega} = \frac{\frac{1}{2} \sqrt{\frac{\epsilon_0}{\mu_0}} E^2 \cdot dS_\Omega}{P_i \frac{dS_\Omega}{r^2}}$$



$$\begin{aligned} \theta_i &: -90^\circ \sim 90^\circ & \theta_s &: -270^\circ \sim 270^\circ \\ \varphi_s &: -90^\circ \sim 90^\circ & \Delta\Omega &: 0.02^\circ \sim 2^\circ \end{aligned}$$

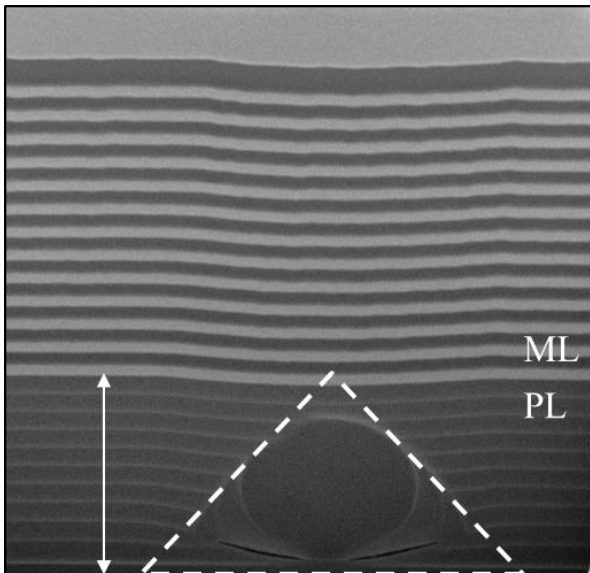
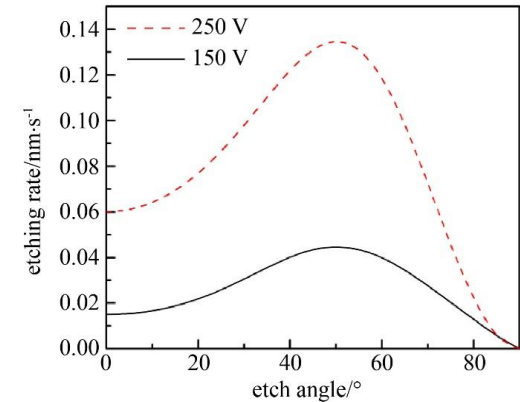
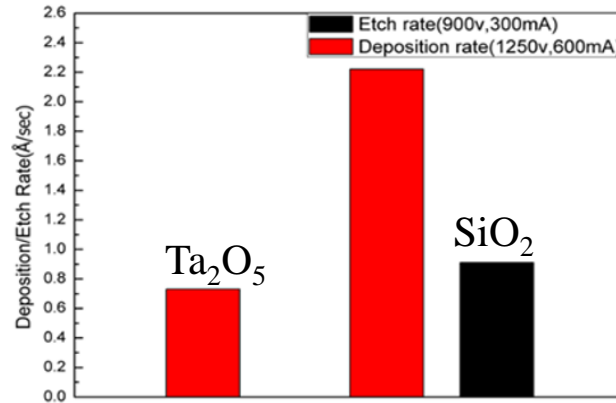
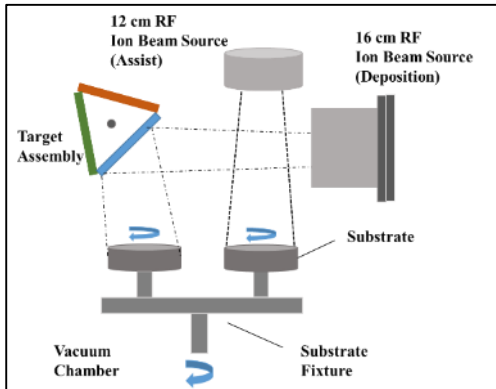
## Scattering measurement results vs. simulation results – s direction



simulation  $\longleftrightarrow$  match  $\longrightarrow$  measurement

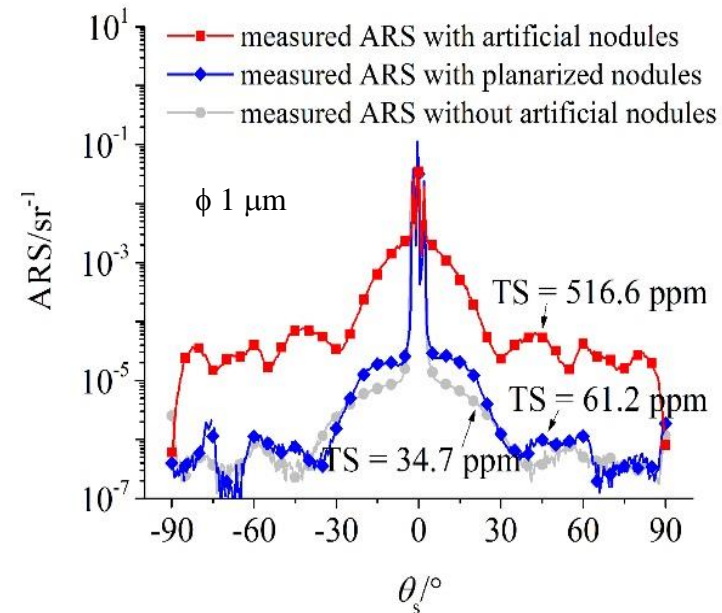
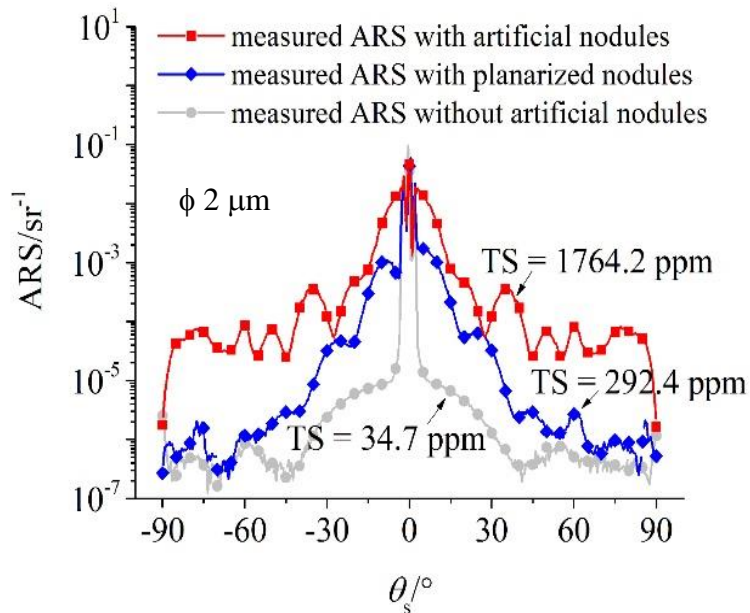
The characteristics of the defect-induced and roughness-induced scattering are significantly different.

## DIBS, 12 cm ion beam source for etching



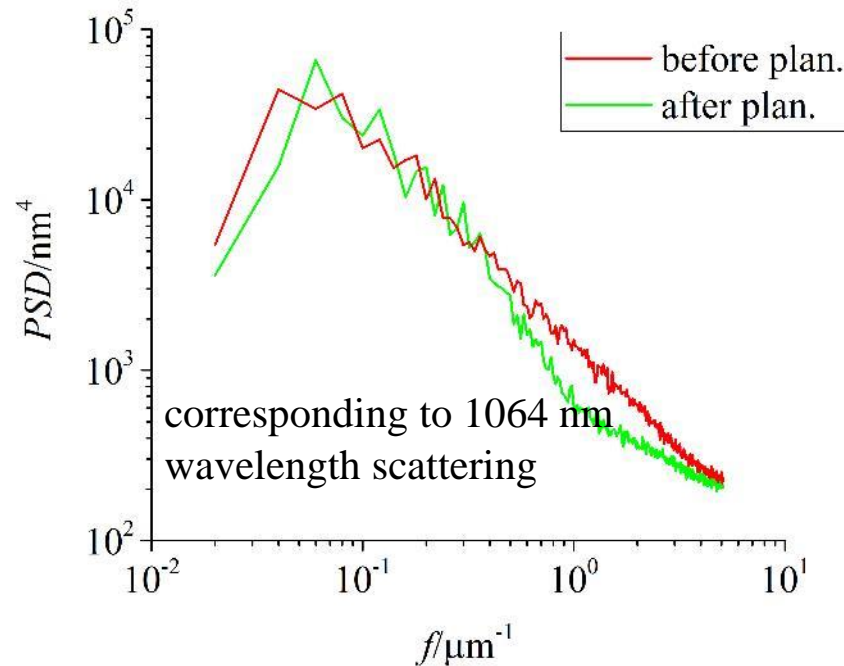
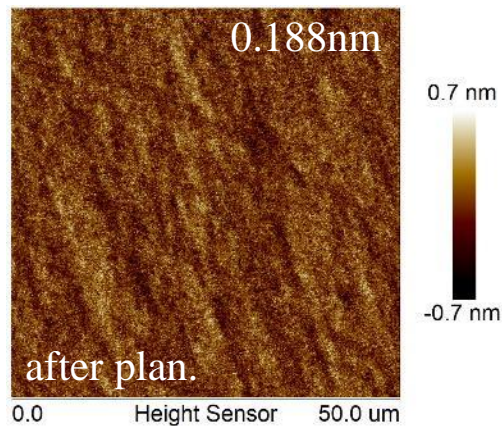
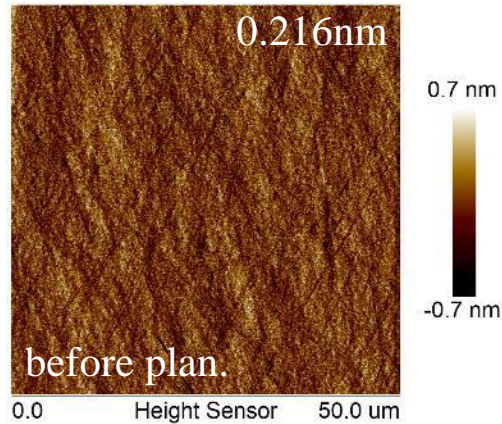
**Seed is completely embedded in the planarization layer, nodule is eliminated effectively.**

## Scattering measurement results before and after planarization



TS is effectively decreased after plan, for  $\phi 1 \mu\text{m}$  seed it almost reach to level of without nodule, but for  $\phi 2 \mu\text{m}$  seed it still large.

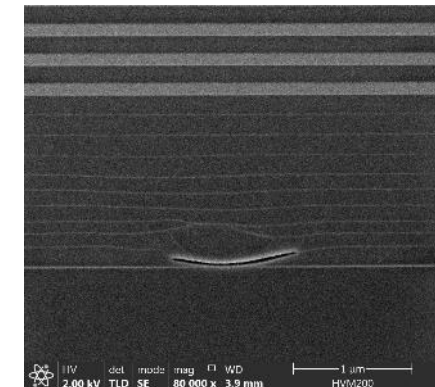
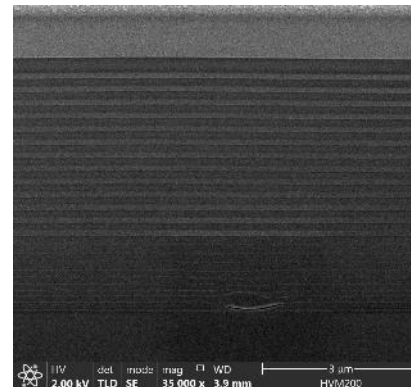
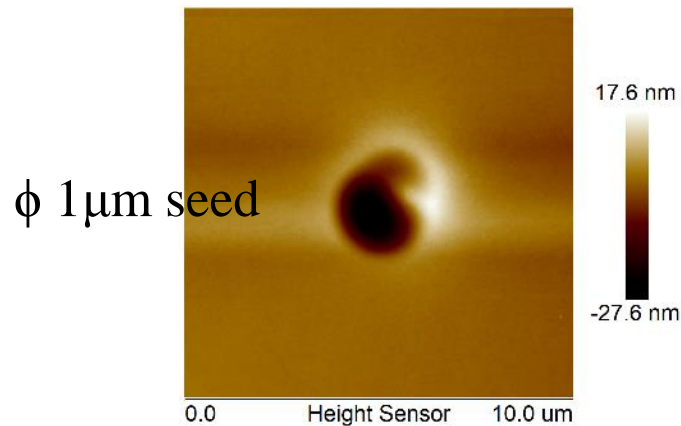
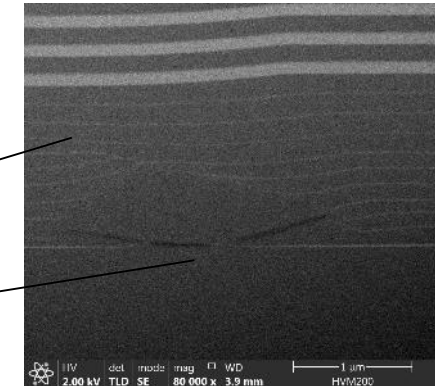
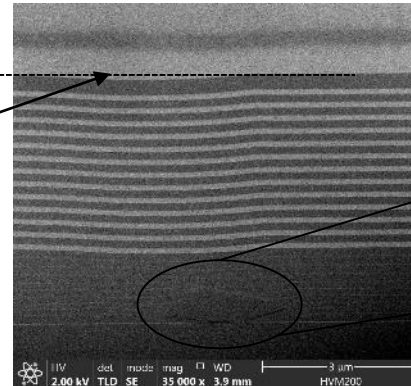
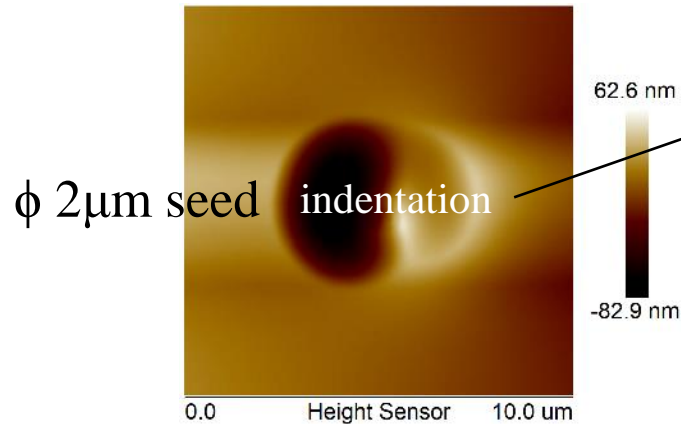




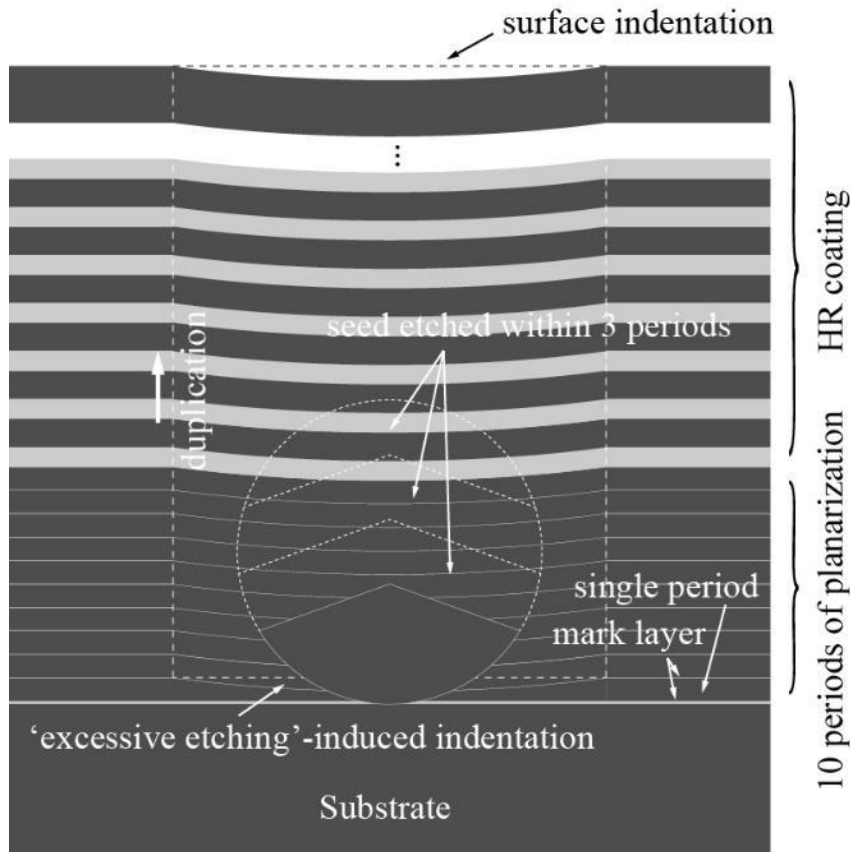
Planarization process decreases the roughness, so the roughness-induced scattering in theory

## AFM micrograph

## SEM cross-section micrograph



The nodule was completely eliminated, even there existed a indentation upon the seed and the seed was etched partly.



- **Surface indentation is the reason for not complete elimination of the nodular defect-induced scattering**
- **Surface indentation may be caused by excessive etching**

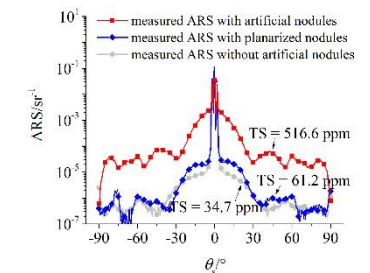
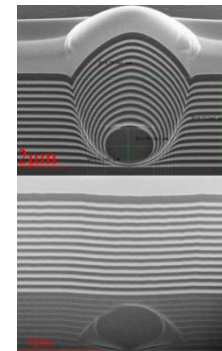
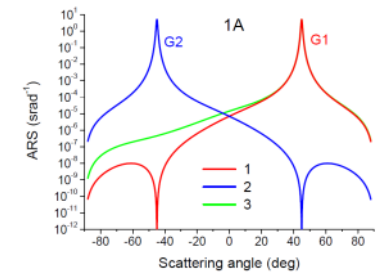
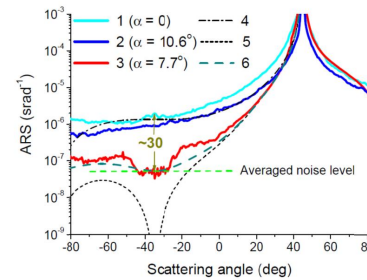
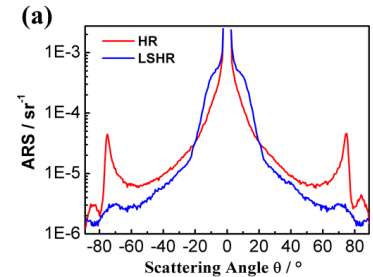
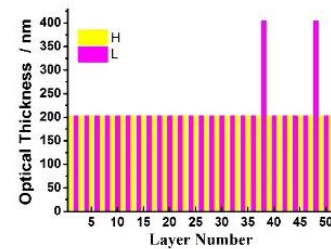
**01 Background**

**02 Recent progress of interface scattering**

**03 Simulation, control of defect-induced scattering**

**04 Conclusion**

- Scattering reduction of HR coatings by destructive interference of scattered waves on fully correlated interfaces
- Interference suppression of light back scattering through oblique deposition
- Quantitative assessment of defect-induced scattering in HR coatings, suppression of nodules with planarization



**Thank you!**

# Acknowledgement

**Han Wu, Lei Zhang, Hongfei Jiao, Xinbin Cheng, Zhanshan Wang**

**Sven Schröder, Marcus Trost** (Fraunhofer Institute for Applied Optics and Precision Engineering IOF)

**Igor V. Kozhevnikov** (Shubnikov Institute of Crystalloraphy of Federal Scientific Research Centre)

**NSFC for financial support**

