

# **FAST INTERACTIONS WITH SURFACES**

## **COHERENCE & DECOHERENCE**

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# OUTLINE

## FAST ATOM DIFFRACTION

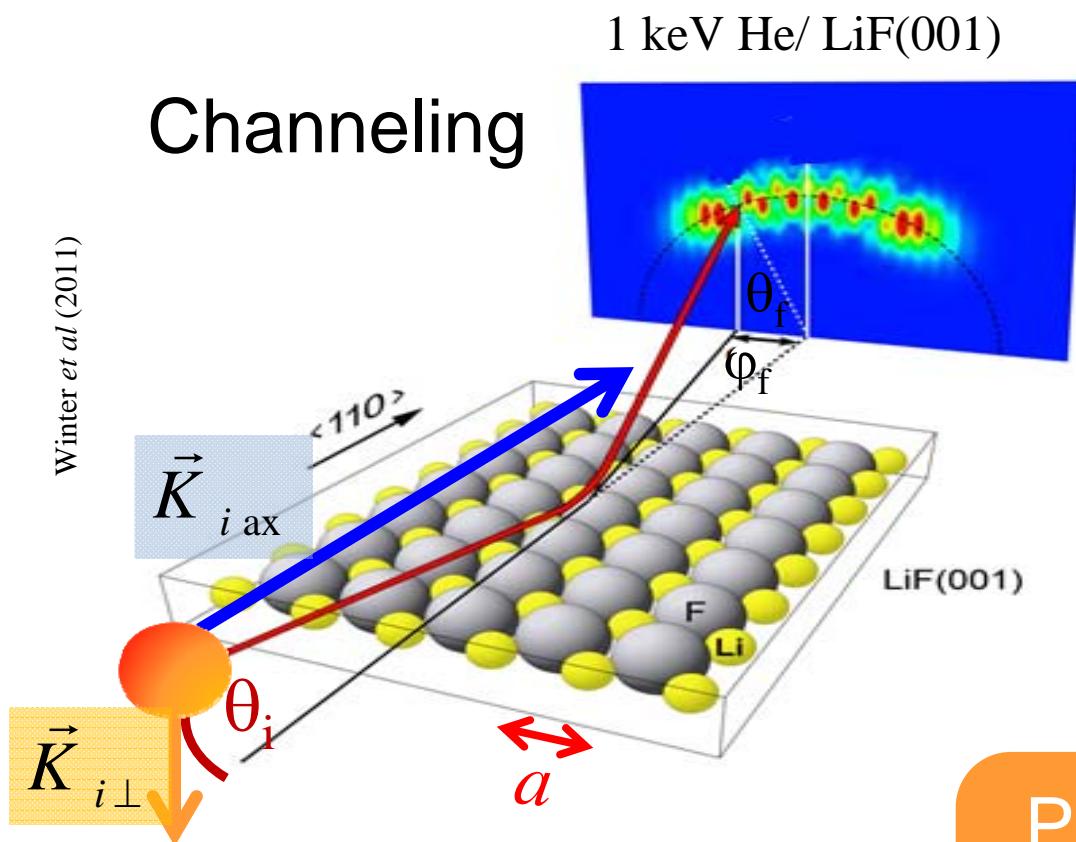
- General features
- Semi-quantum method
- Coherent lighting:  
van Cittert-Zernike theorem
- *Transversal* coherence effects:  
slit width, energy, and crystal spotting
- *Axial* coherence effects:  
normal momentum spread
- Decoherent contributions:  
influence of the temperature

# OUTLINE

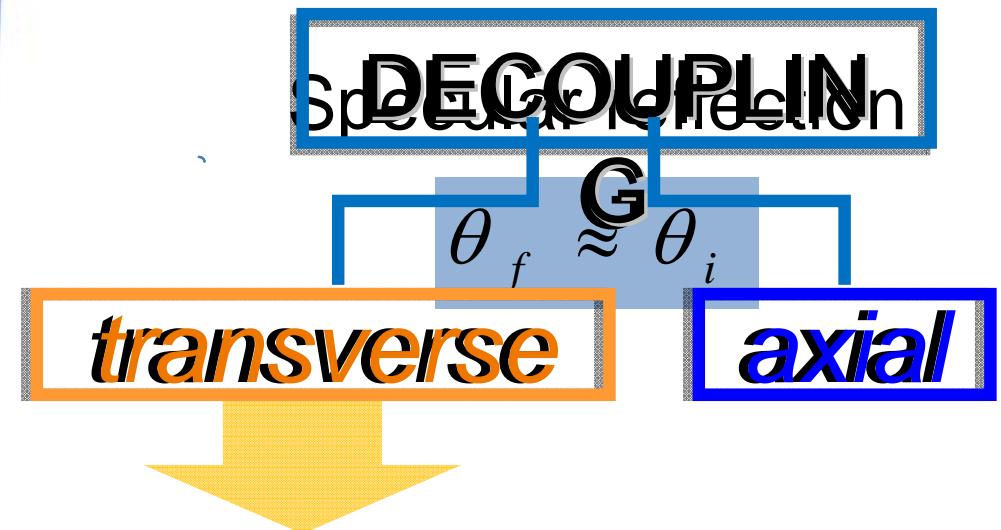
- 
- SURFACE ANALYSIS with:  
fast atoms and laser pulses
  - FINAL REMARKS

# FAST ATOM DIFFRACTION

Winter *et al* (2011)

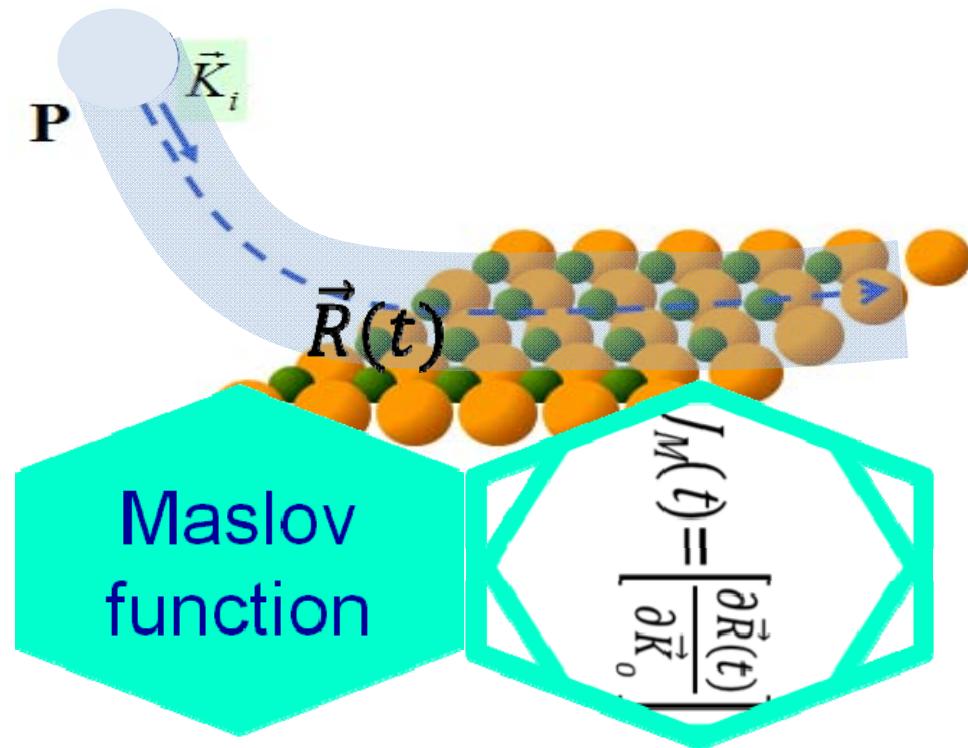


$$\lambda = \frac{2\pi}{K_i} \approx 0.008 \text{ a.u.} \ll a \approx 4 \text{ a.u.}$$

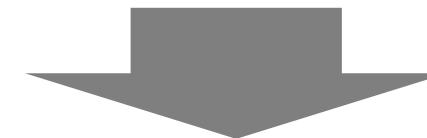


$$\lambda_{\perp} = \frac{2\pi}{K_{i\perp}} \approx 0.4 \text{ a.u.}$$

# Surface Initial Value Representation (SIVR)



Based on the IVR method by Miller (1970)



Feynman path integral  
formulation

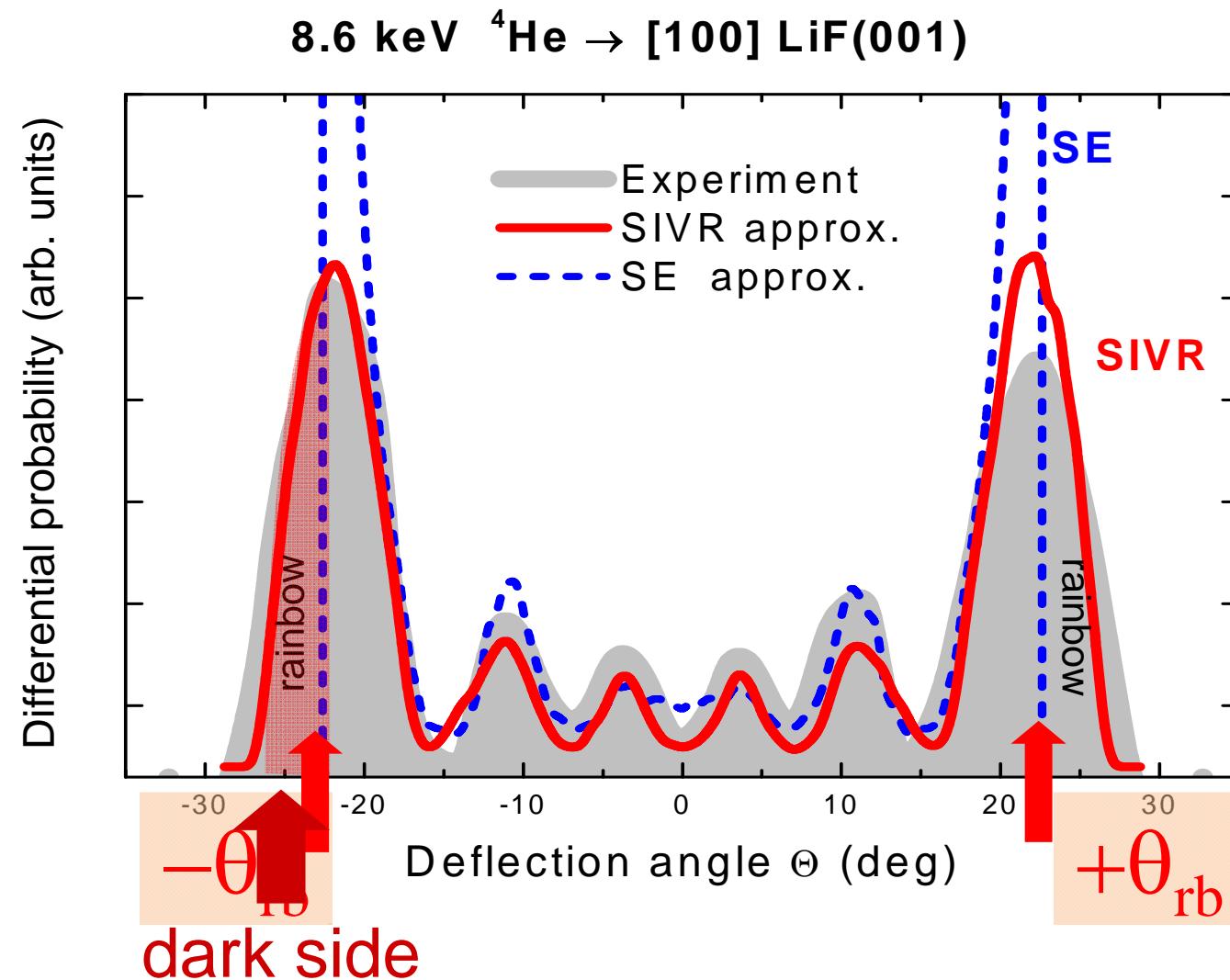


Semi-quantum method  
*without the stationary phase approx.*

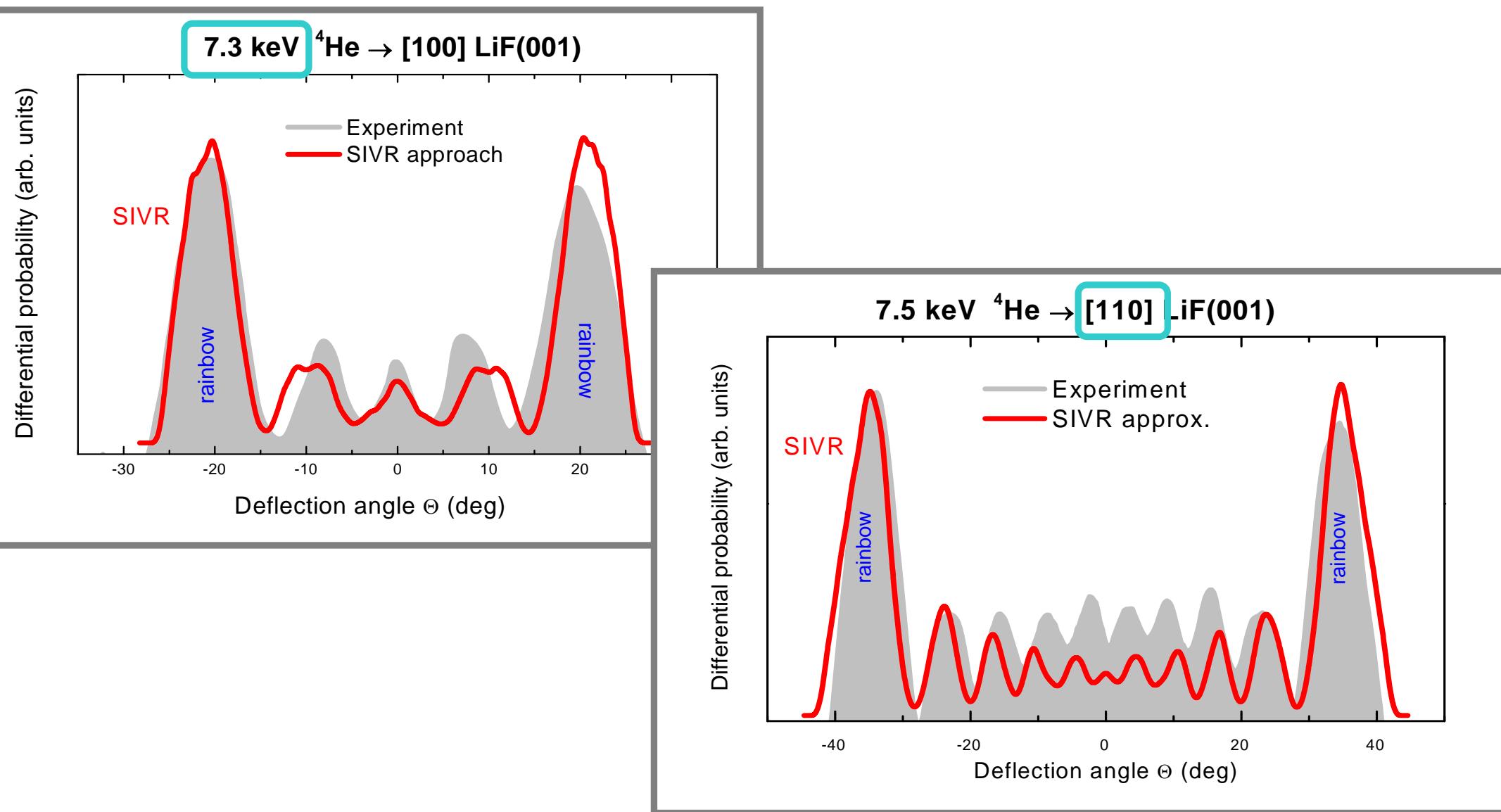
QUANTUM INTERFERENCE OF  
TRANSITION AMPLITUDES

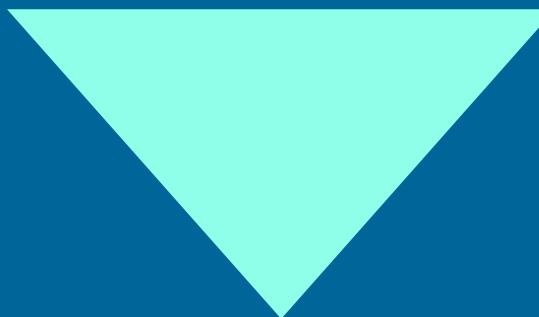
Classically forbidden  
transitions

# Surface Initial Value Representation (SIVR)



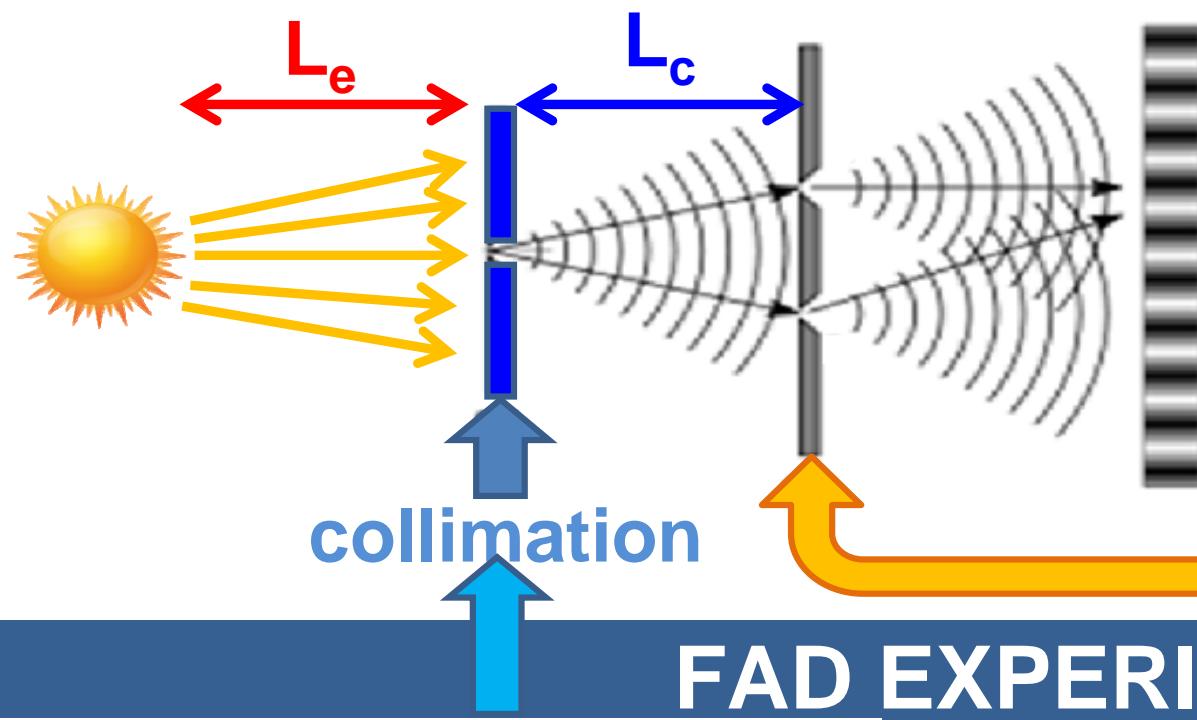
# Surface Initial Value Representation (SIVR)





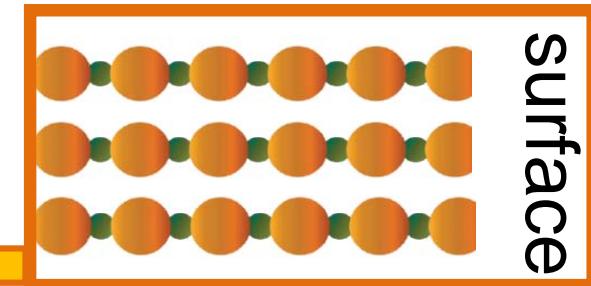
# COHERENT LIGHTING

# Atom interferometry

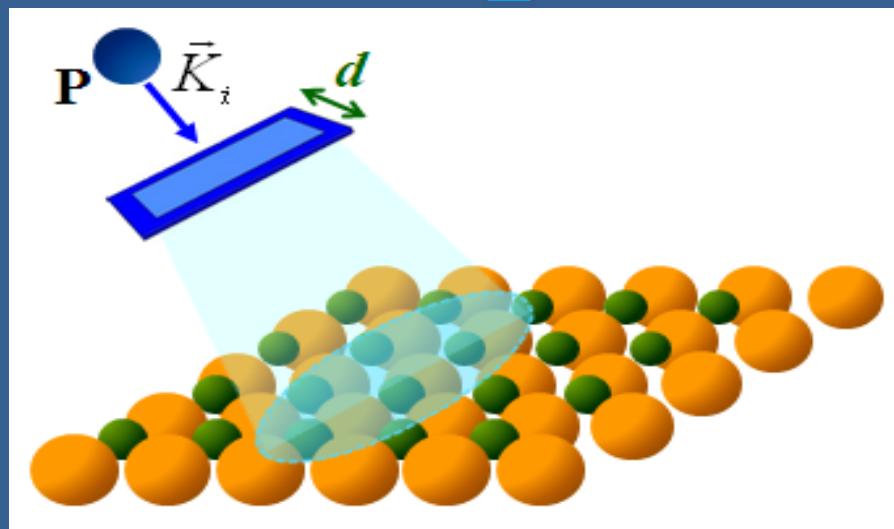


Needed:

**COHERENCE**



**FAD EXPERIMENTS**



1 keV He atoms:  $\lambda \cong 0.5 \text{ pm}$

$$L_e, L_c \leq \frac{d^2}{\lambda}$$

Near-field regime  
(Fresnel)

# The van Cittert-Zernike theorem (1938)

“The wavefront from an incoherent extended quasi-monochromatic source will appear mostly coherent at large distances”

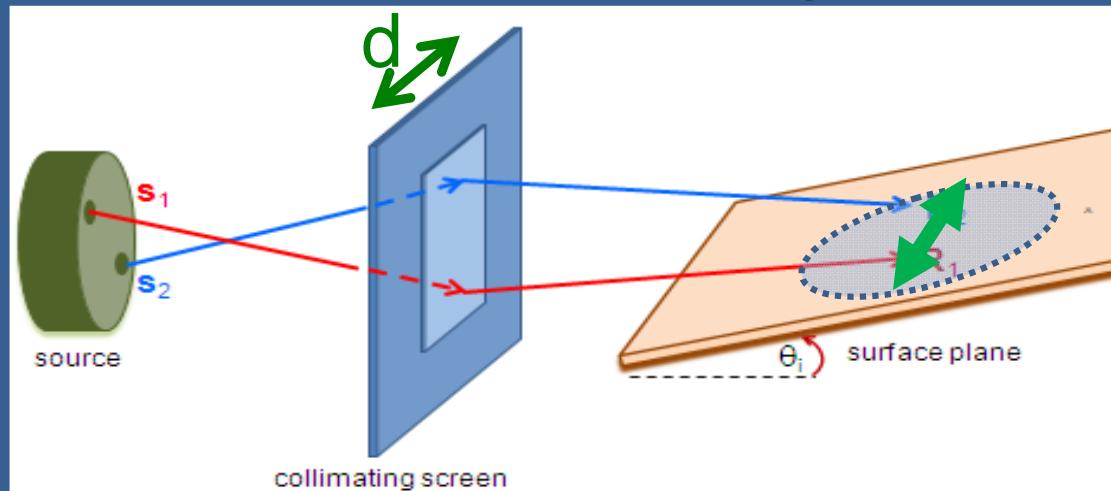
Knox, Alonso and Wolf, Phys. Today **63**, 11 (2010)



coherent waves

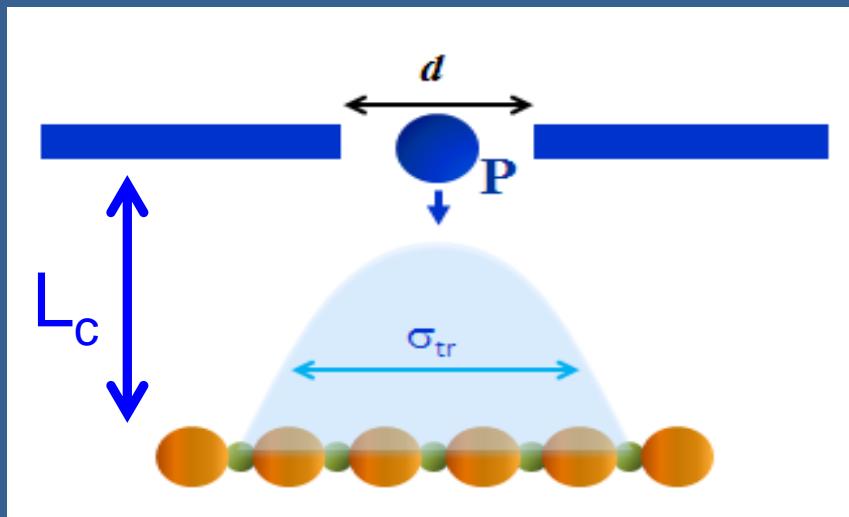
# Degree of coherence: van Cittert-Zernike

Extended incoherent quasi-monochromatic source



Size of the wave packet:

**Complex degree of coherence**

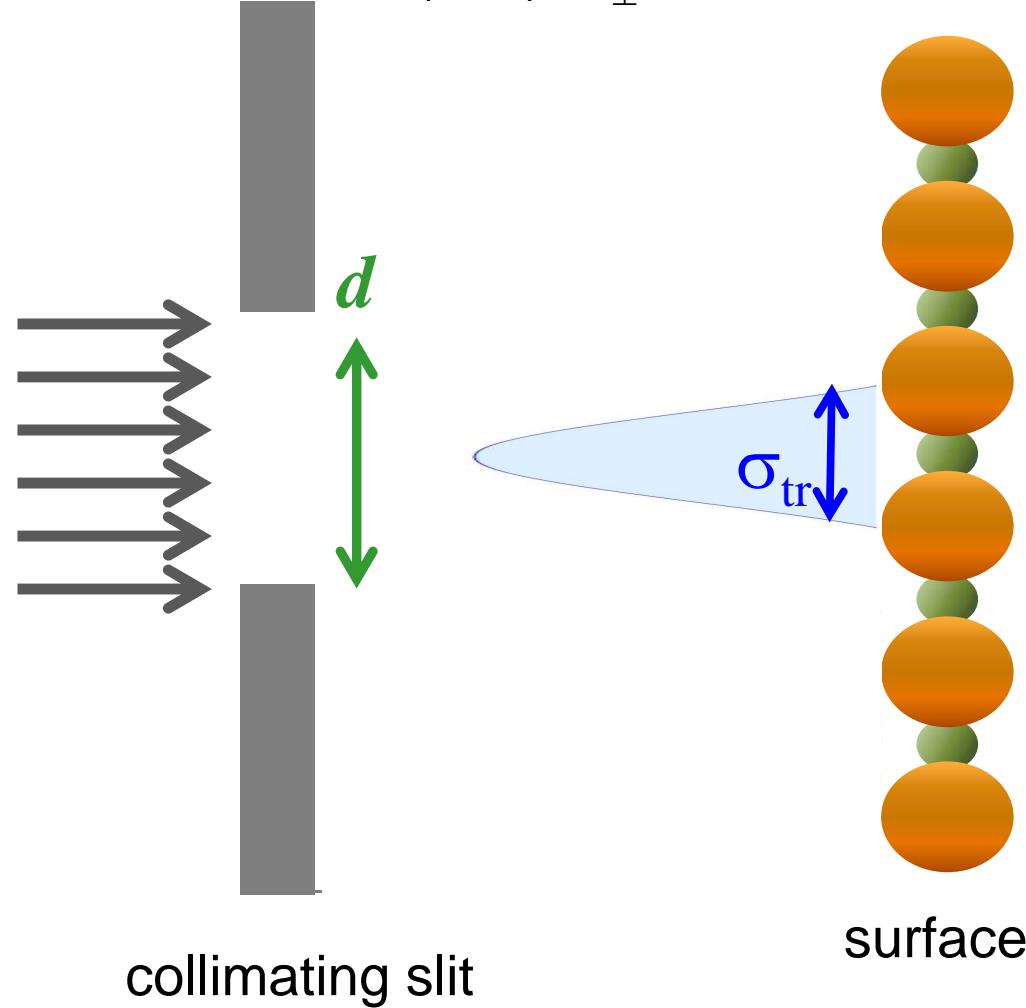


*transversal coherence length*

$$\sigma_{tr} = \frac{\lambda}{\sqrt{2}} \frac{L_c}{d}$$

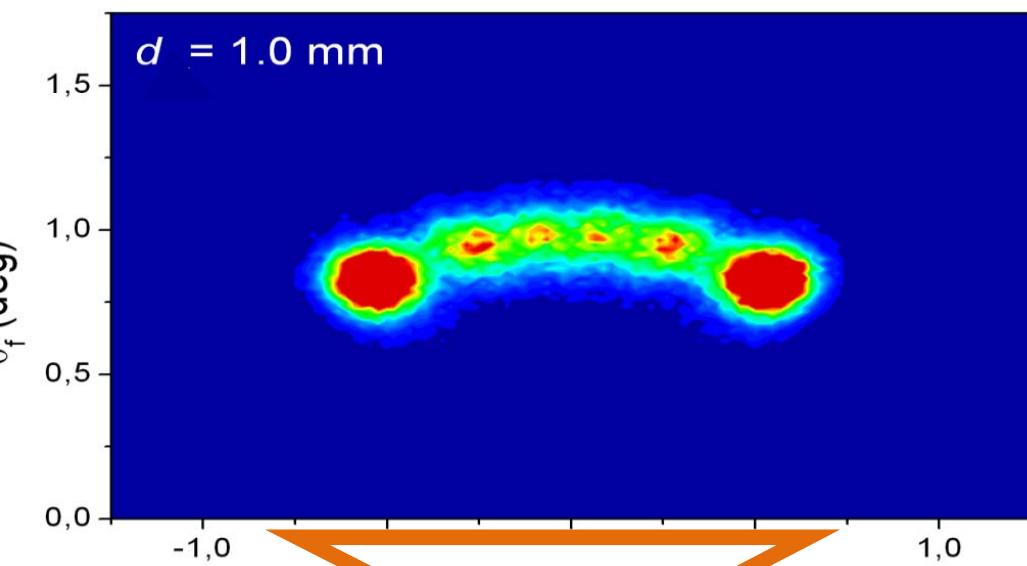
# Transversal coherence: slit width

${}^4\text{He} \rightarrow <110> \text{LiF}(001)$ ,  $E_{\perp} = 0.3 \text{ eV}$



surpernum. rainbows

unit-cell interference

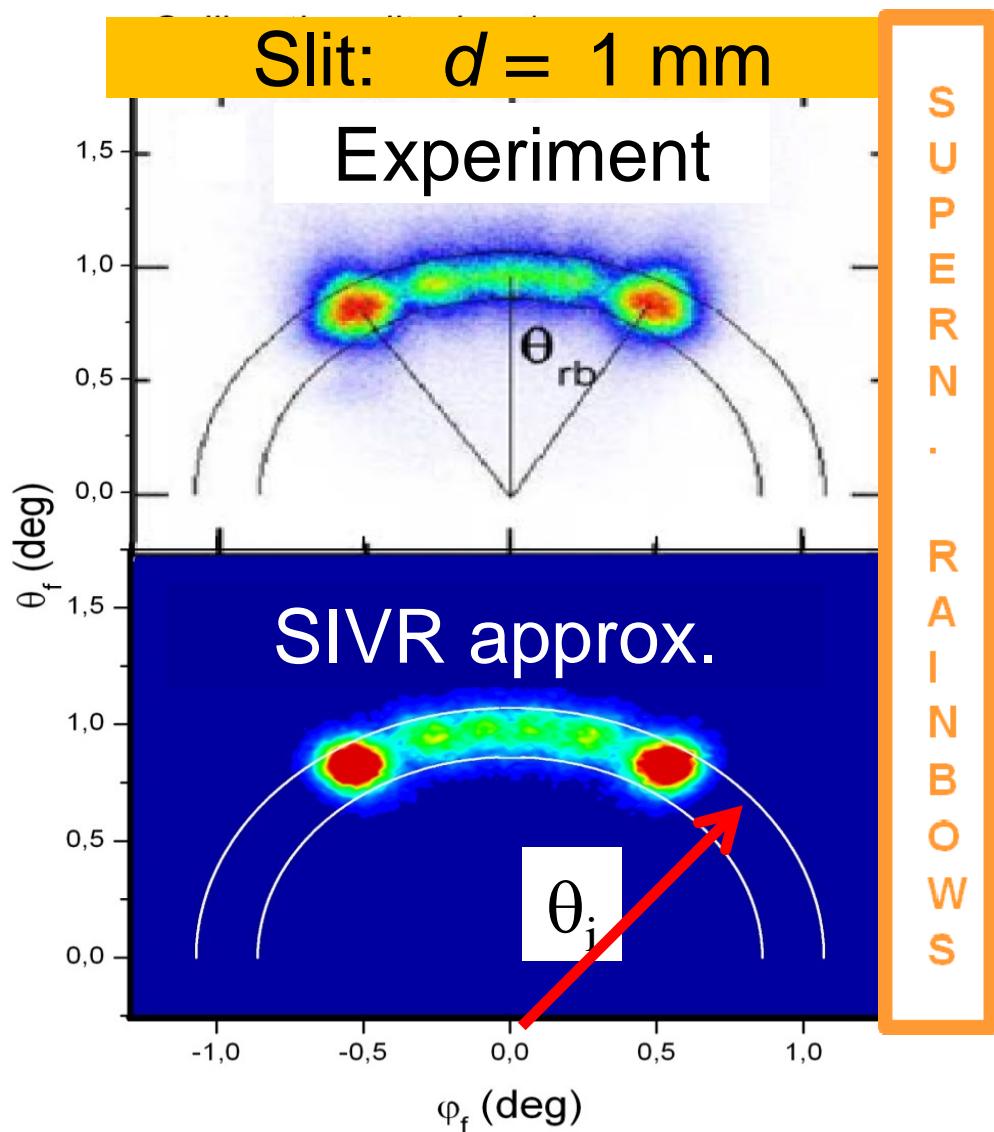
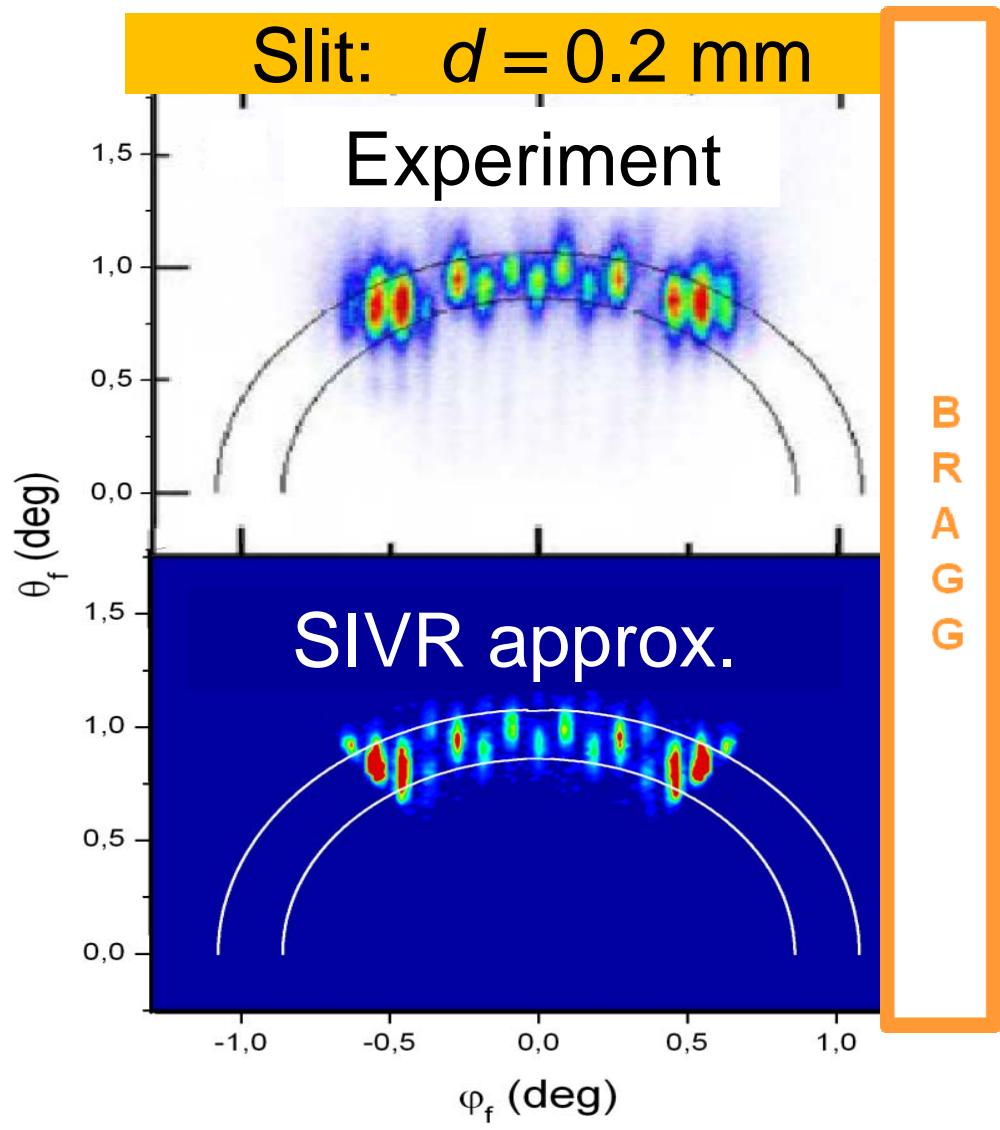


Corrugation of the potential  
inter-cell interference

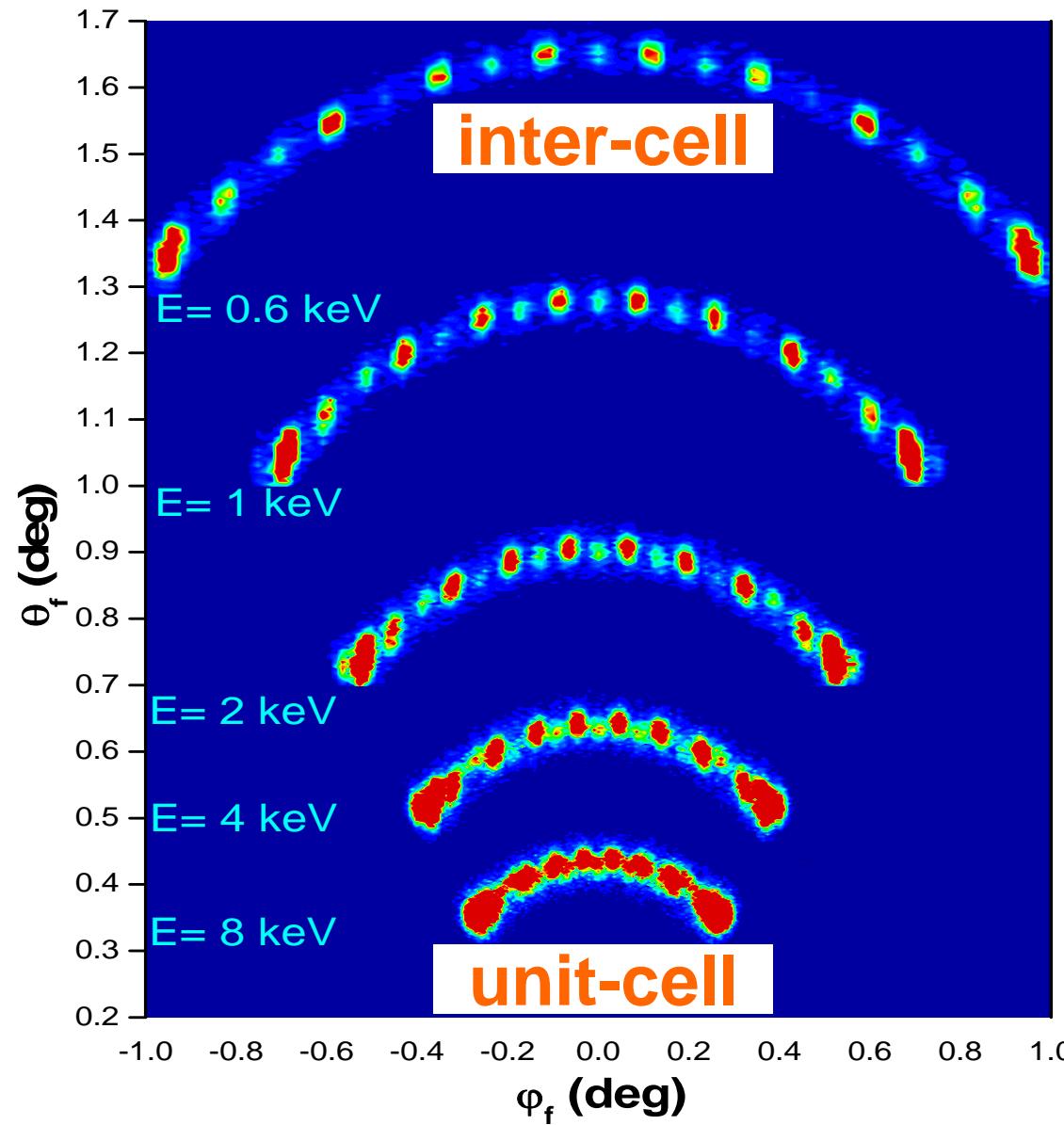
# Experimental confirmation

Expt. : Seifert *et al.*, Nucl. Instr. Meth. B 350 (2015) 99

${}^4\text{He} \rightarrow <110> \text{LiF}(001)$ ,  $E_{\perp} = 0.3 \text{ eV}$



# Transversal coherence: impact energy



${}^4\text{He} \rightarrow <110> \text{LiF}(001)$   $E_{\perp} = 0.5 \text{ eV}$

Fixed collimation:  $d = 0.2 \text{ mm}$

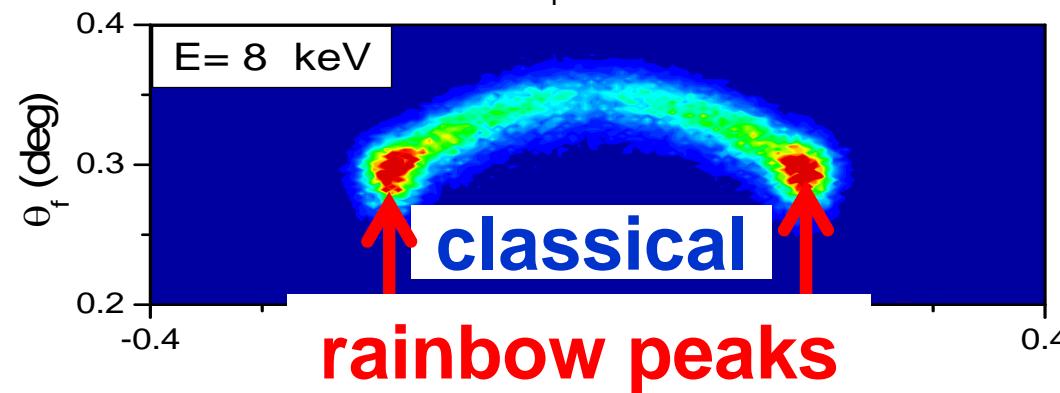
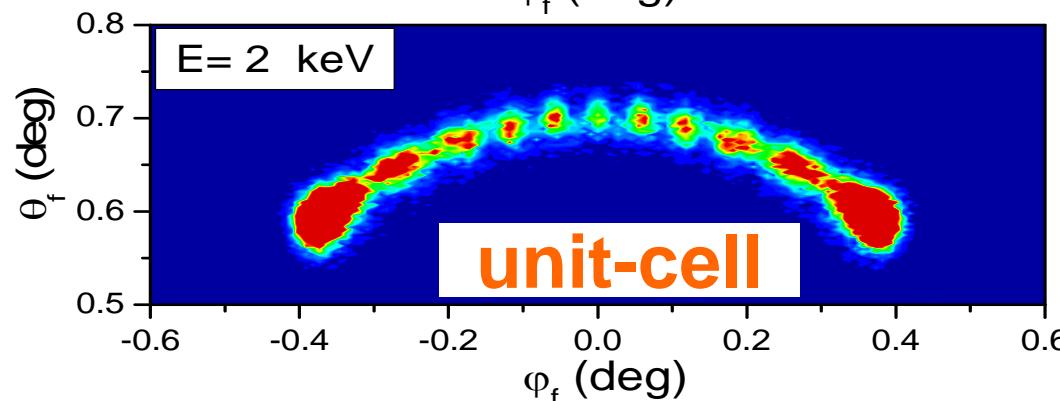
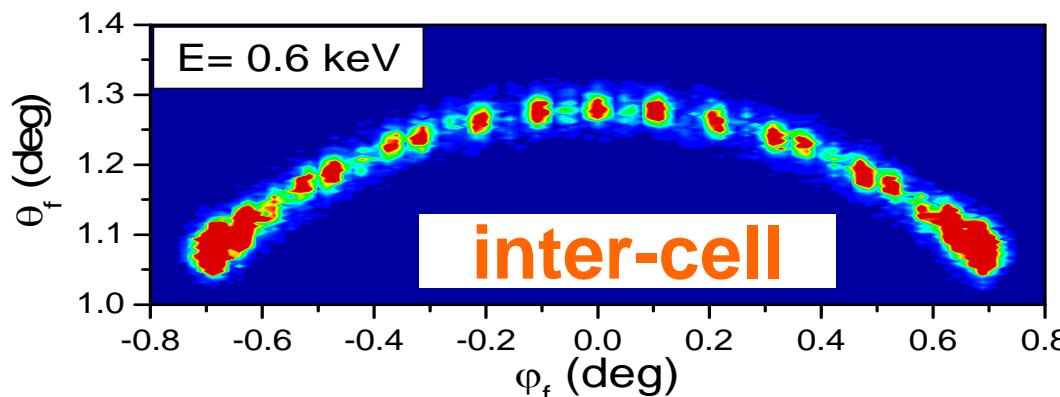
transversal coherence length

$$\sigma_{tr} = \frac{\lambda}{\sqrt{2}} \frac{L_c}{d} \propto \frac{1}{\sqrt{E}}$$

Independent of:

- inelastic contributions
- detector resolution

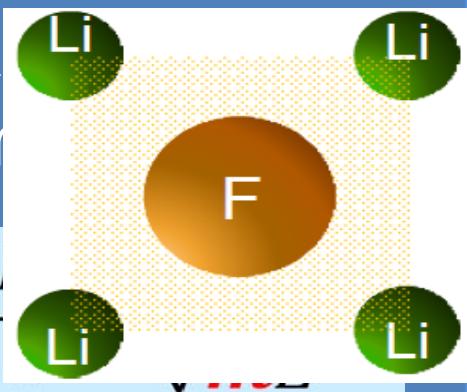
# Transversal coherence: atomic mass



$^{20}\text{Ne} \rightarrow <110> \text{LiF}(001)$ ,  $E_{\perp} = 0.3 \text{ eV}$

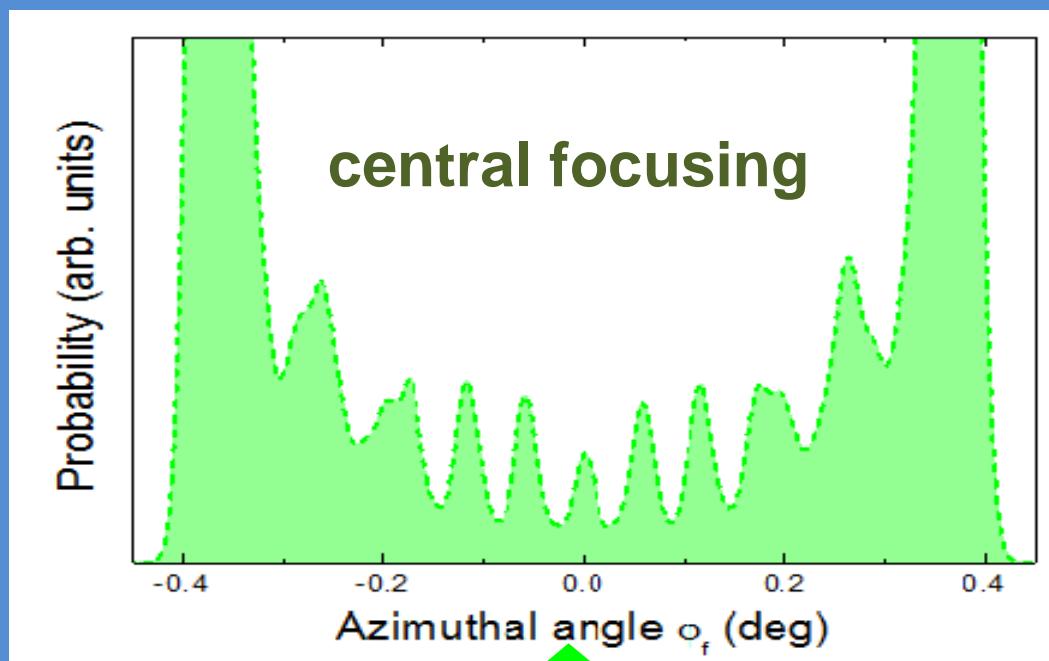
CRYSTAL SPOTTING

transversal  
supernum.  
rainbows

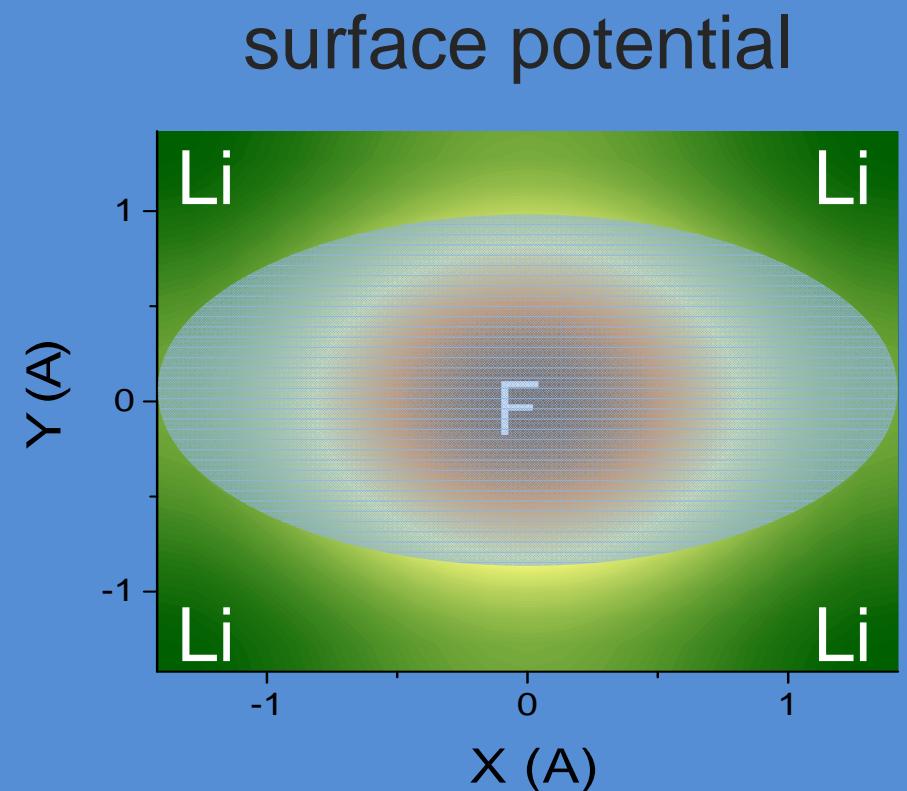


# Crystal spotting

2 keV Ne  $\rightarrow$   $<110>$  LiF(001),  $E_{\perp} = 0.3$  eV



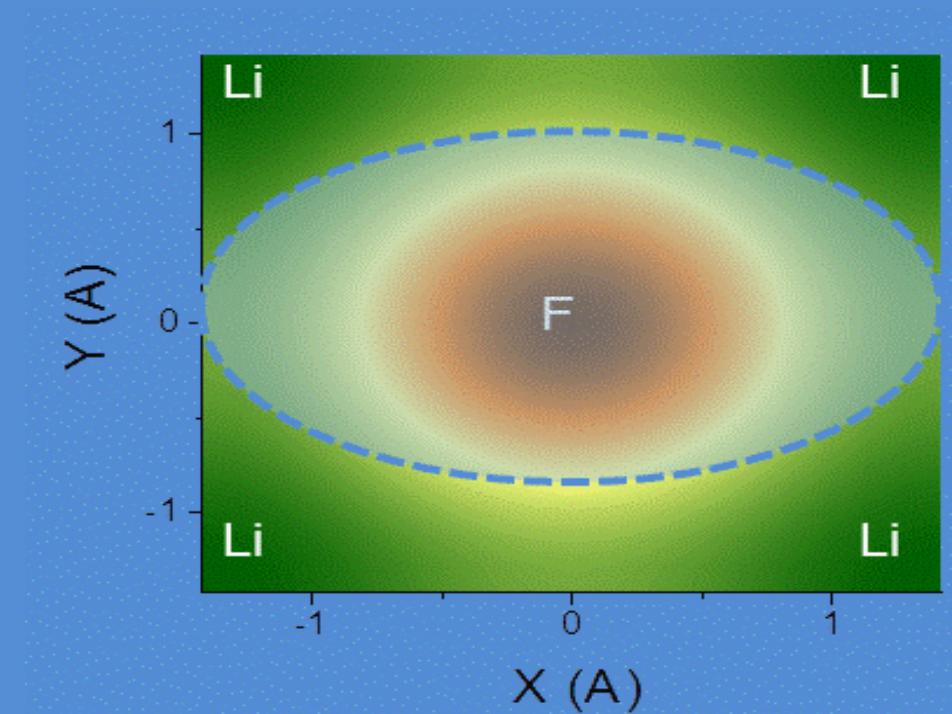
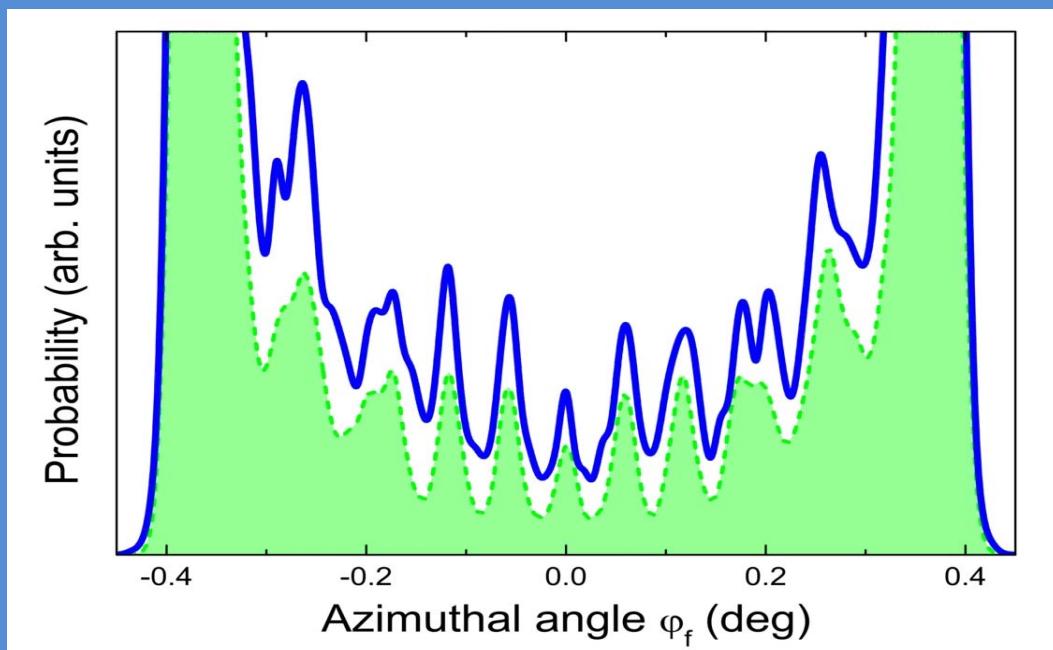
incidence direction



# Crystal spotting

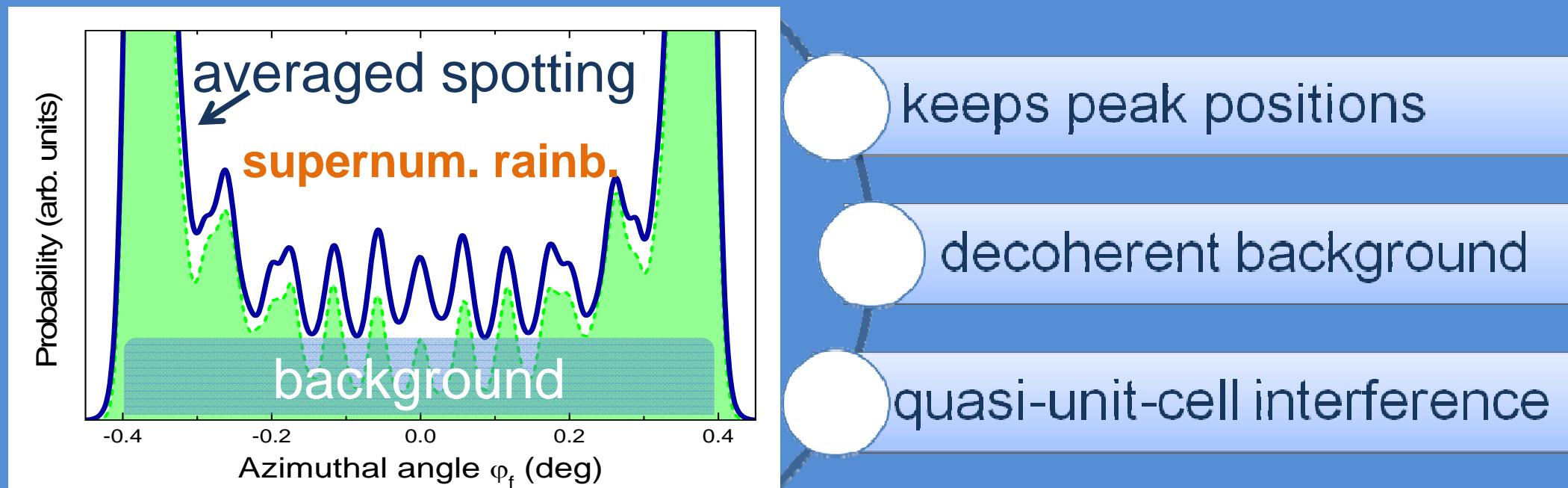
2 keV Ne  $\rightarrow$   $<110>$  LiF(001),  $E_{\perp} = 0.3$  eV

surface potential



# Crystal spotting

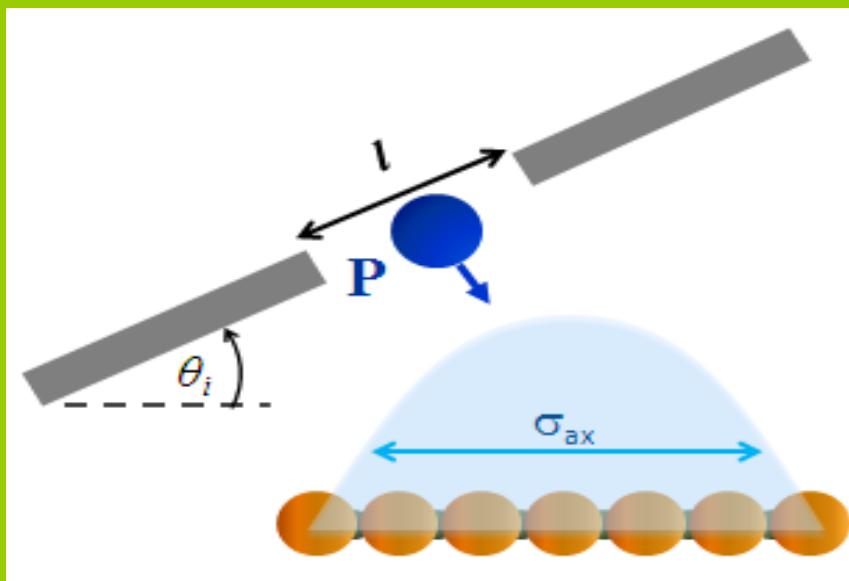
2 keV Ne  $\rightarrow$  <110> LiF(001),  $E_{\perp} = 0.3$  eV



Several coherently lighted cells: negligible

# Axial coherence: slit length

Initial wave-packet:  
axial width

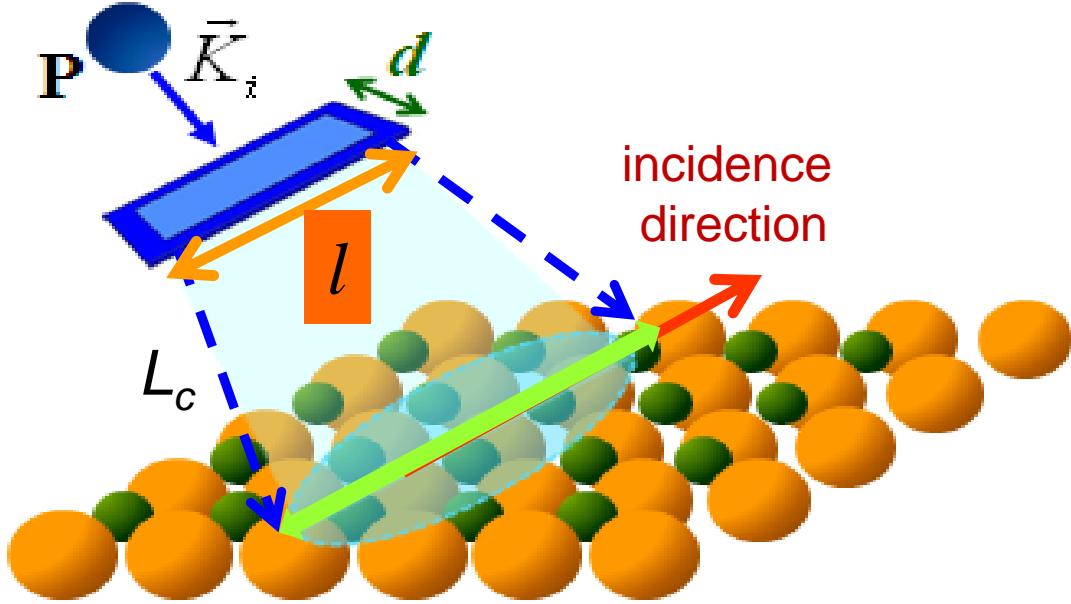


Uncertainty principle

$$\Delta X_o \Delta K_{ox} \approx 1$$

polar angle spread

$$\Delta\theta_o$$



$$\sigma_{ax} = \frac{\lambda_{\perp} L_c}{\sqrt{2} l}$$

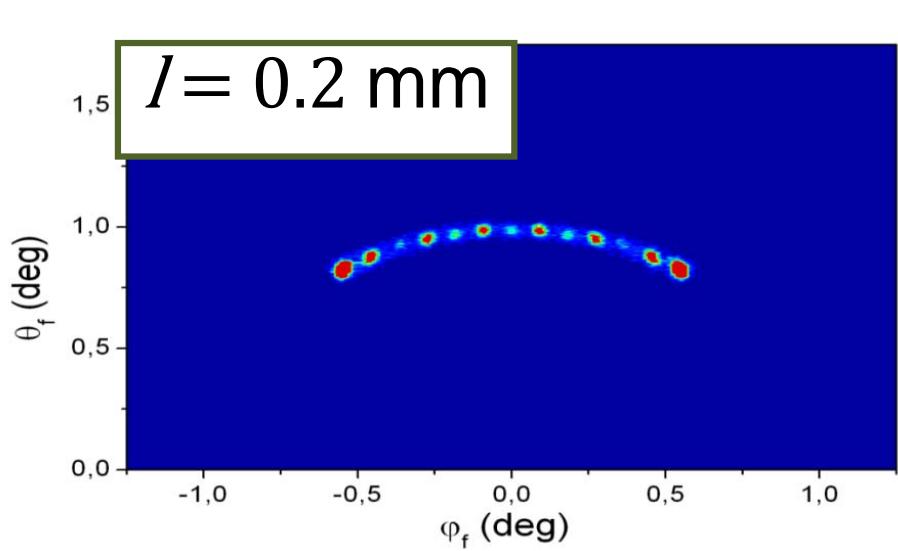
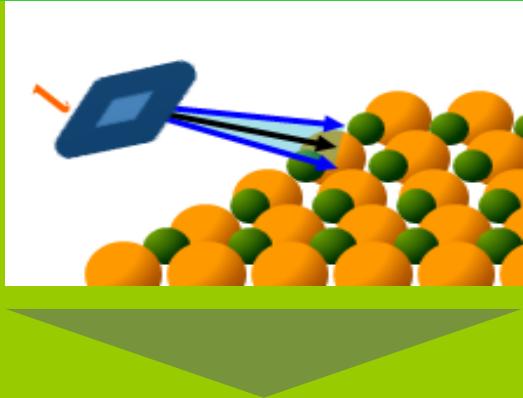
axial coherence  
length

$$\lambda_{\perp} = 2\pi / (K_i \sin\theta_i)$$

perpendicular de Broglie wavelength

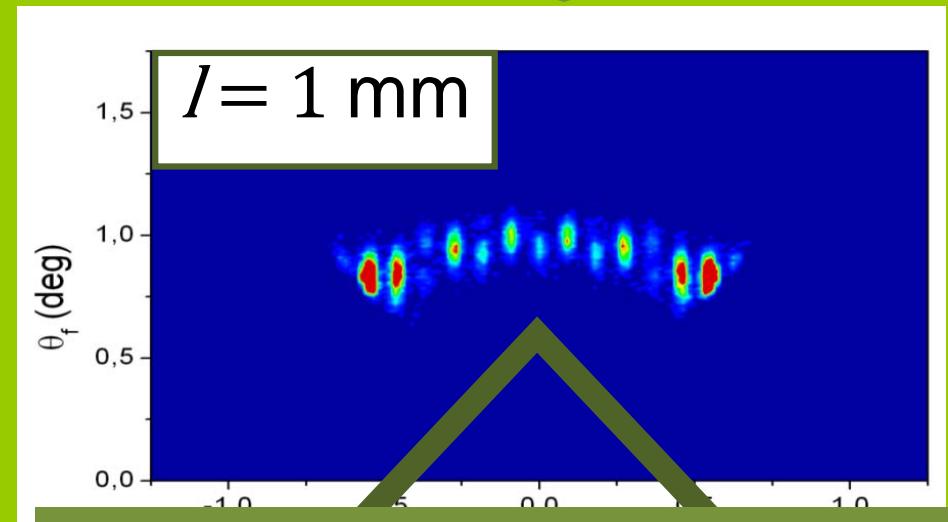
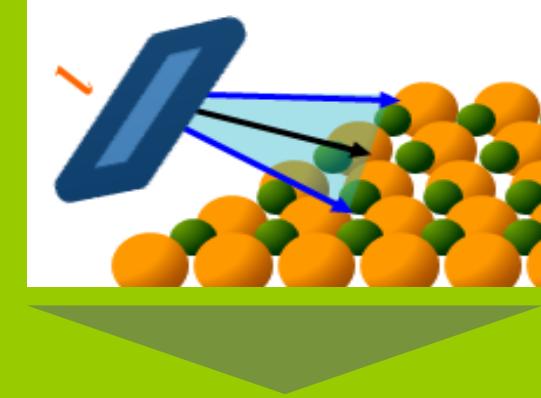
# Slit length: normal momentum spread

*small* square slit

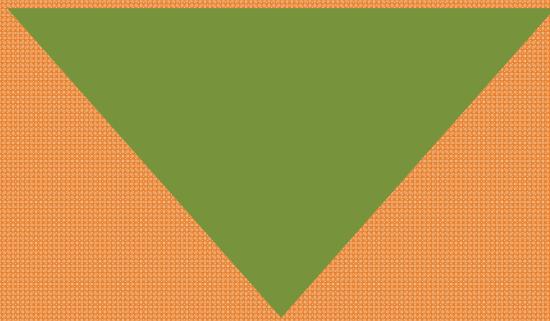


${}^4\text{He} \rightarrow <110> \text{LiF}(001), E_{\perp} = 0.3 \text{ eV}$

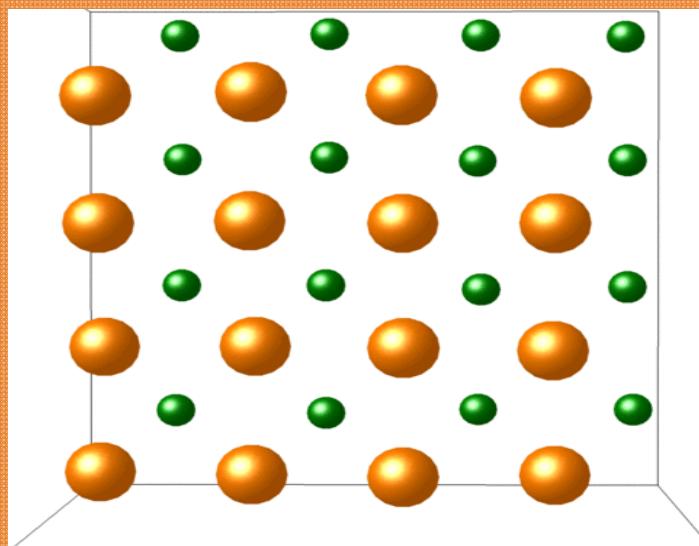
*long* rectangular slit



Probing different distances

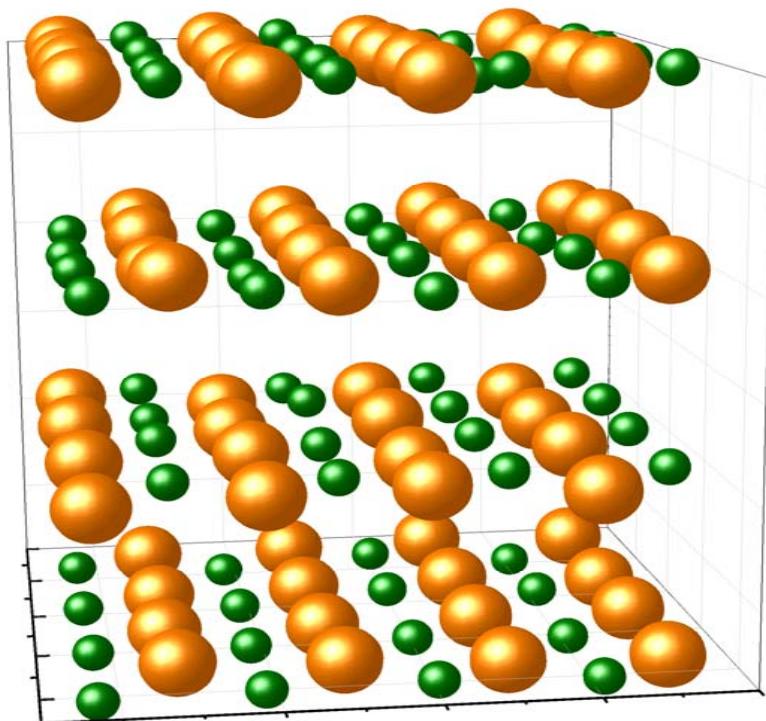


# DECOHERENT HEATING



# Influence of the temperature

T= 300 K

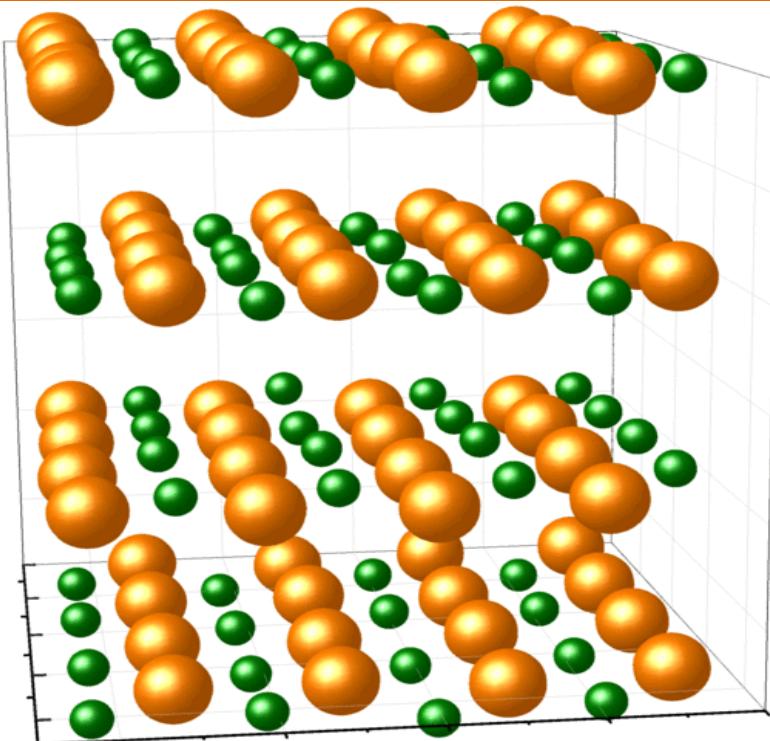


LiF(001)

$^{20}\text{Ne} \rightarrow <110> \text{ LiF}(001)$ ,  $E_{\perp} = 0.3 \text{ eV}$

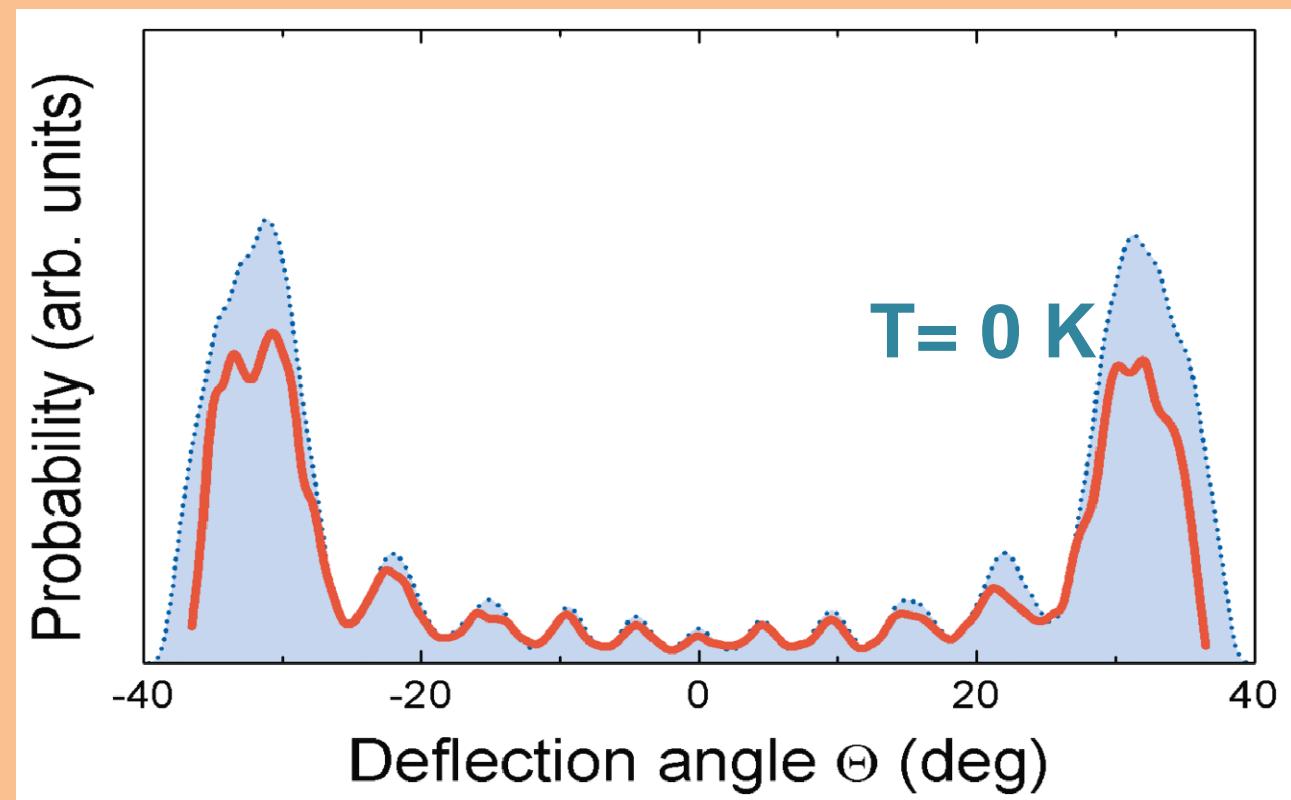
# Influence of the temperature

$T = 300 \text{ K}$



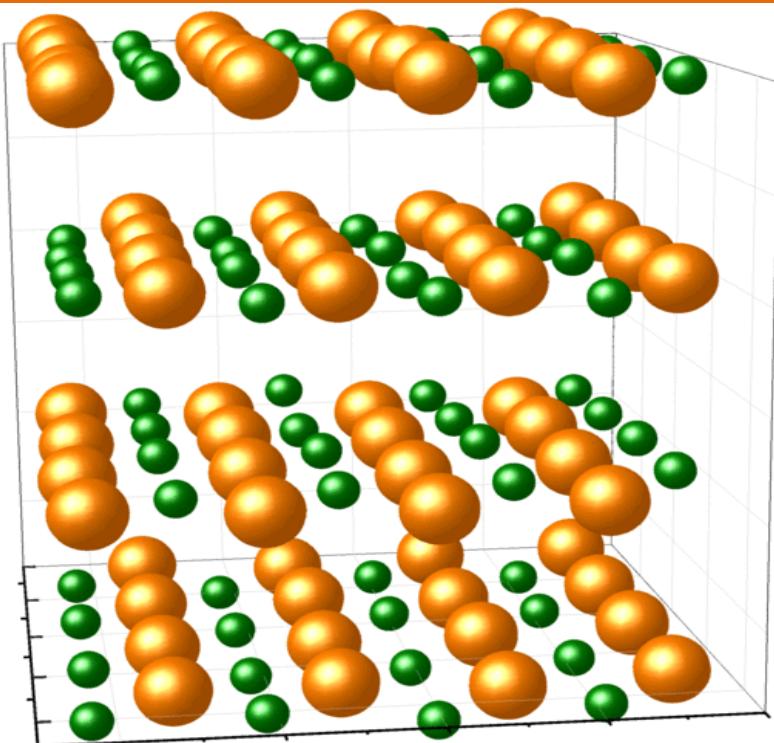
LiF(001)

$^{20}\text{Ne} \rightarrow <110> \text{ LiF}(001), E_{\perp} = 0.3 \text{ eV}$



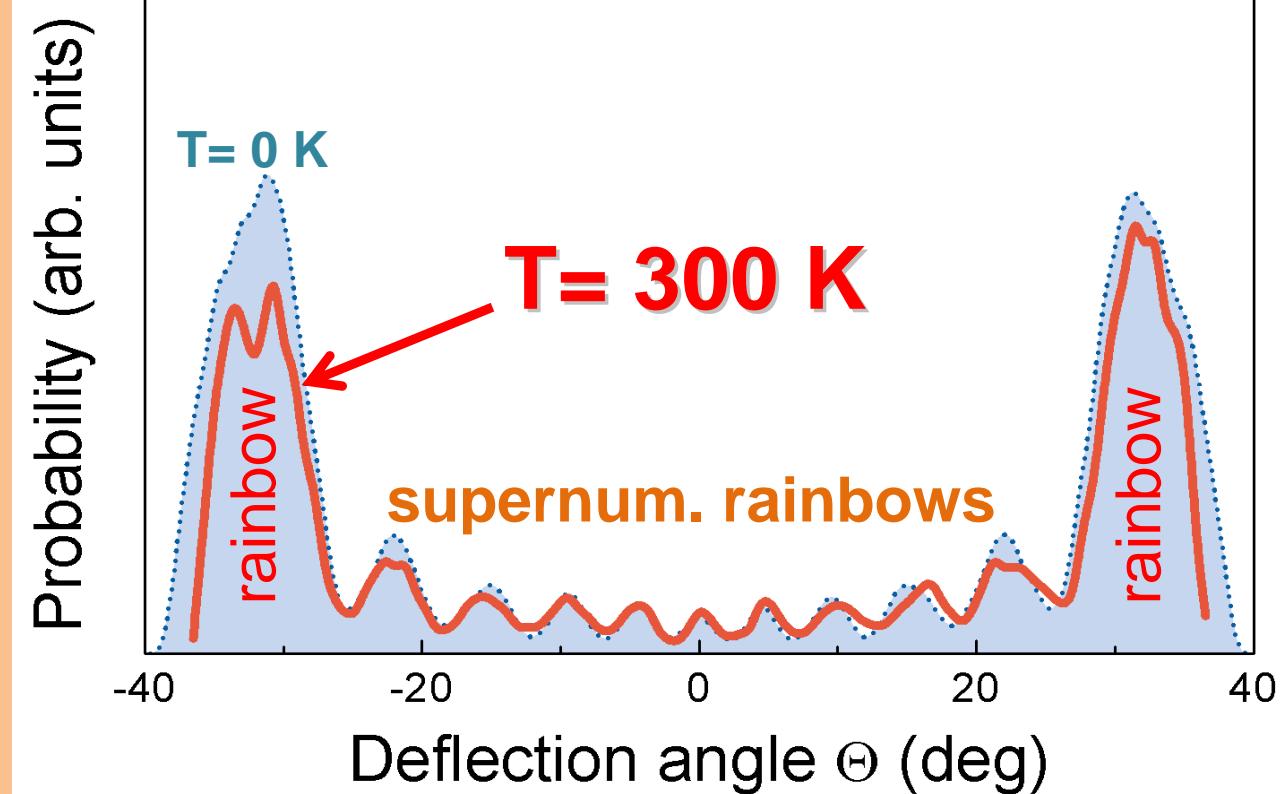
# Influence of the temperature

$T = 300 \text{ K}$

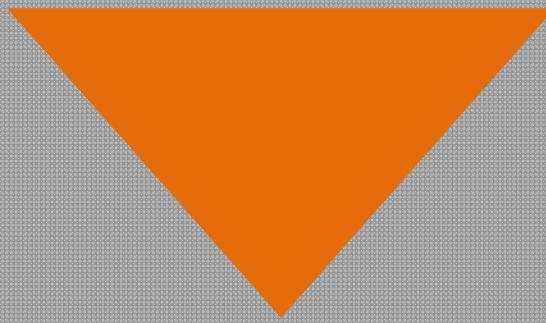


**LiF(001)**

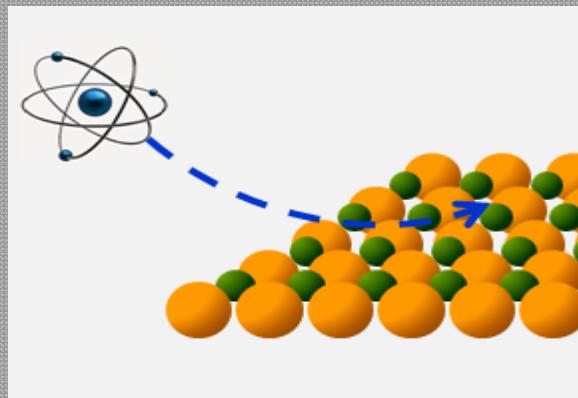
$^{20}\text{Ne} \rightarrow <110> \text{LiF}(001), E_{\perp} = 0.3 \text{ eV}$



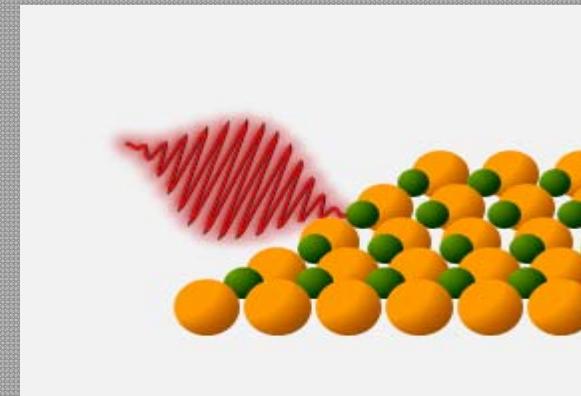
Manson *et al.*, Phys. Rev. B **78** (2008)  
Aigner *et al.*, J. Phys. Conf. Ser. **133** (2008)



# SURFACE ANALYSIS



Atoms

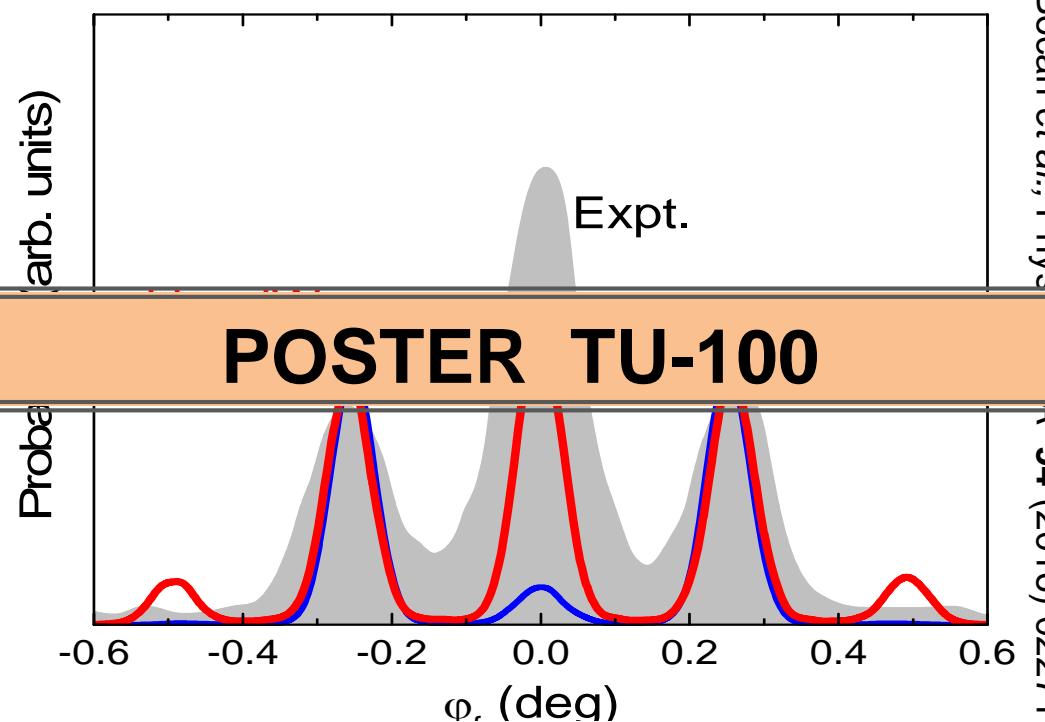


Laser pulses

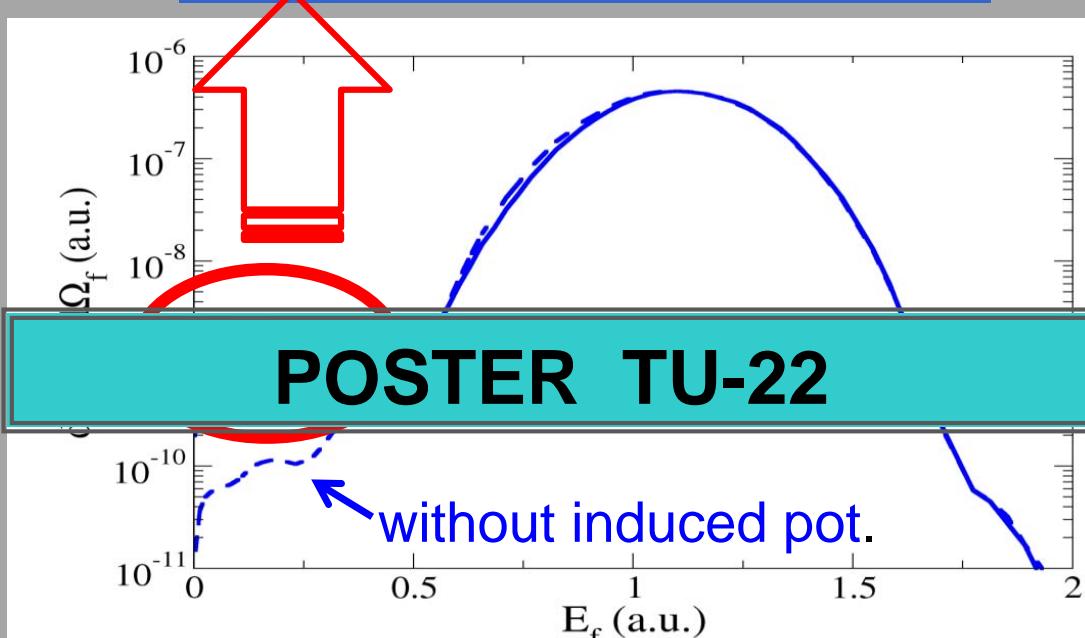
# SURFACE ANALYSIS



van der Waals effects



surface electronic states



XUV pulse  $\rightarrow \text{Al}(001), \omega = 1.5 \text{ a.u.}$

Ríos Rubiano *et al.*, Phys. Rev. A 94 (2016) 022711

# FINAL REMARKS

SIVR  
approach

Semi-quantitative  
• very good  
• intuitive

coherent  
lighting

- governs
- defines

collimating  
slit

- width
- length

decoherent  
heating

- broadens

## COHERENCE for DIFFERENT TARGETS:

clusters

molecules

atoms

patterns  
conditions

classic

# COLLABORATORS

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## ATOMS:

- J. Miraglia
- G. Bocan
- J. Fuhr

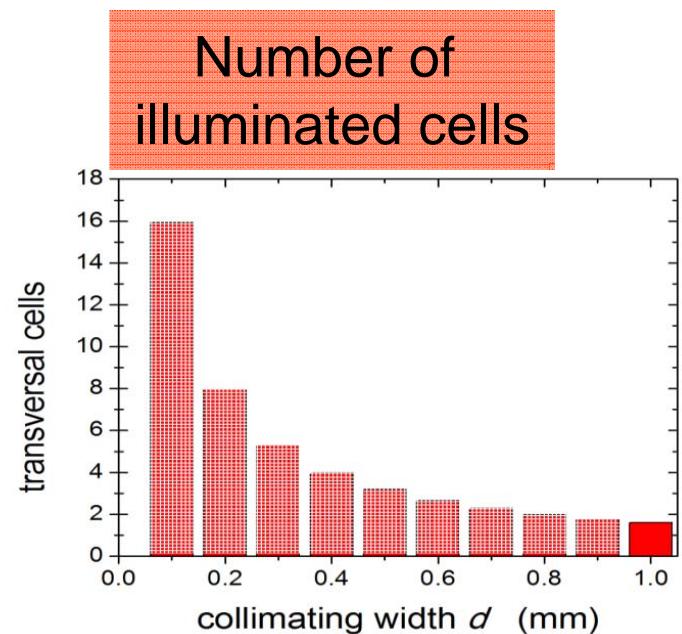
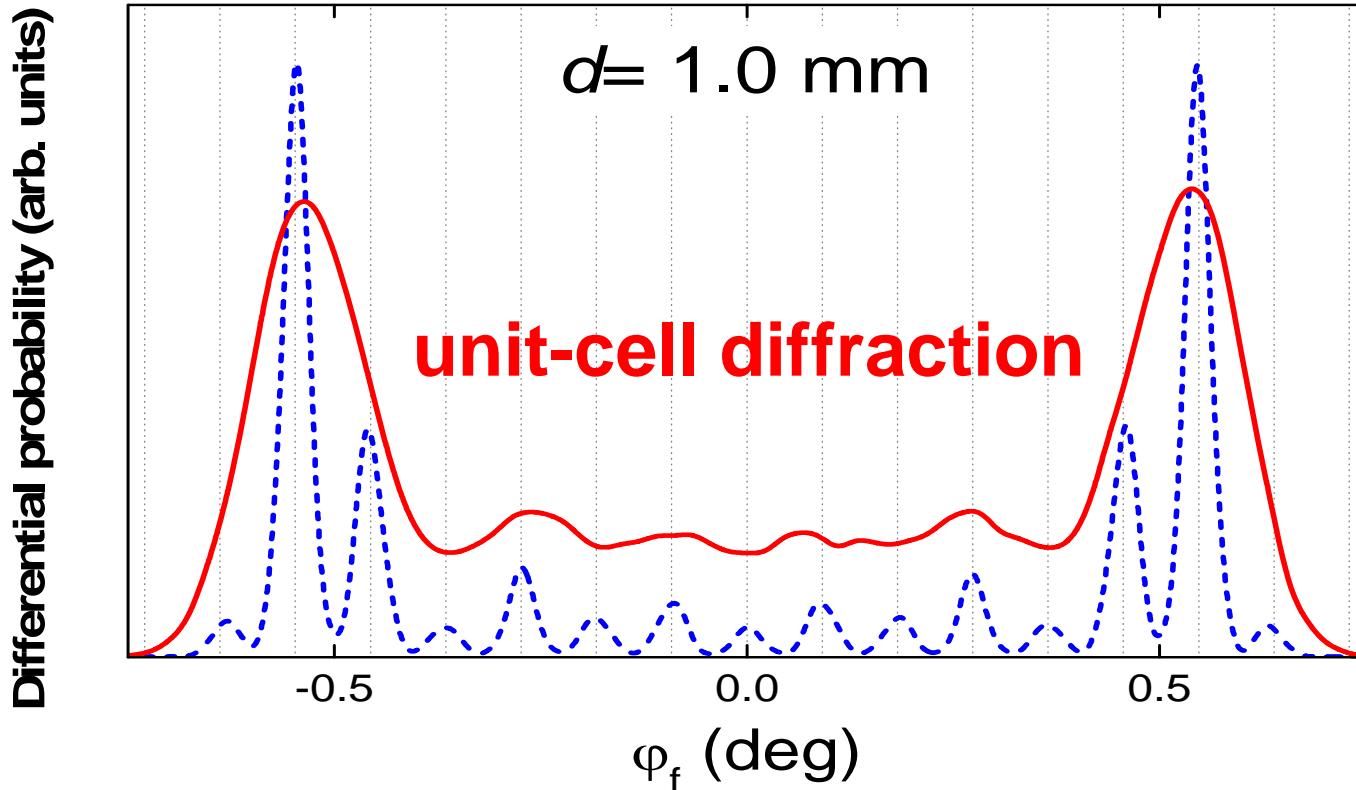
## LASER PULSES:

- C. Ríos Rubiano
- R. Della Picca
- D. Mitnik
- V. Silkin (Spain)

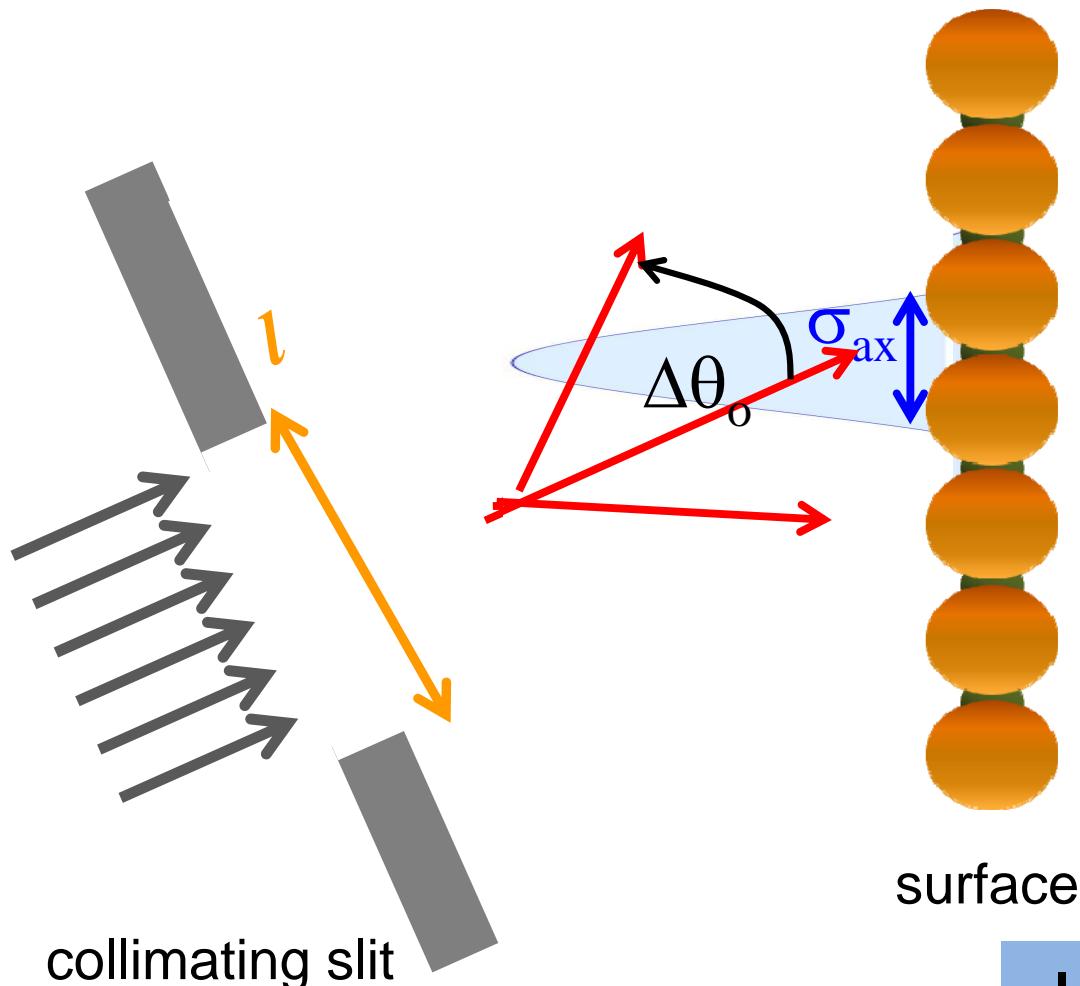
**THANKS FOR THE ATTENTION**

# FAD spectra vs. slit width

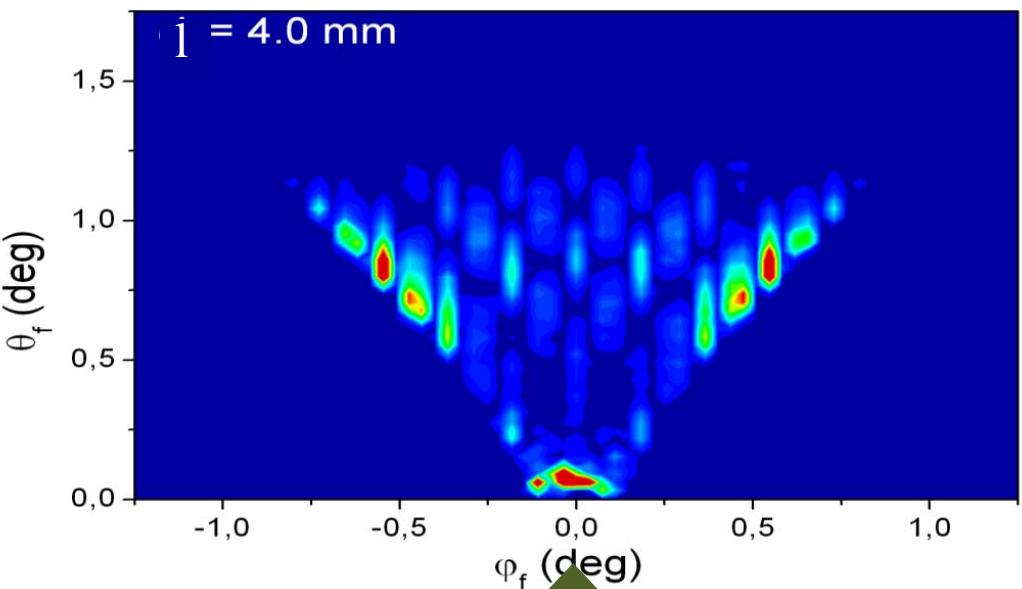
${}^4\text{He} \rightarrow <110> \text{LiF}(001)$ ,  $E = 1 \text{ keV}$ ,  $\theta = 0.99 \text{ deg}$



# Slit length: normal momentum spread



${}^4\text{He} \rightarrow <110> \text{LiF}(001)$ ,  $E_\perp = 0.3 \text{ eV}$



surface

Incident slit  
To probe different distances

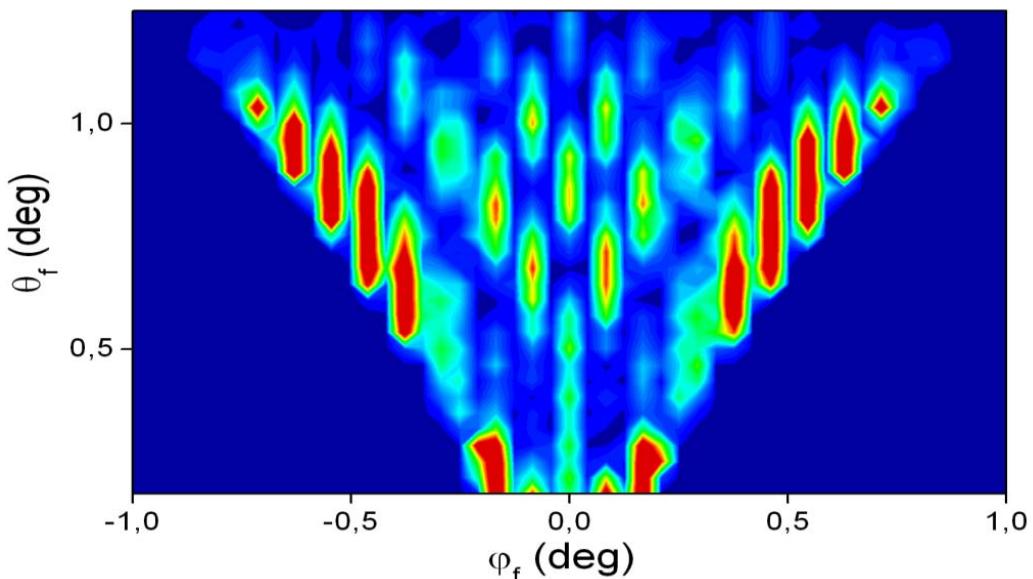
# Long slit collimation vs. diffraction chart

Angular spectrum

Long slit :  $l = 5 \text{ mm}$

Useful for probing potentials

Fixed  $\theta_i$

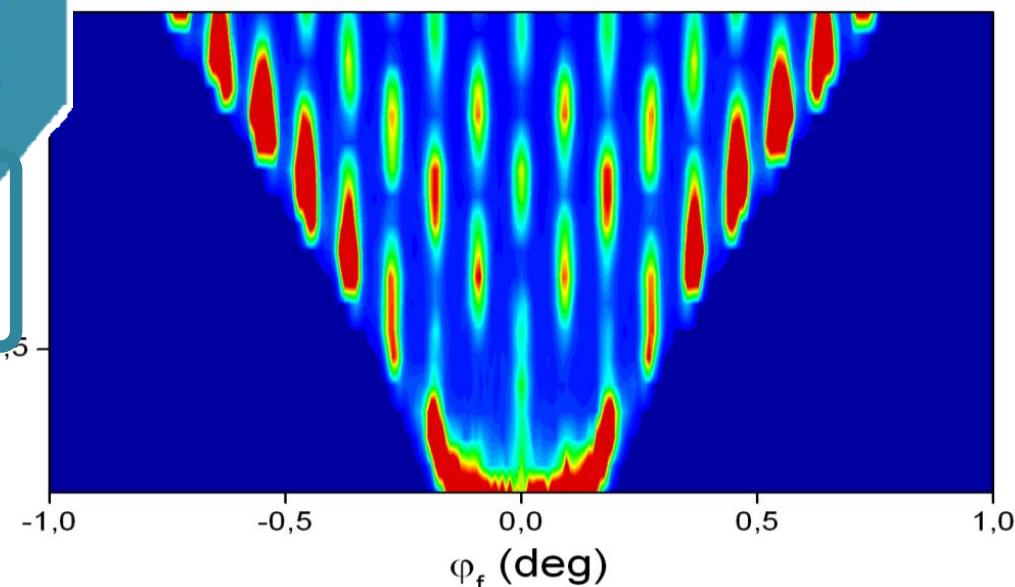


Diffraction chart

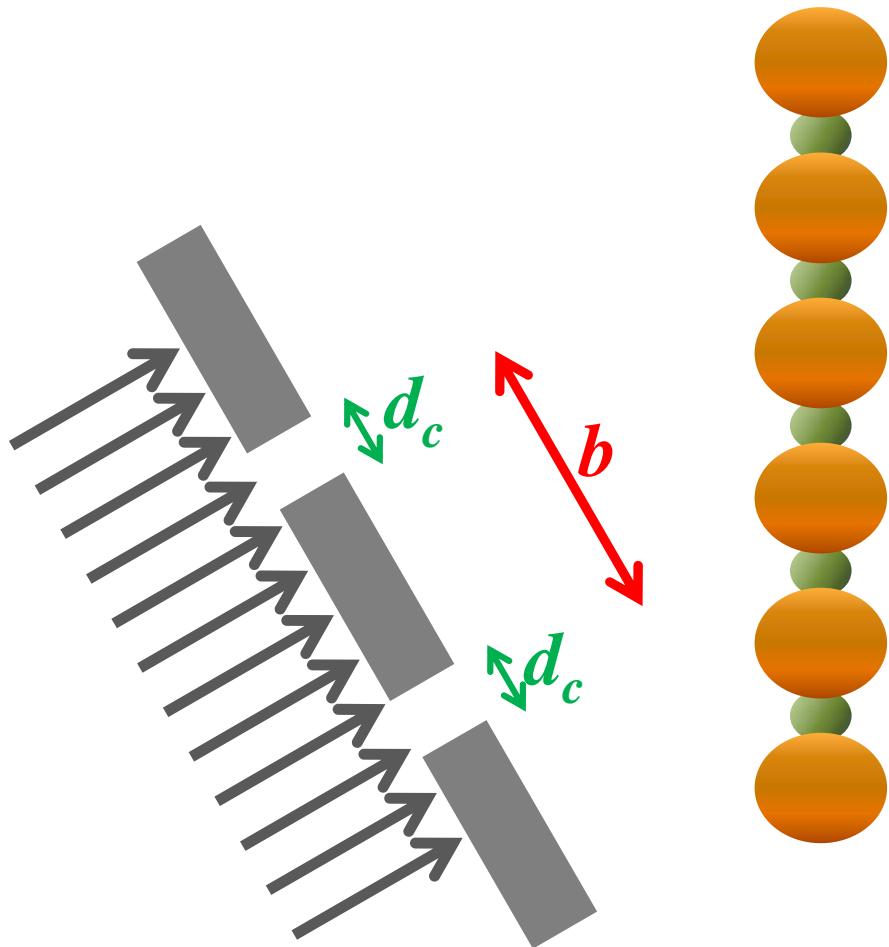
Short slit :  $l = 0.2 \text{ mm}$

Normal energy  
 $\theta_i$  (deg)

Different  $\theta_i$  values



# DOUBLE SLIT COLLIMATION



${}^4\text{He} \rightarrow <110> \text{LiF}(001)$ ,  $E = 1 \text{ keV}$ ,  $\theta_i = 0.99 \text{ deg}$

Double slit:  $d = 0.2 \text{ mm}$ ,  $b = 0.2 \text{ mm}$

