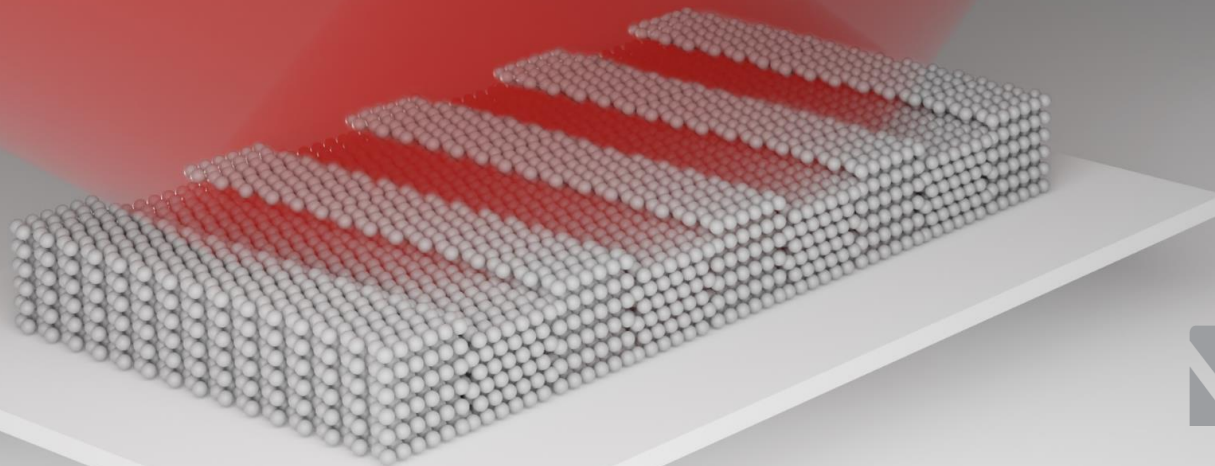


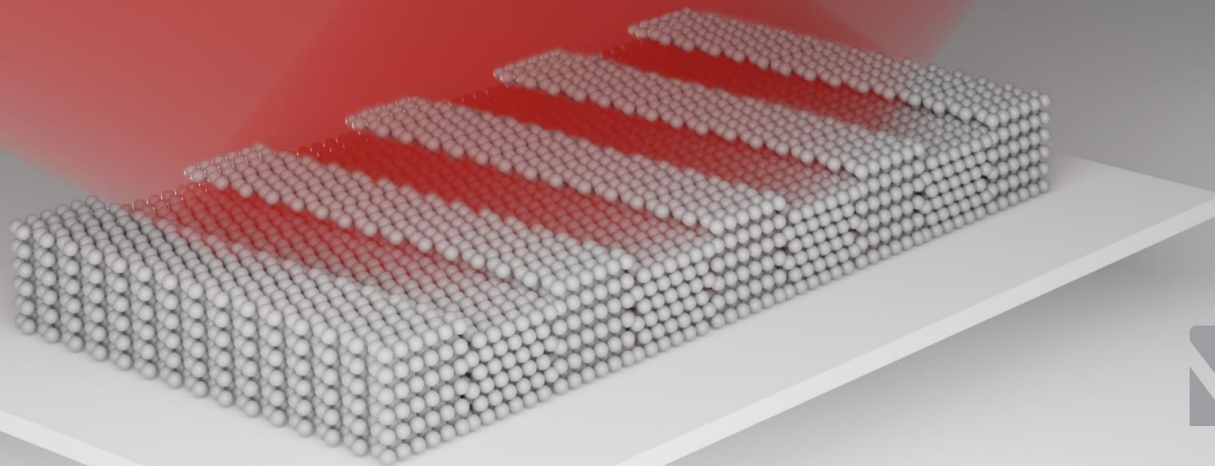
# Lattice reconfiguration driven by metastable electronic phase transition in TMDs

Igor Vaskivskyi

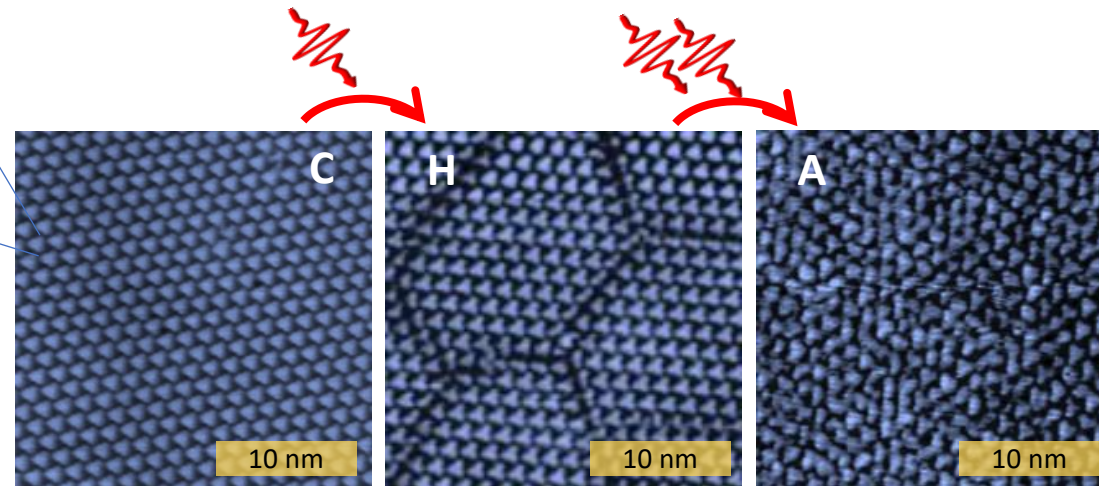
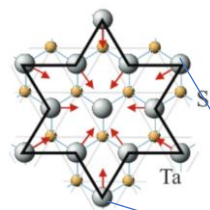
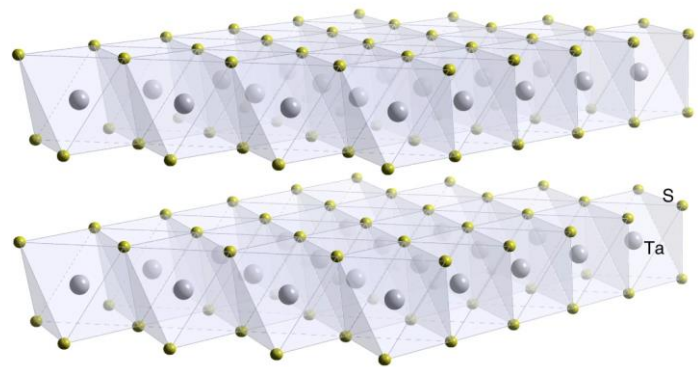


# Lattice reconfiguration driven by metastable electronic phase transition in **1T-TaS<sub>2</sub>**

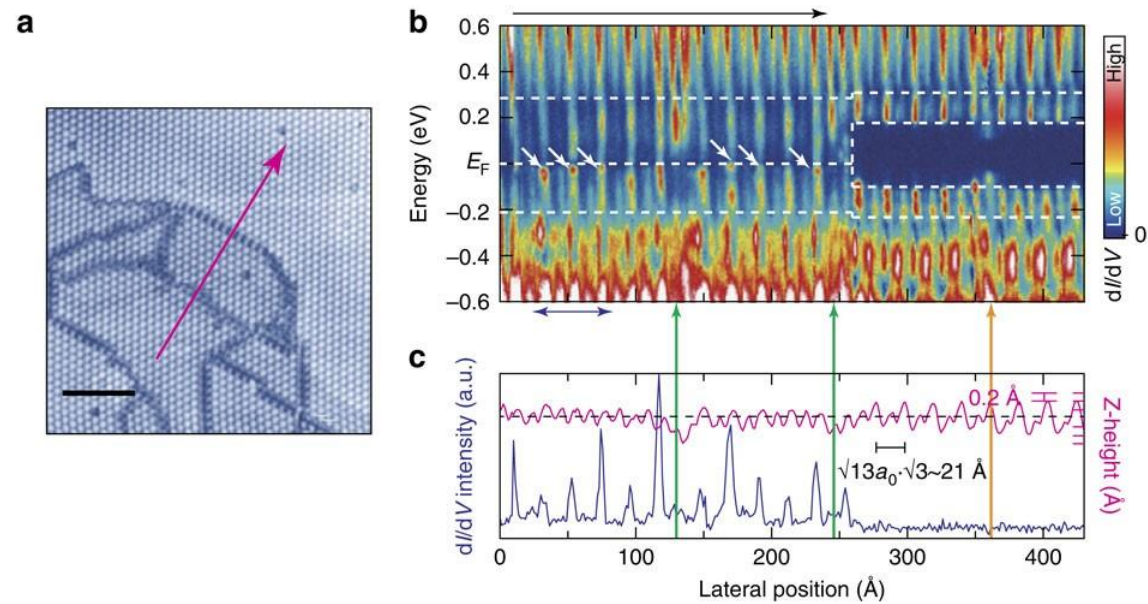
Igor Vaskivskiy



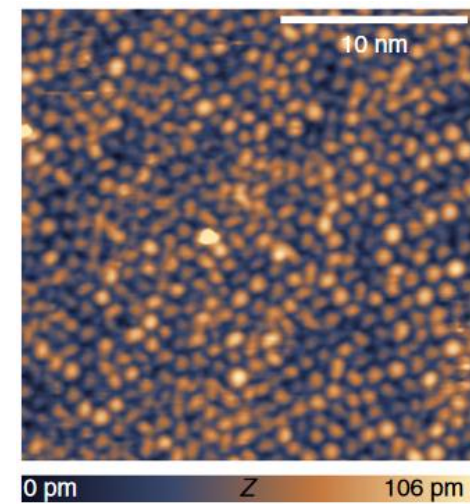
# 1T-TaS<sub>2</sub> & photoinduced states



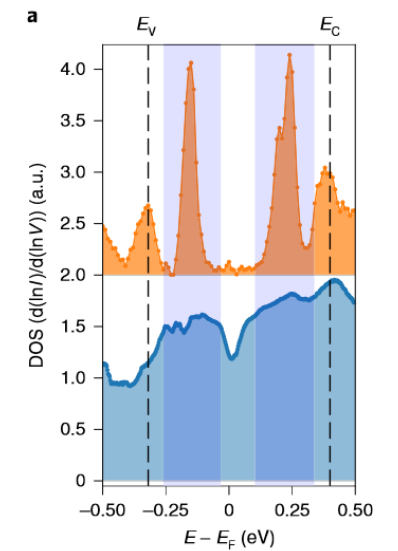
# Insulator vs. metal



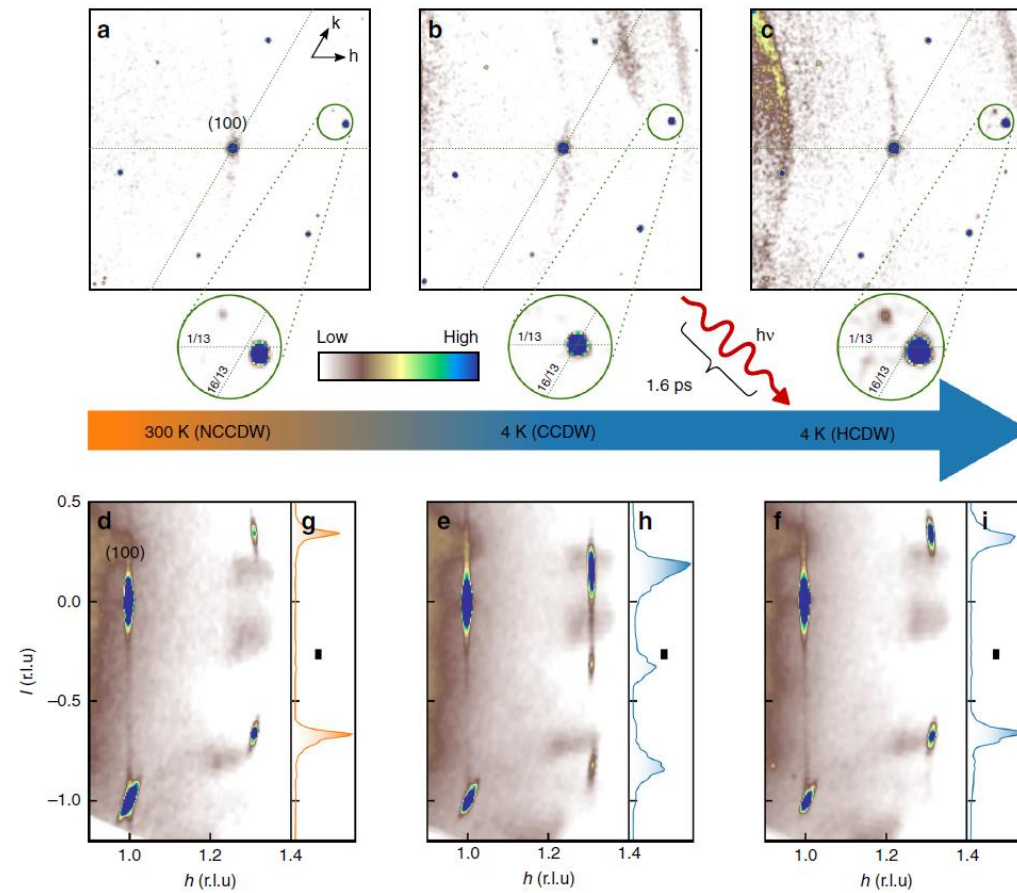
Cho *et al.*, Nat. Commun. 7, 10453 (2016)



Gerasimenko, IV et al. Nat. Mat. 18, 1078 (2019)



# Insulator vs. metal

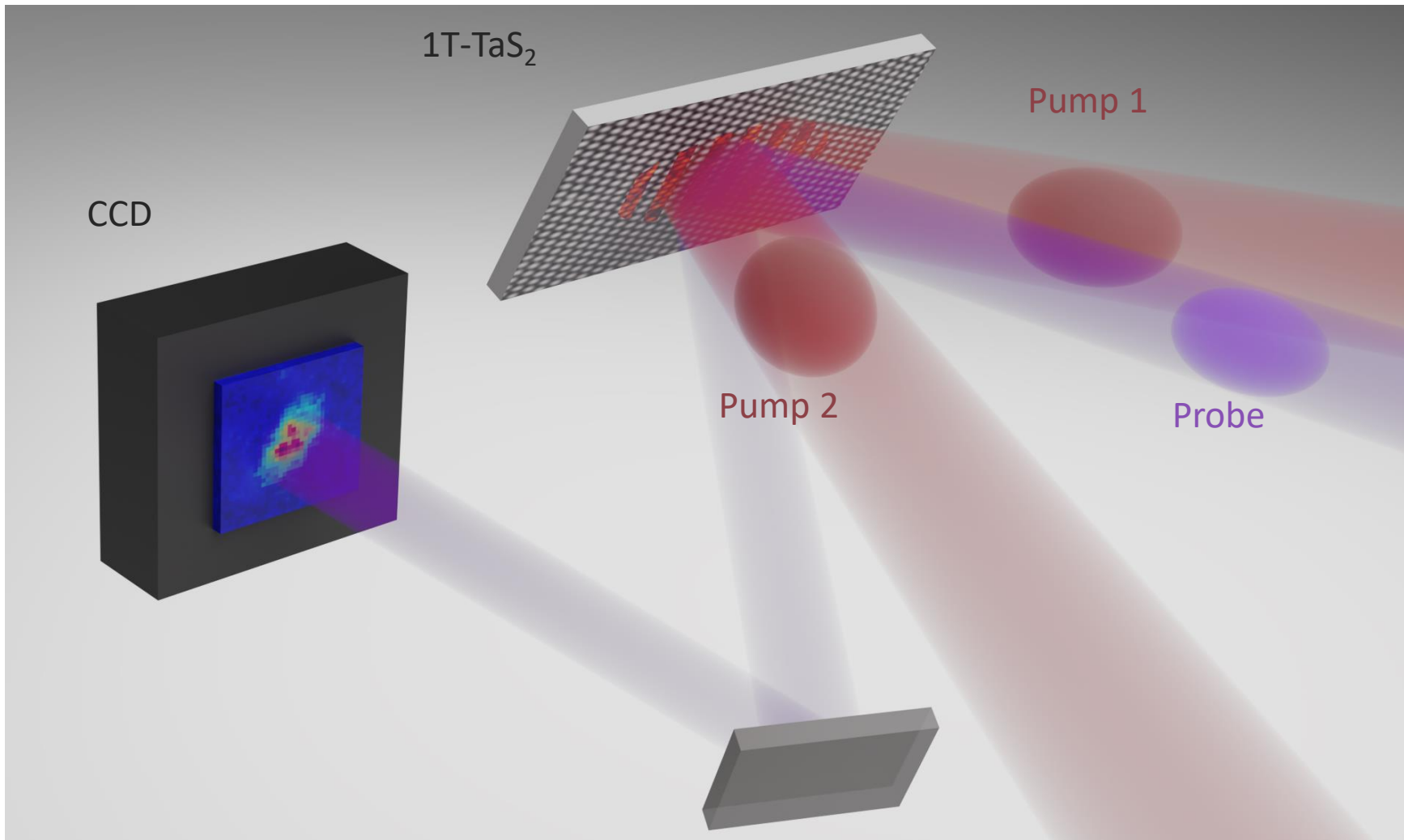


Stahl *et al.*, Nat. Comm. (2019)

- Lattice reconfiguration during C  $\rightarrow$  H transition
- Dynamics of CDW restacking

- Lattice reconfiguration during C  $\rightarrow$  H transition
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# Transient grating spectroscopy

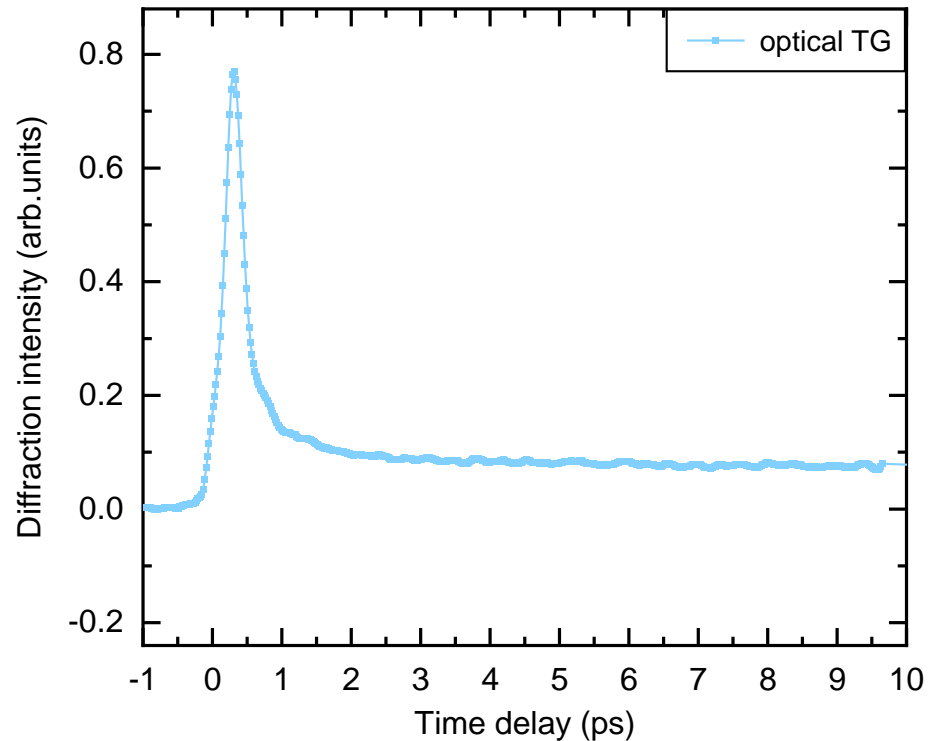


- Electron dynamics
- Spin dynamics
- Phonon dynamics
- Heat transport
- .....

$$\mathbf{q} \neq 0$$

$$\Lambda = \frac{\lambda}{2 \sin \Theta/2}$$

# Transient grating spectroscopy: **300 K**



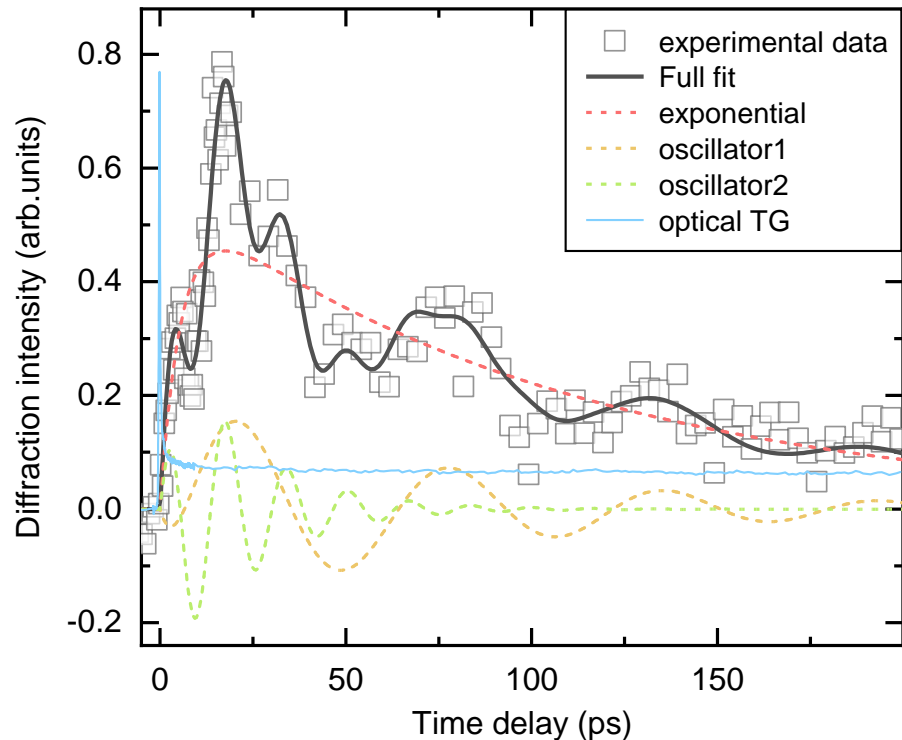
## Optical TG:

Sub-ps rise time – melting of CDW

Recovery – reemergence of CDW

Grating period:  $\sim 10$   $\mu\text{m}$

# Transient grating spectroscopy: 300 K



IV *et al.*, Nat. Photon. (2024)

## Optical TG:

Sub-ps rise time – melting of CDW

Recovery – reemergence of CDW

Grating period:  $\sim 10$   $\mu\text{m}$

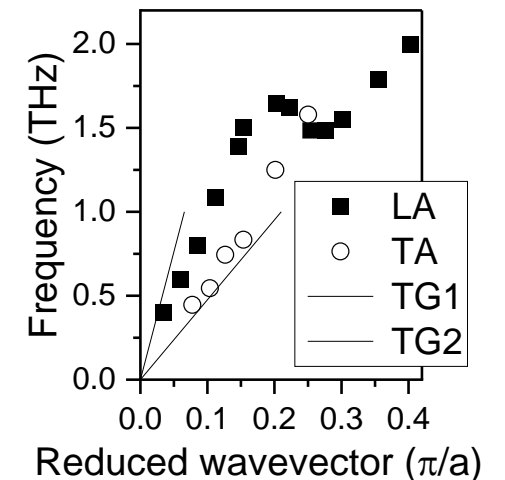
## EUV TG:

Rise time  $\sim 4.8$  ps – electron-lattice thermalization

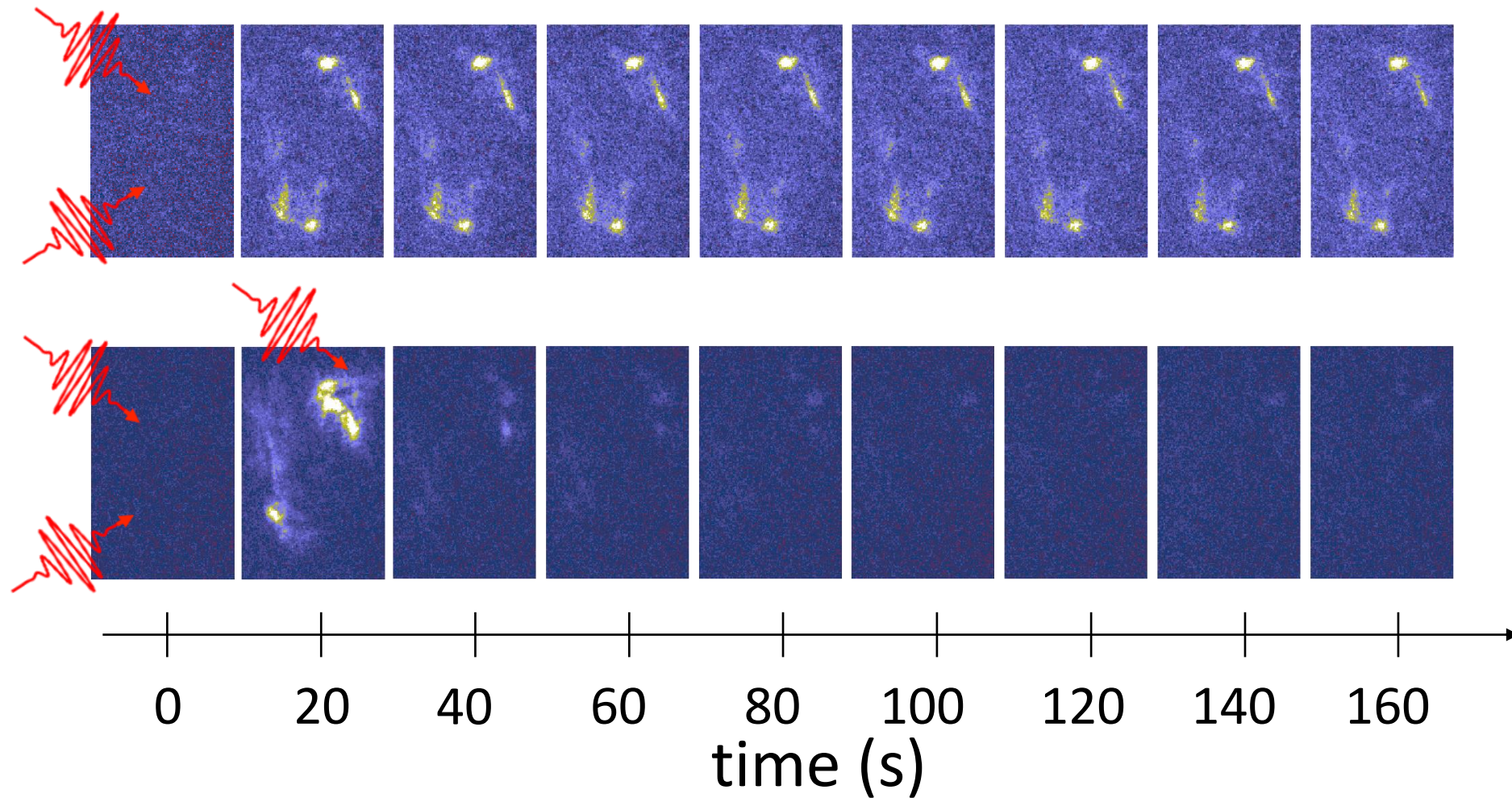
Exp recovery – heat diffusion

Oscillations: LA and TA phonon modes

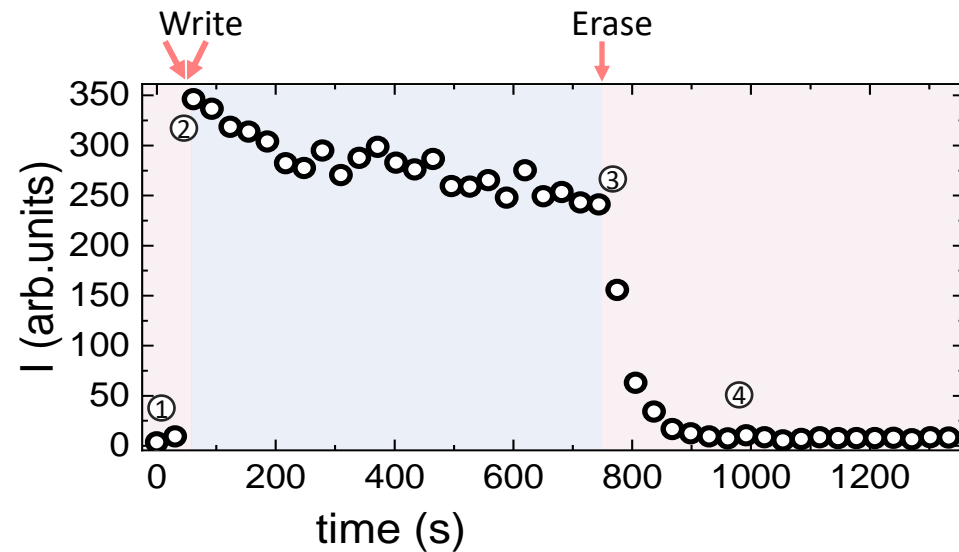
Grating period:  $\sim 83$  nm



# "Transient" grating spectroscopy: **100 K**



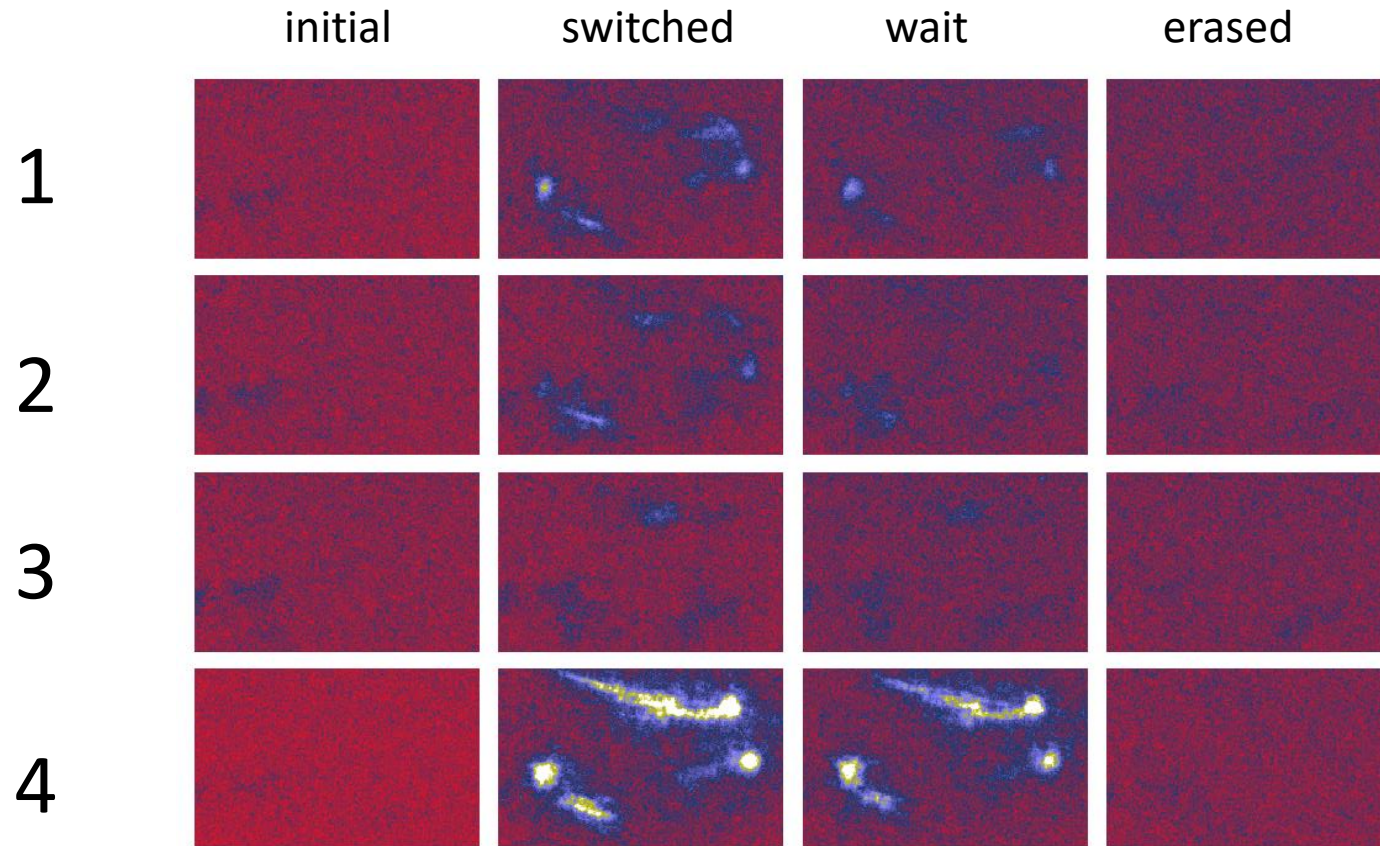
# "Transient" grating spectroscopy: **100 K**



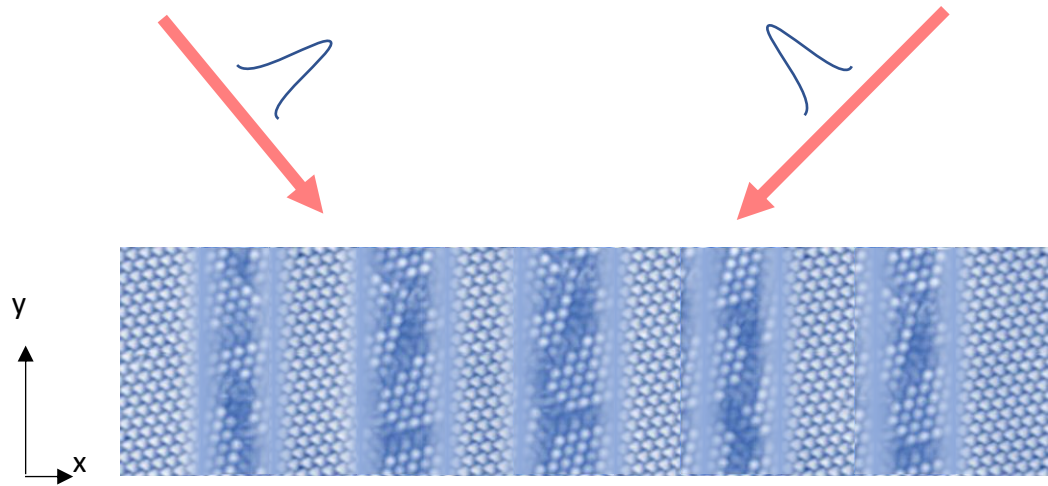
## EUV TG:

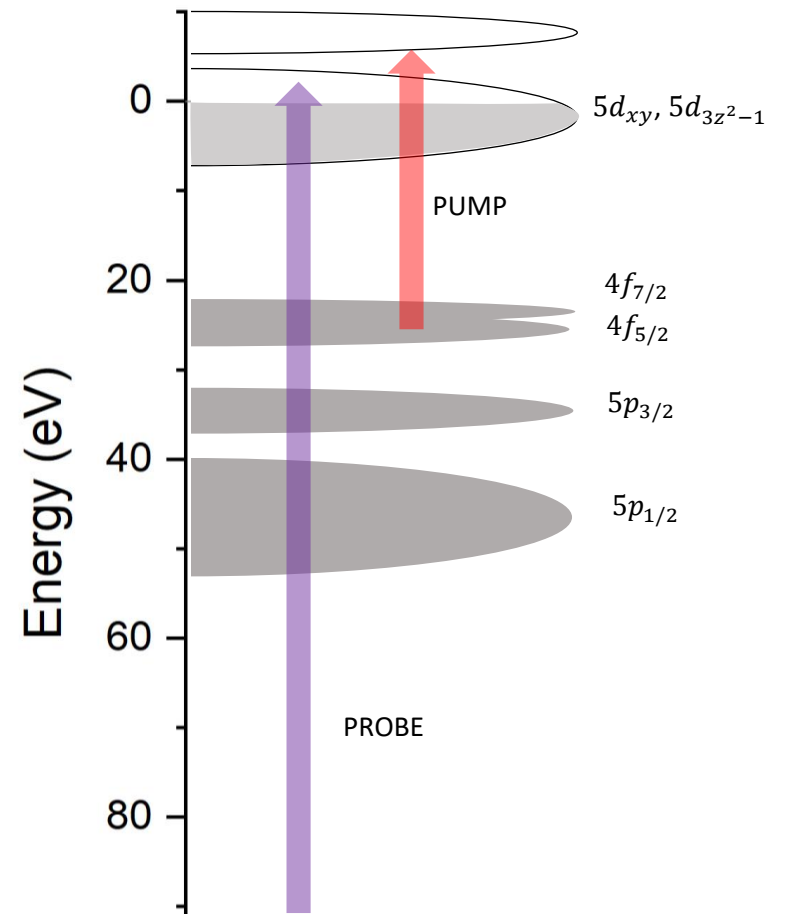
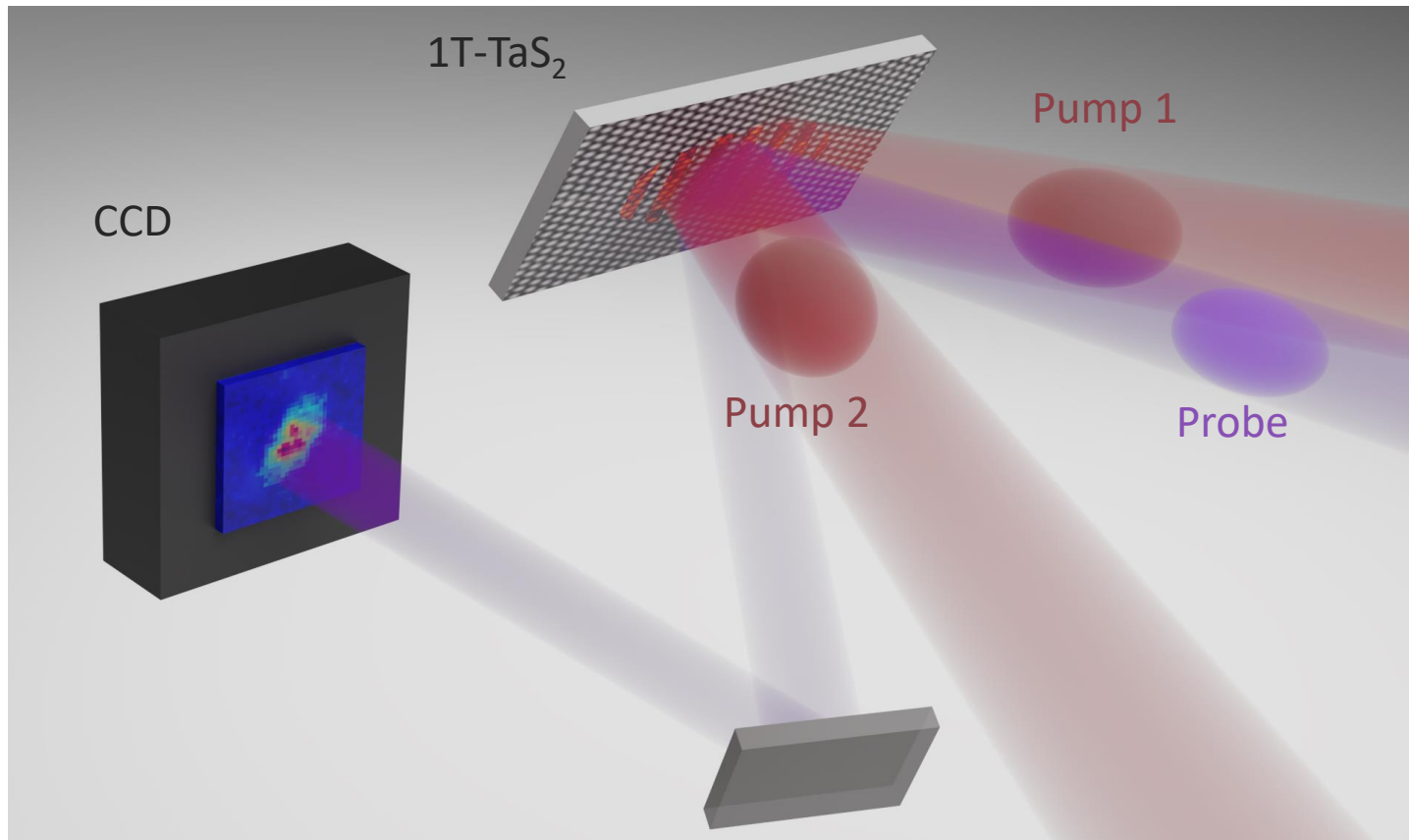
- Extremely strong signal
- Almost no relaxation
- Erases by heating
- Grating period: ~83 nm

~~"Transient"~~ *metastable* grating spectroscopy: **100 K**

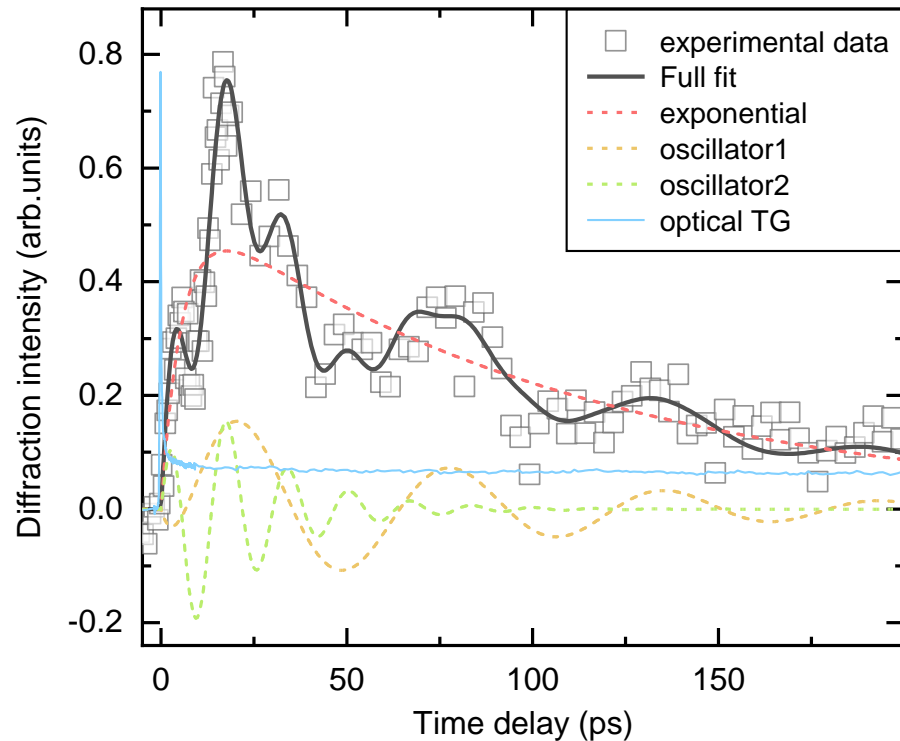


# "Transient" grating spectroscopy: **100 K**





# Transient grating spectroscopy: **300 K**



## Optical TG:

Sub-ps rise time – melting of CDW

Recovery – reemergence of CDW

Grating period:  $\sim 10 \mu\text{m}$

## EUV TG:

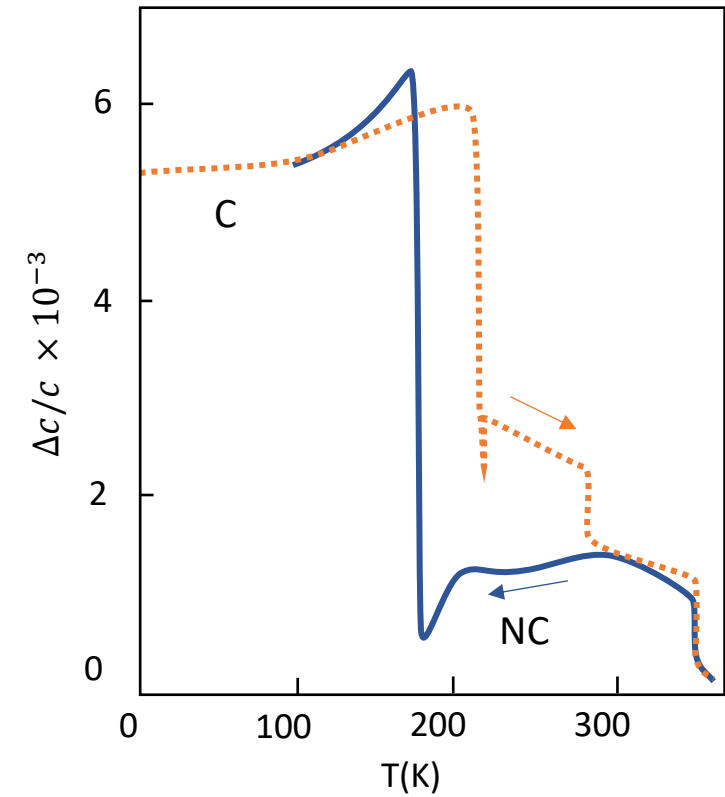
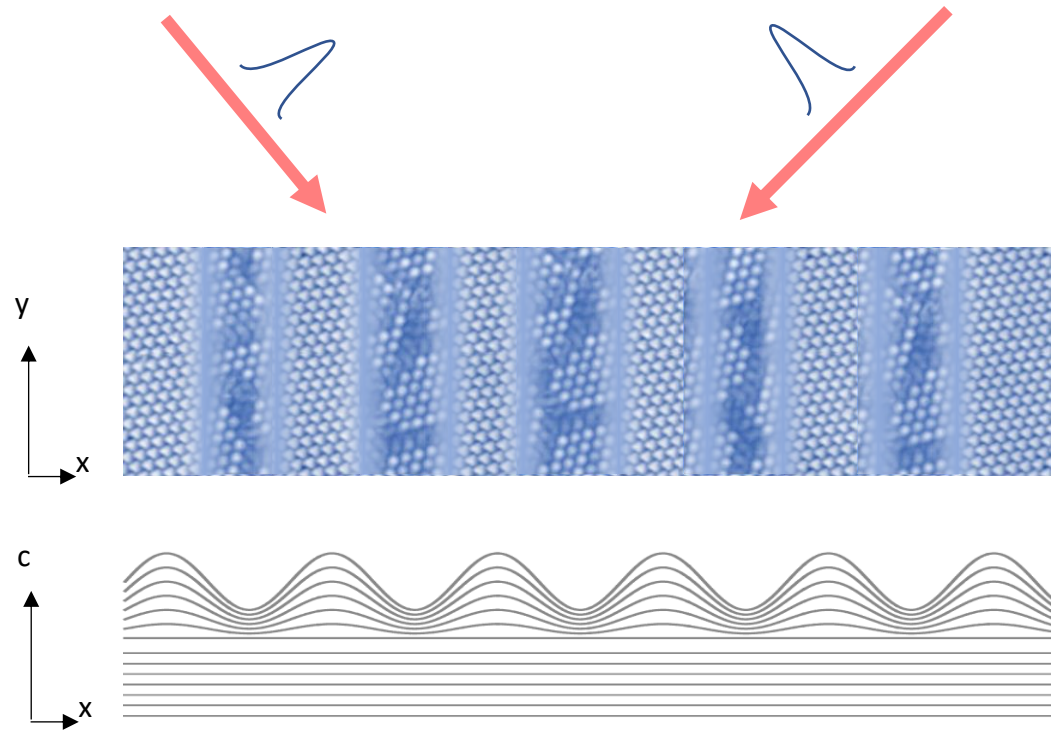
Rise time  $\sim 4.8 \text{ ps}$  – electron-lattice thermalization

Exp recovery – heat diffusion

Oscillations: LA and TA phonon modes

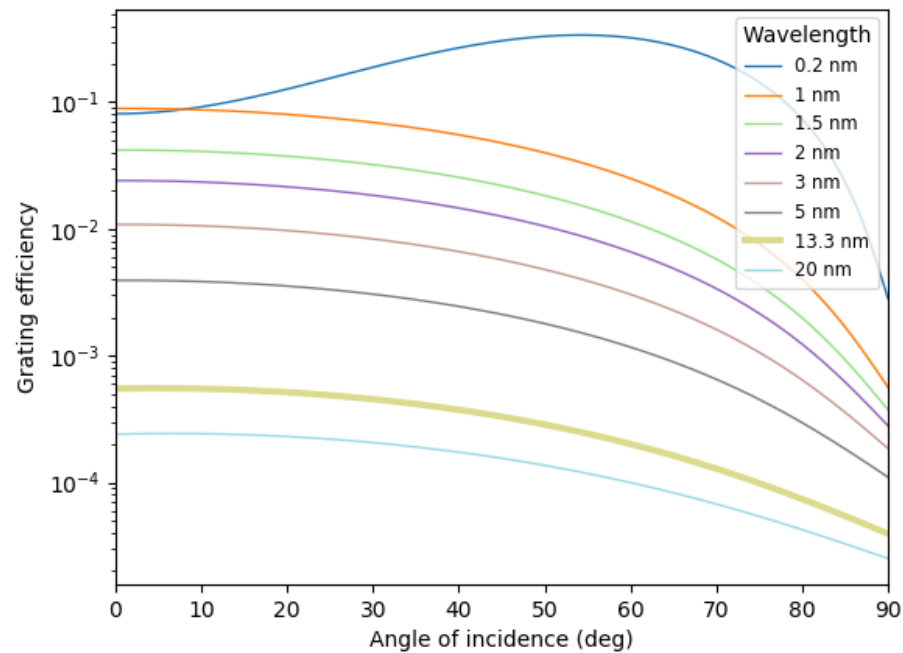
Grating period:  $\sim 83 \text{ nm}$

# "Transient" grating spectroscopy: **100 K**



Sezerman *et al.*, Solid State Communications, **36**, 9 (1980)

# Efficiency of the grating



$$\eta = \frac{I_d}{I_0} = R J_1^2 \left\{ \frac{4\pi h}{\lambda} \right\}$$

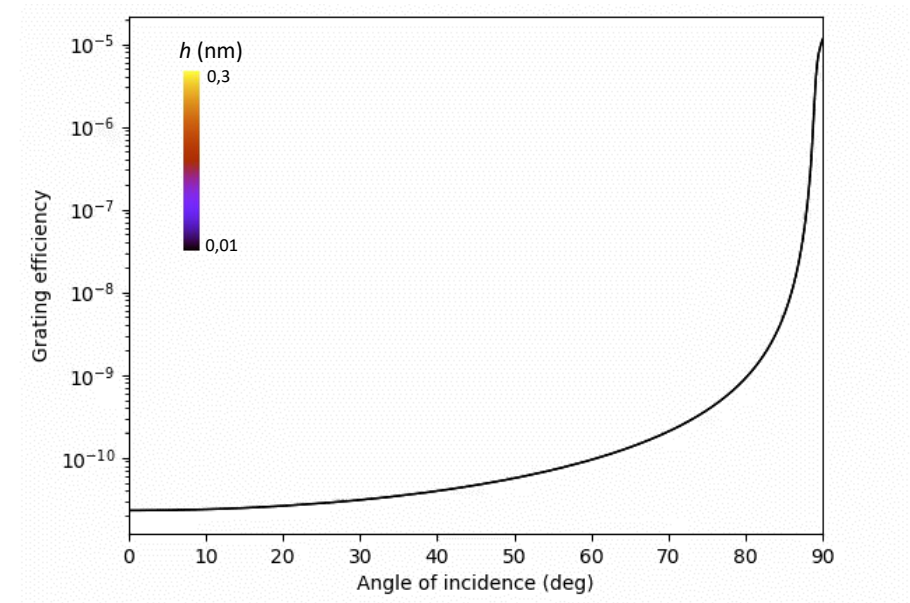
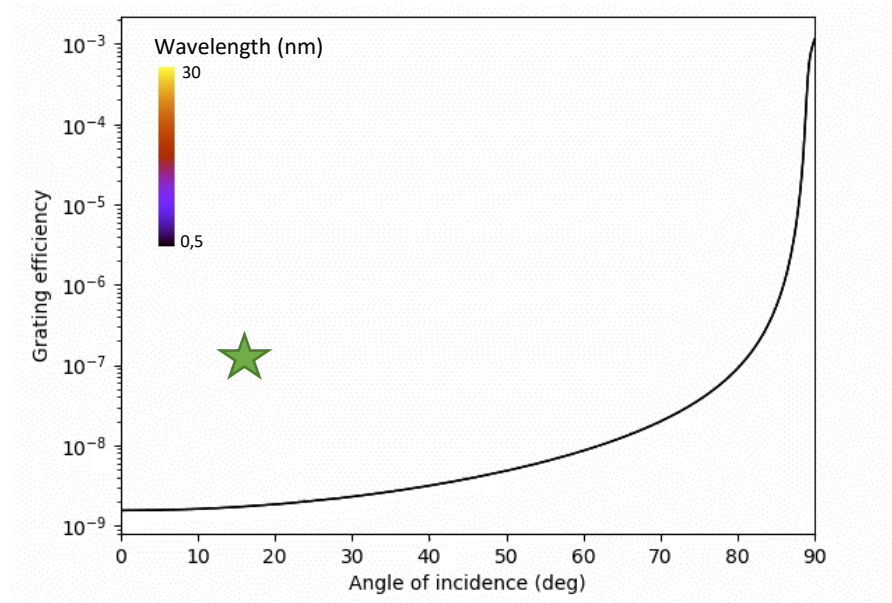
$R$  – reflectivity

$J$  – Bessel function

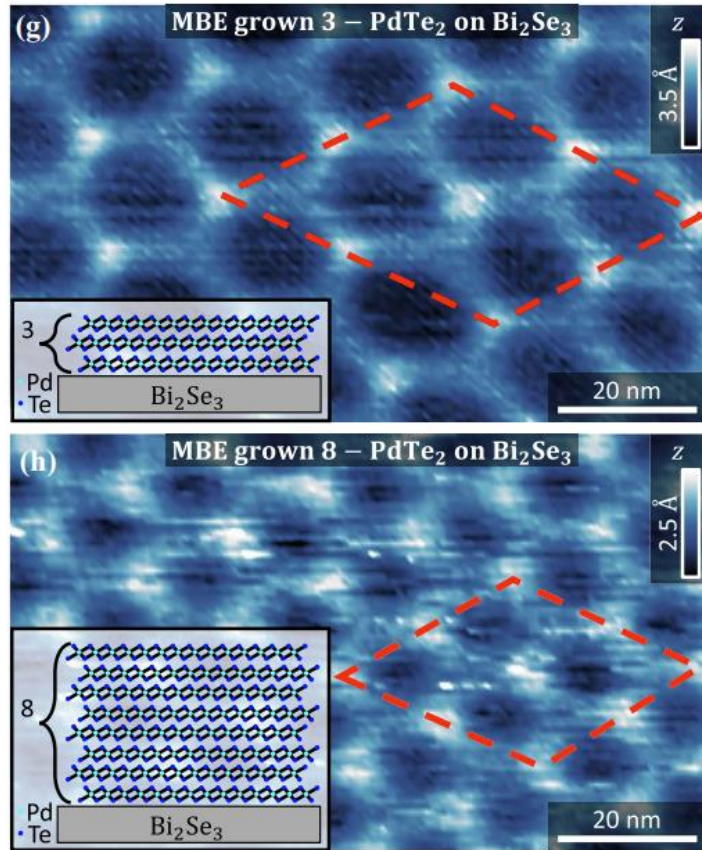
$h$  – height of modulation

$\lambda$  – phonon wavelength

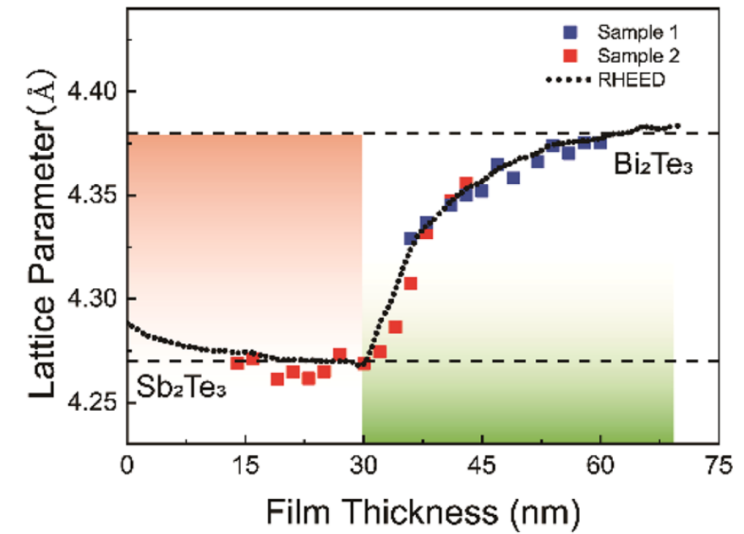
# Efficiency of the grating



# Strain in 2D materials

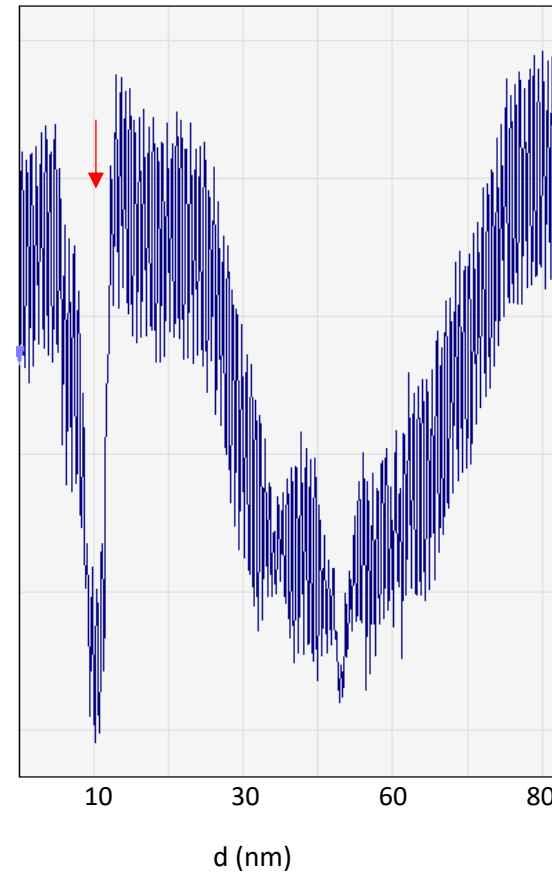
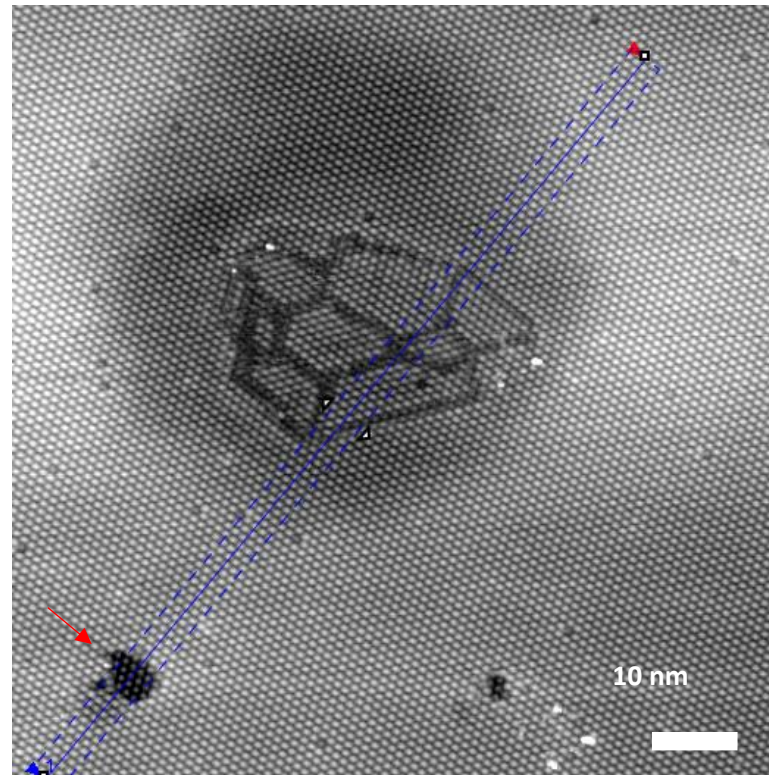


Halbertal et al. Phys. Rev. X 13, 011026 (2023)

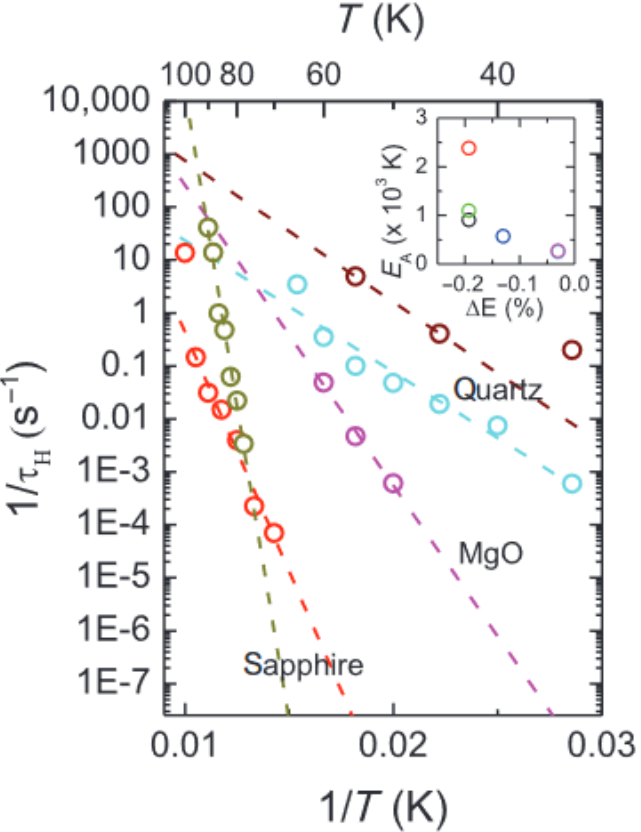


Zhang et al. ACS Nano. 15, 2 (2021)

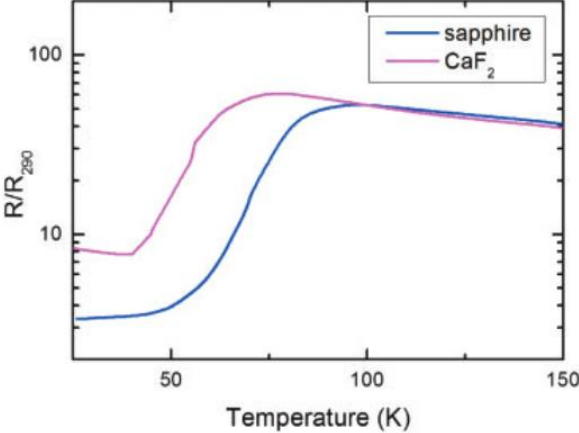
# How much deformation to expect?



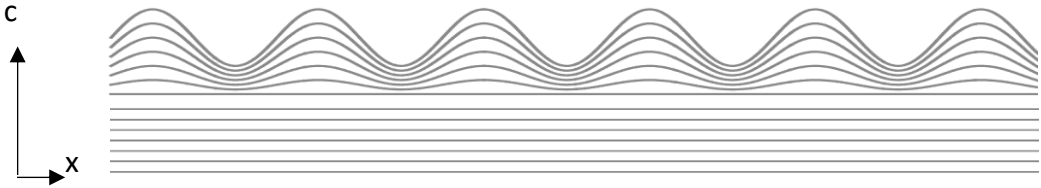
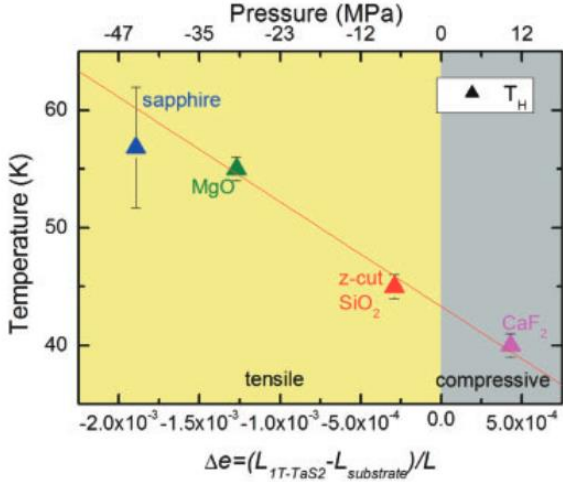
# H state vs. strain



I.V. et al, Science Advances (2015)



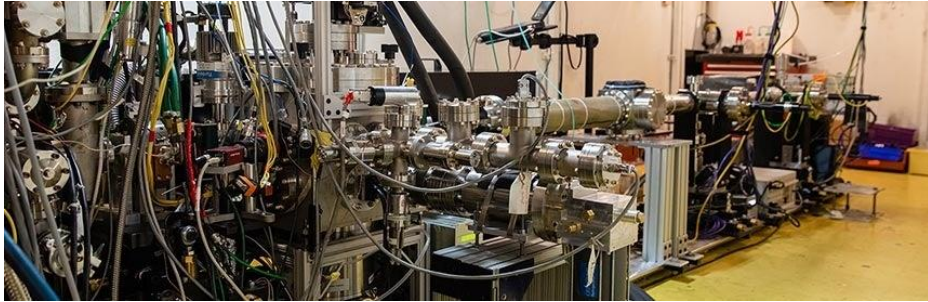
D. Svetin, I.V. et al, Appl. Phys. Exp. (2014)



- Lattice reconfiguration during C  $\rightarrow$  H transition
- Dynamics of CDW restacking

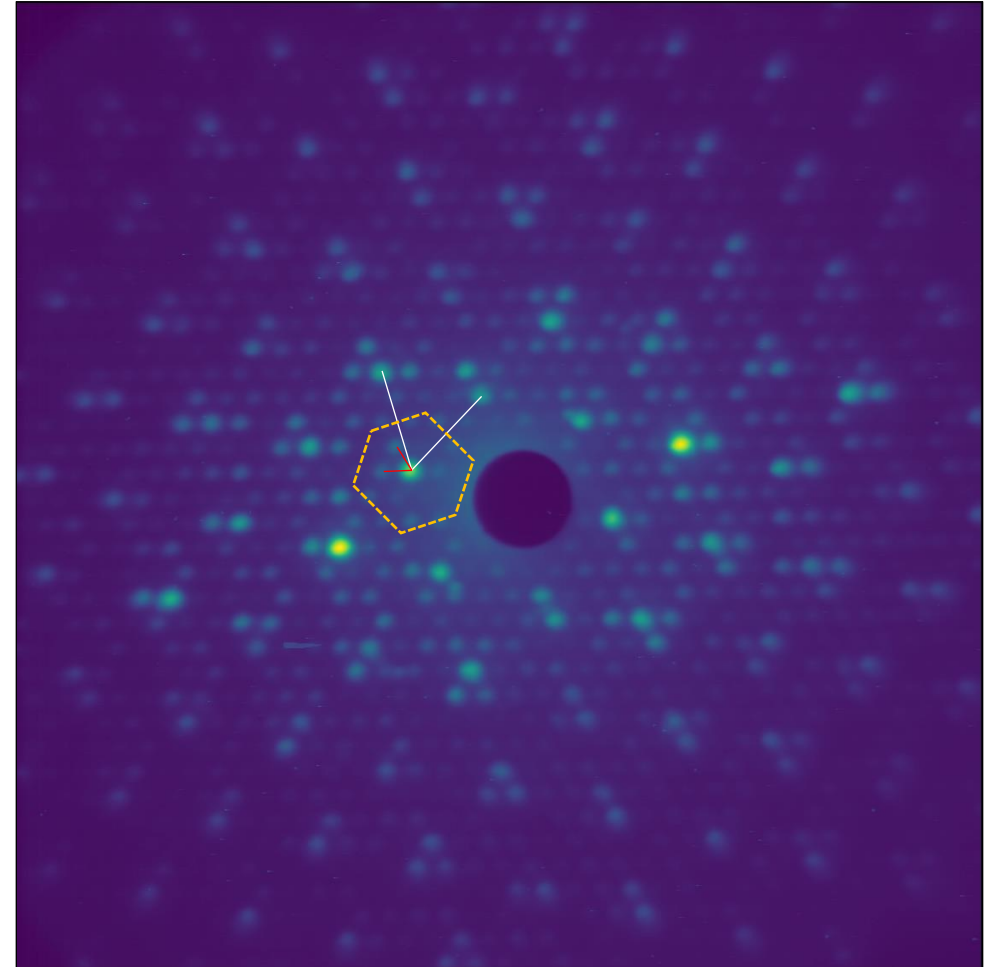
# Stacking dynamics

SLAC

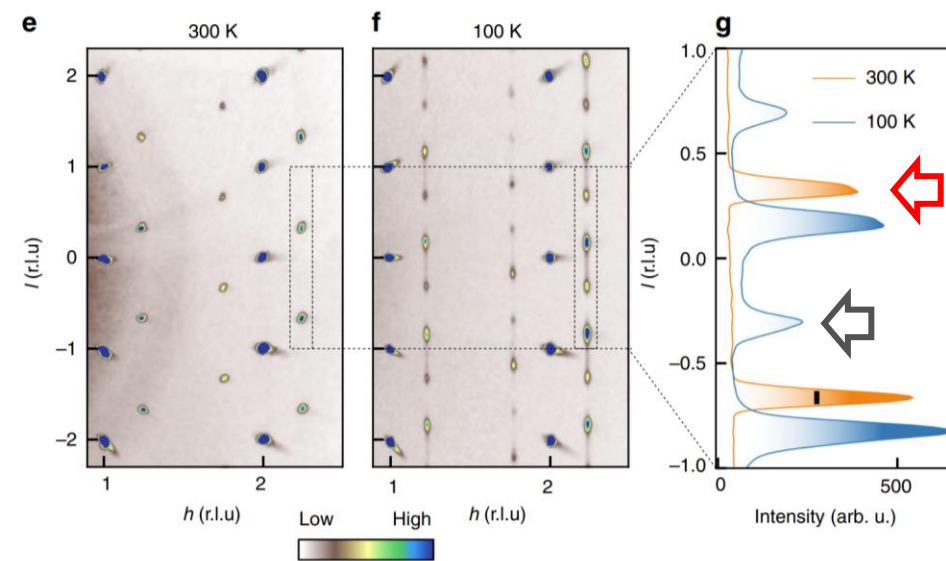
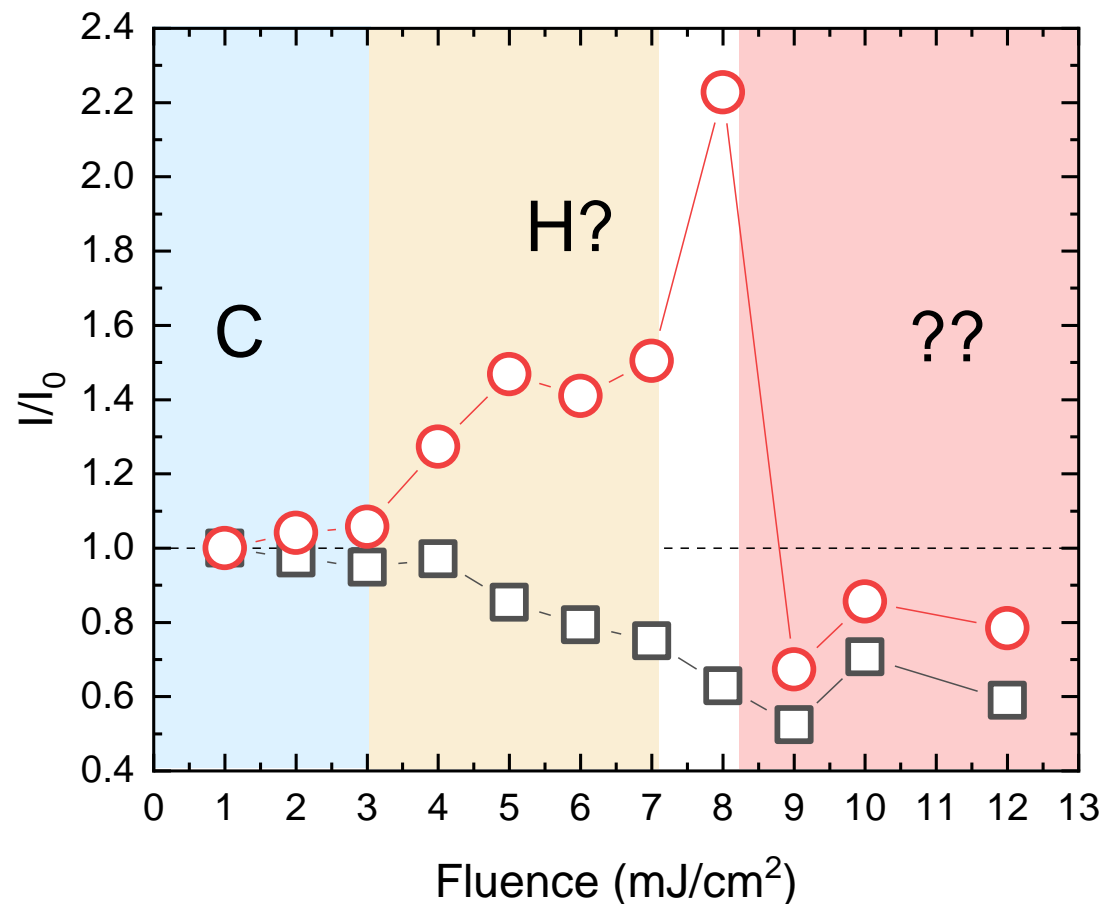


MeV Ultrafast electron diffraction:

- Very flat Ewald sphere
- Reasonable attenuation length
- Large scattering cross section

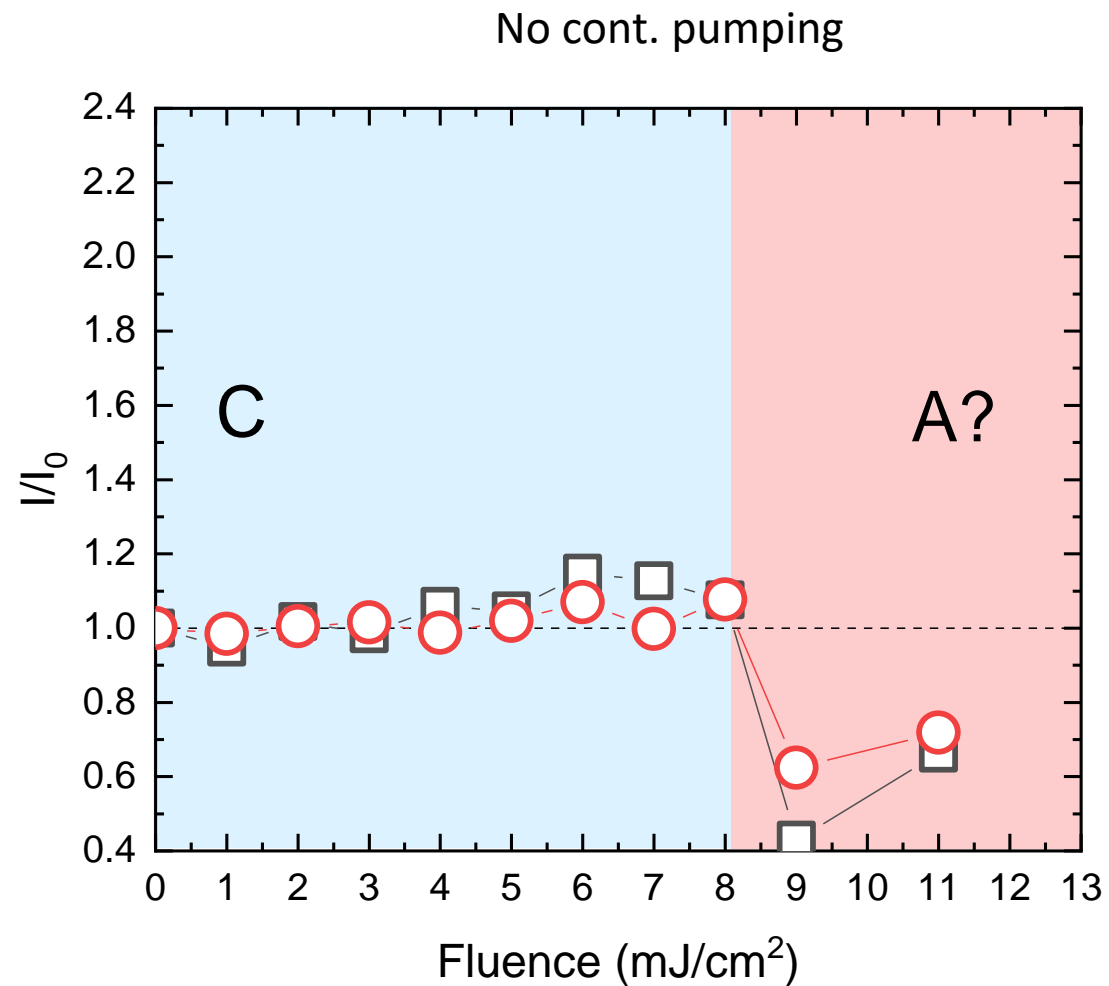
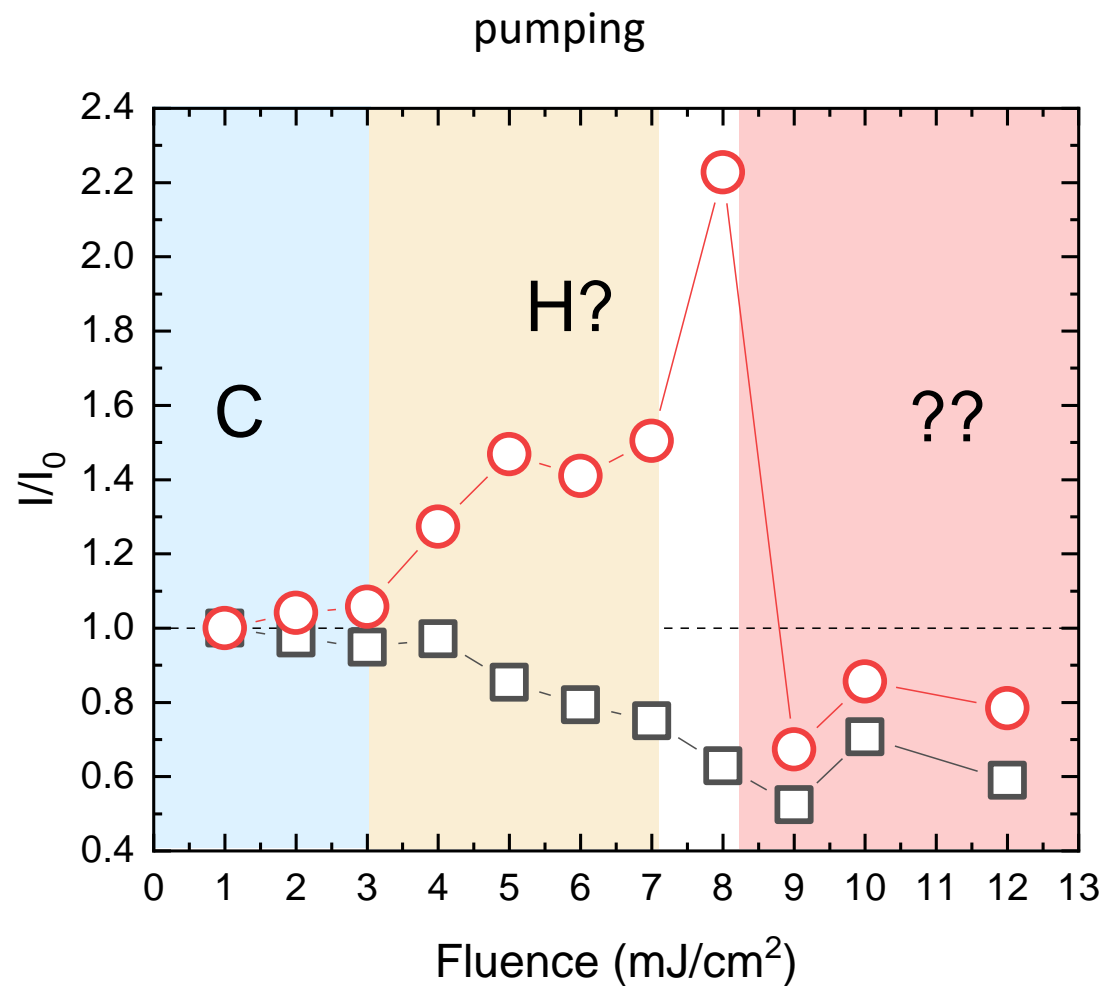


# Stacking after the photoexcitation

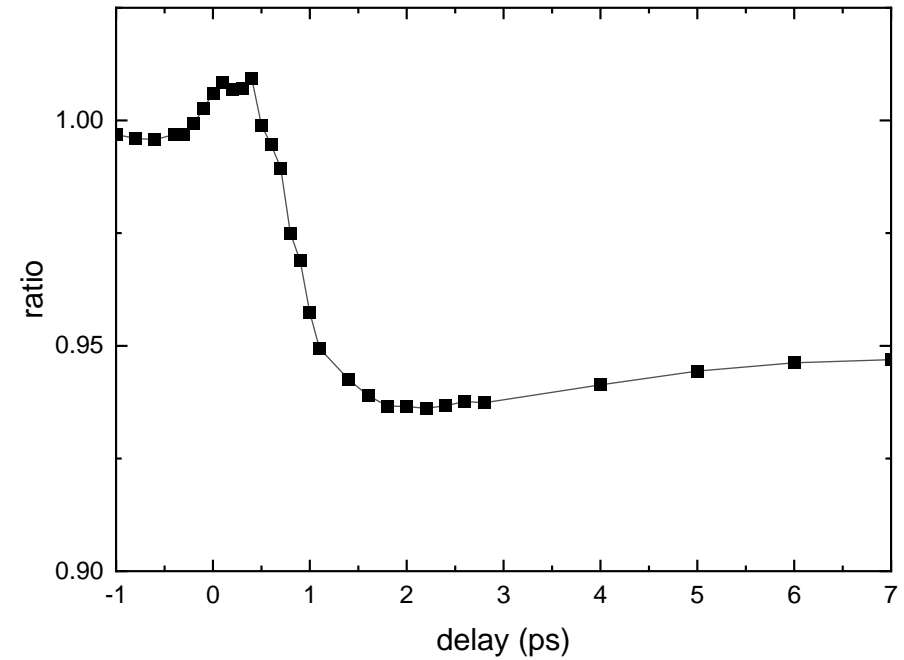
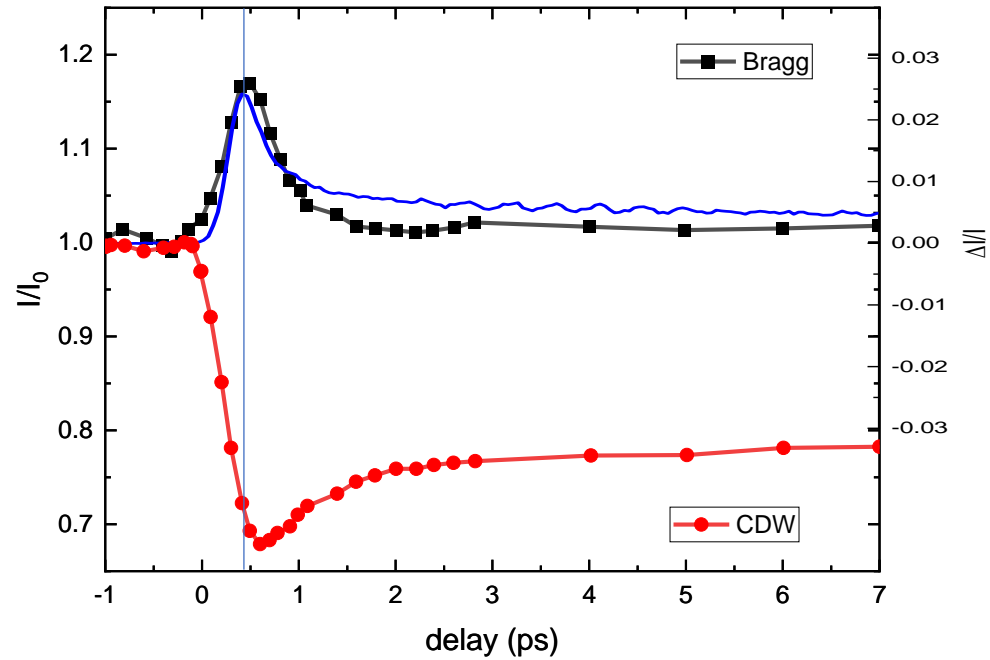


Ritschel et al. Nat Comm. (2018)

# Stacking after the photoexcitation



# How fast is the transition to the H state?



# Summary

- Electronic transition to the H state is accompanied by strong out-of-plane lattice contraction.
- The strain textures in inhomogeneously excited sample can stabilize the H state.
- The effect can be used for tunable X-ray optics.
- The breaking of dimerization occurs on  $\sim 1$  ps timescale.
- There is no stacking order in the A state.

# Acknowledgement



G. Jecl  
Y. Vaskivskyi  
A. Mraz  
R. Venturini  
J. Ravnik

D. Svetin  
P. Sutar  
T. Mertelj  
D. Mihailovic



D. Turenne  
X. Wang  
V. Shokeen  
H. A. Dürr



R. Mincigrucci  
F. Bencivenga  
L. Foglia  
D. De Angelis

J. Pelli-Cresi  
E. Paltanin  
D. Fainozzi  
C. Masciovecchio



A. H. Reid  
X. Shen  
M.-F. Lin  
X. Cheng  
F. Li  
M. Hoffmann



**THANK YOU FOR ATTENTION!**