



UNIVERSITY OF TARTU



# Radiation induced damage in nuclear materials studied with UED and modelling

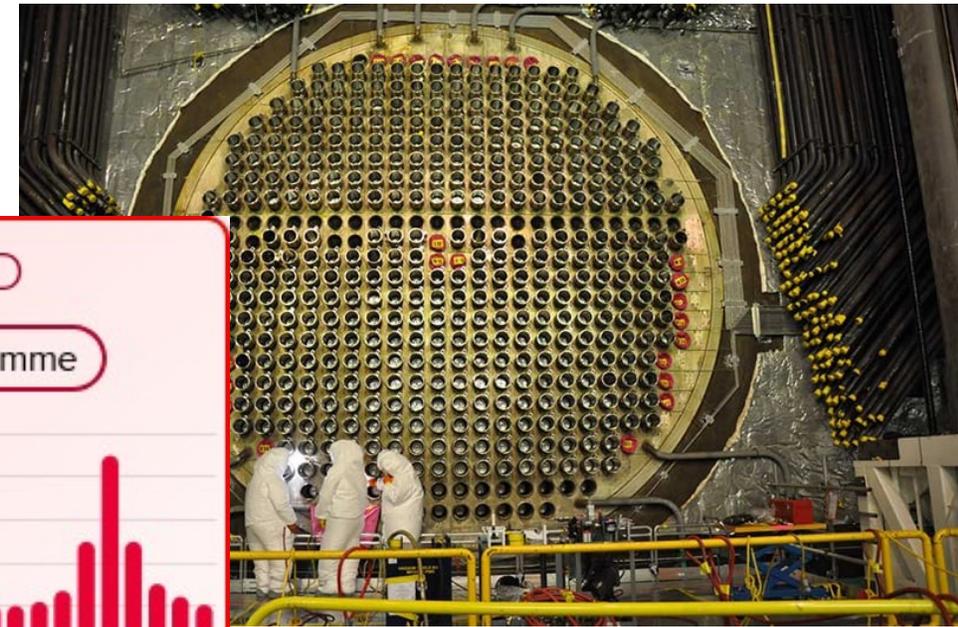
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FUSE @ SLAC  
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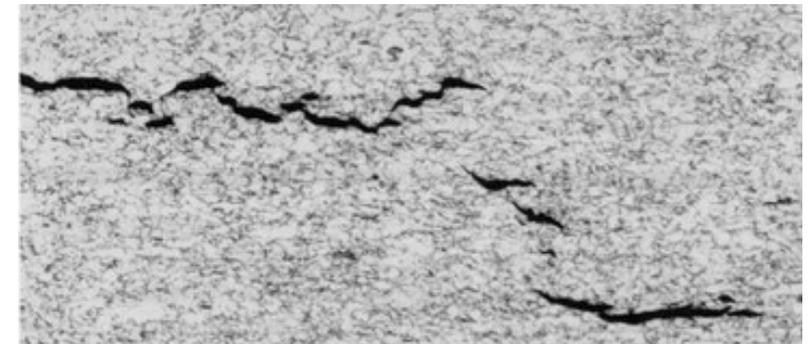
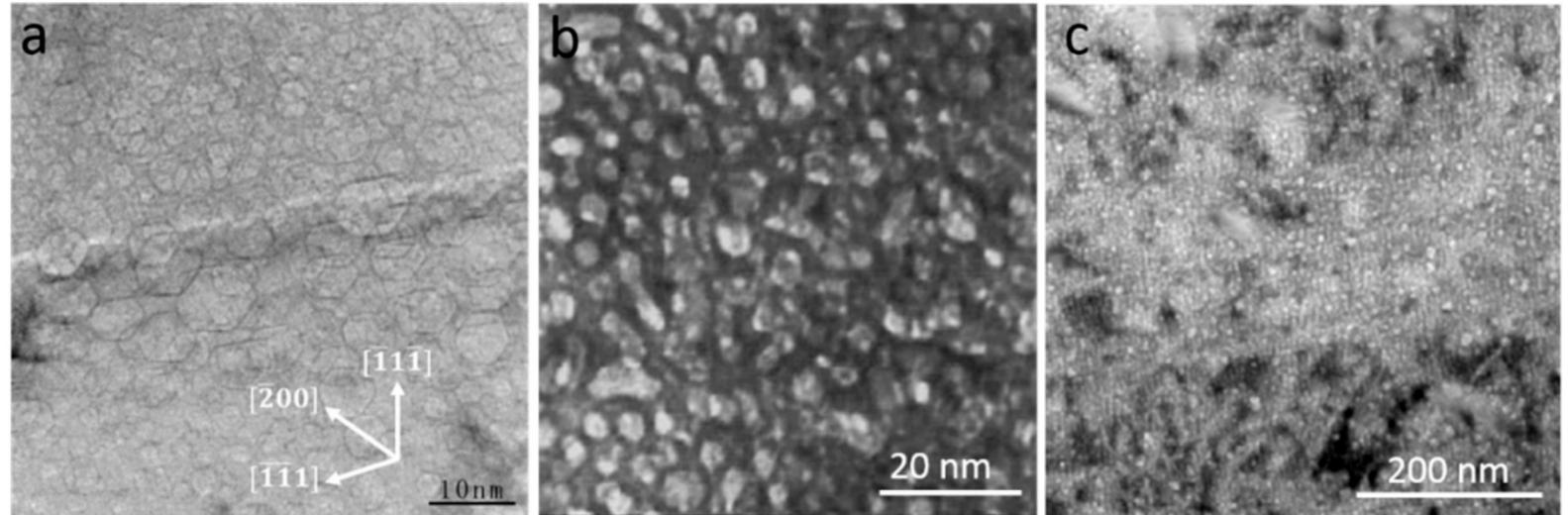
# Motivation

- Recent changes in electricity production have created a need for stabilizing the grid
- Nuclear energy is being actively pursued as a controllable energy source
- Many countries are looking into deploying small modular reactors into the grid as well as extending the lifetime of current reactors



# Radiation damage in materials

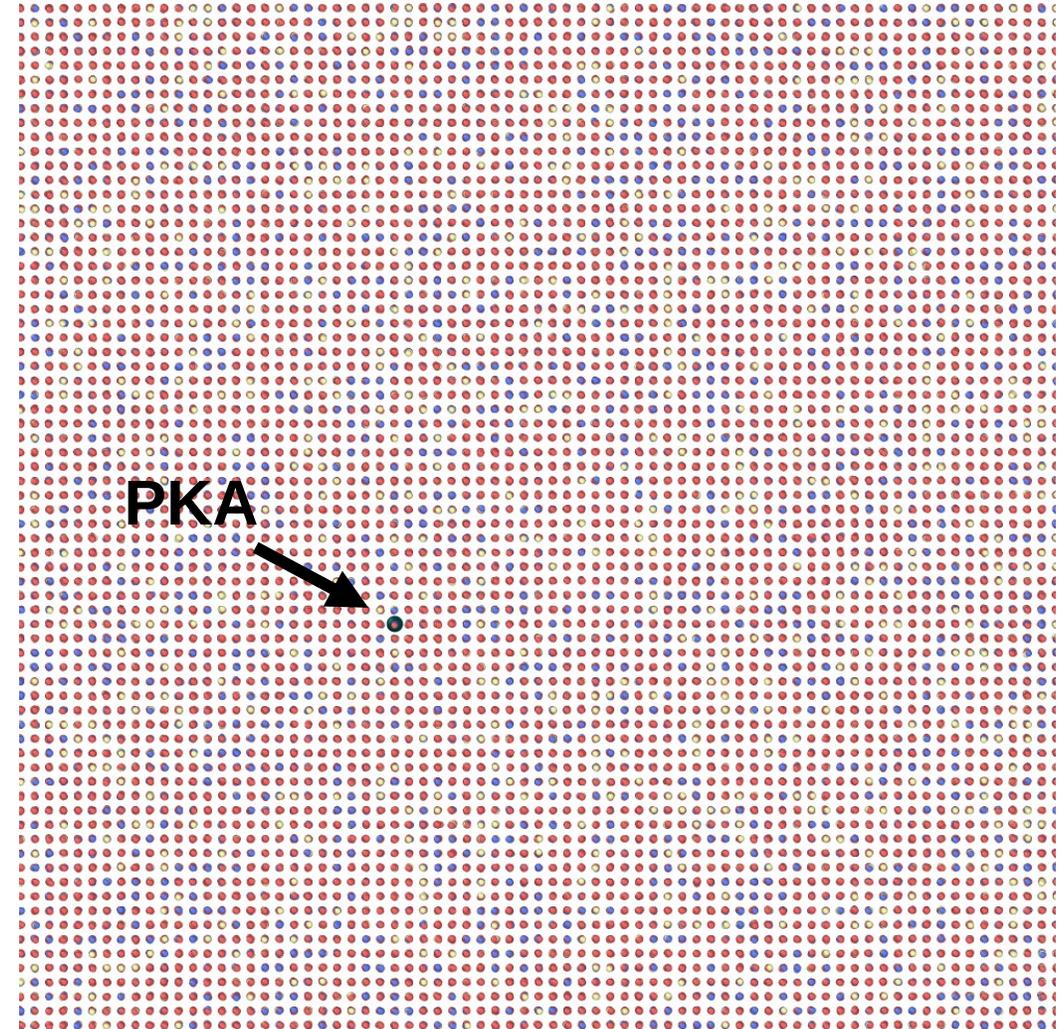
- Extreme conditions in reactors pose a significant challenge for materials
- Void and bubble formation causes hardening and swelling
- High operating temperature enhances corrosion and hydrogen embrittlement
- Crack formation due to temperature gradients
- Radiation induced precipitation



\* stock images from the Web  
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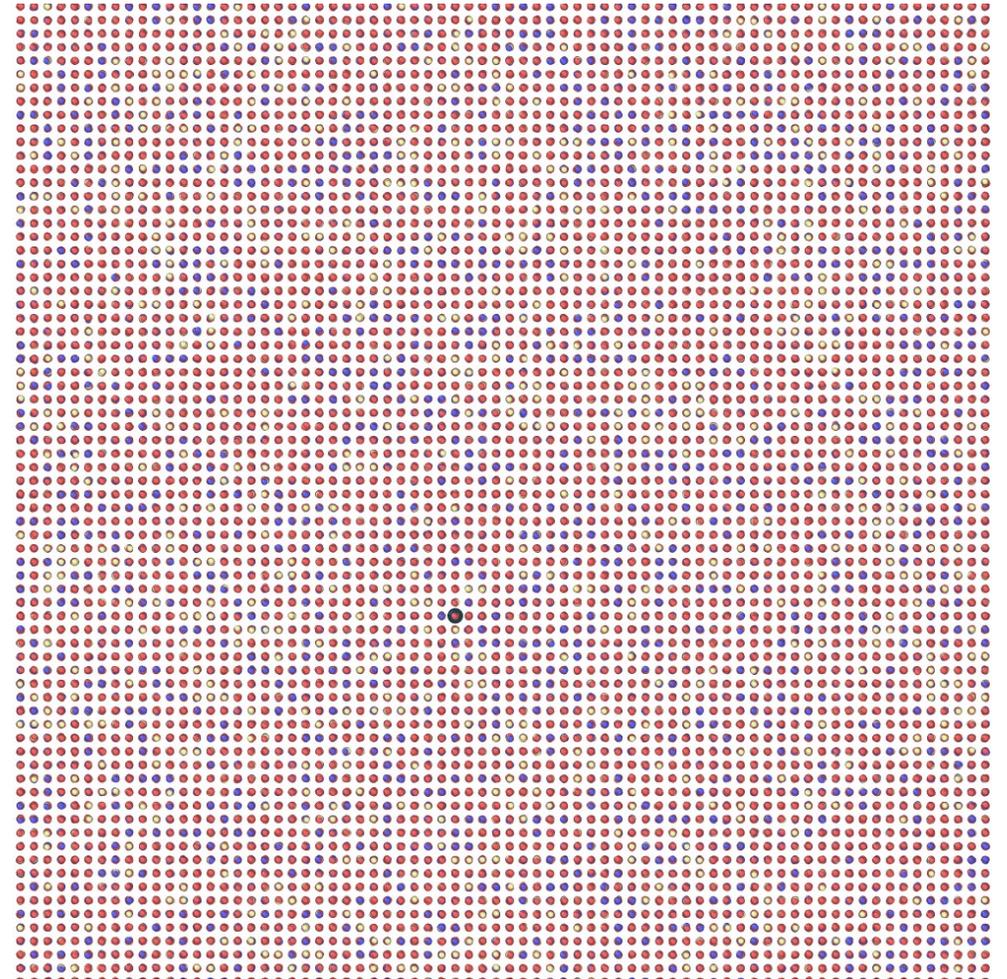
# Radiation damage: primary

- Material degradation in nuclear reactors start with a neutron colliding with an atom in the material
- This primary knock on atom (PKA) receives a lot of kinetic energy (keV and MeV) and starts colliding with other atoms.
- This causes a collision cascade
- Finally energy is distributed throughout the material and several defects remain resulting in primary damage



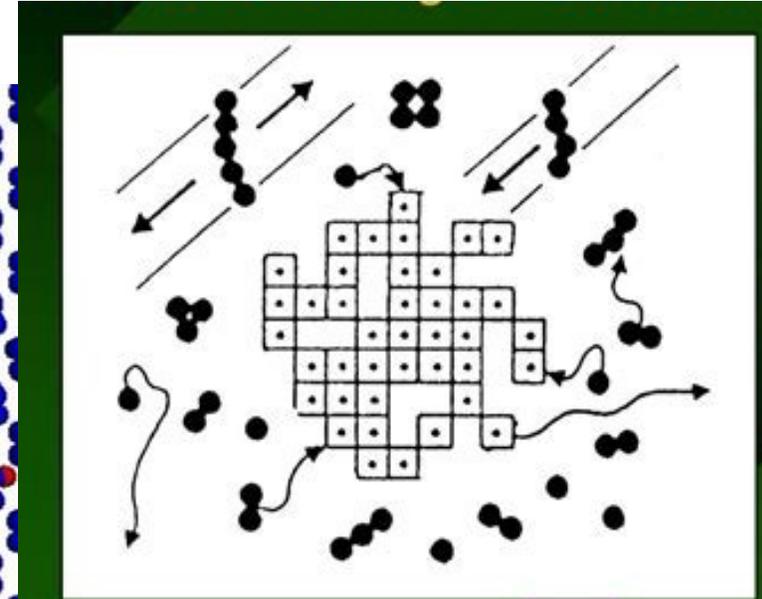
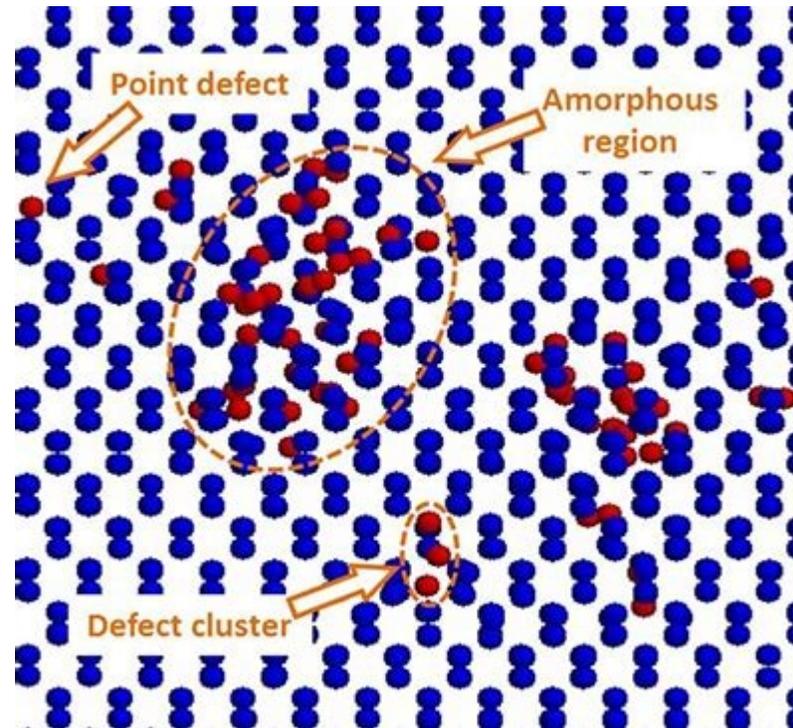
# Radiation damage: primary

- Collision cascade has three distinct stages
- First, binary collision – energetic ions are colliding with each other and distribute energy in a small region
- Second, thermal spike – disordered region forms where ionic temperature is high and pressure waves are emitted
- Third, recrystallisation – the disordered region disappears where most of the defects recombine leaving behind only a few interstitials and vacancies



# Radiation damage: ageing

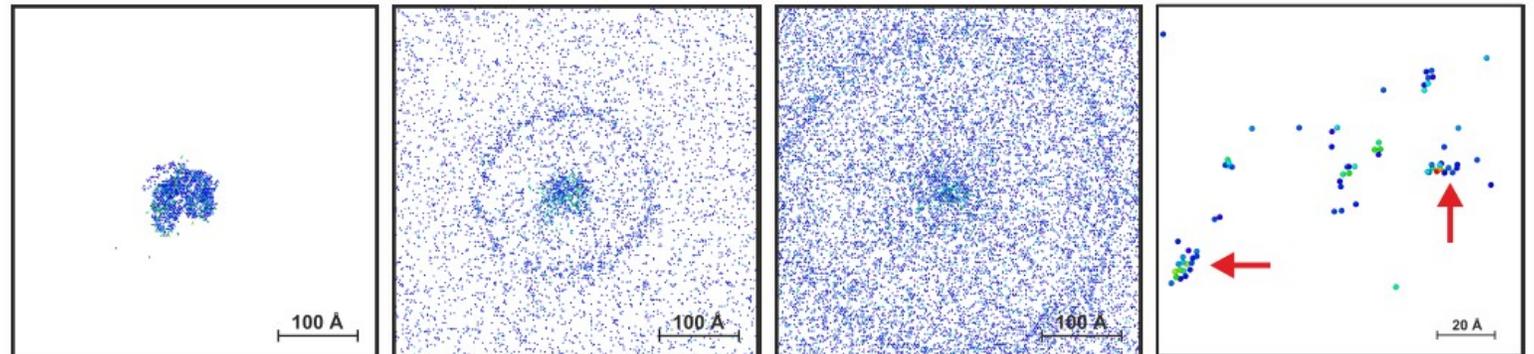
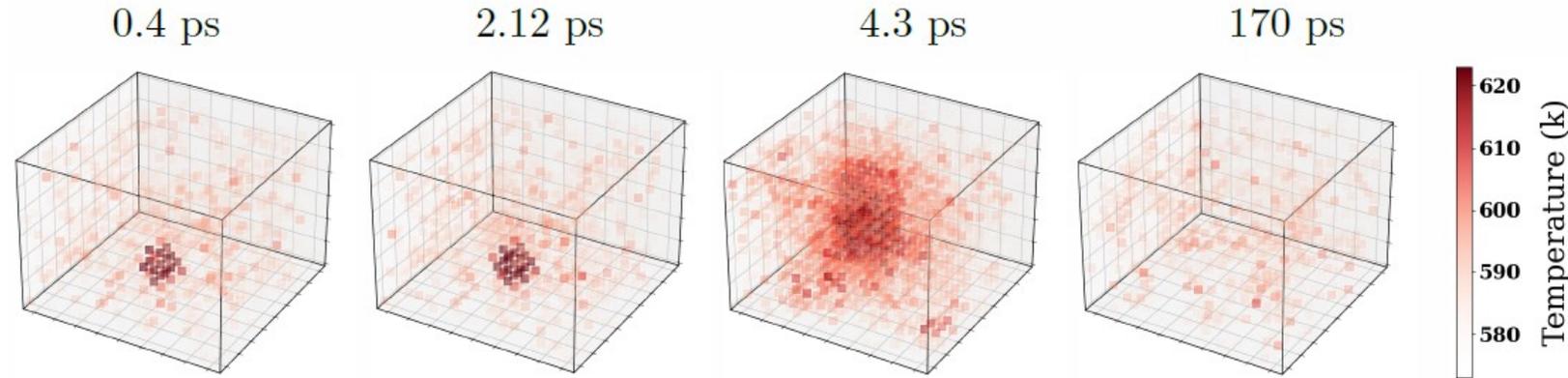
- At a longer timescale point defects created in the primary damage start to diffuse
- They can recombine or exit the material through sinks (surface, grain boundary)
- They can cluster creating larger defects
- They can become trapped at dislocations
- All of this happens at macroscopic times



\* stock images from the Web

# Radiation damage simulations

- Molecular dynamics (MD) is the only tool able to model primary damage
- Interatomic potentials
  - Point-defect energies
  - Short-range interaction
  - Solid-liquid transition
- Electron-ion coupling
  - Electronic stopping
  - Electron-phonon coupling



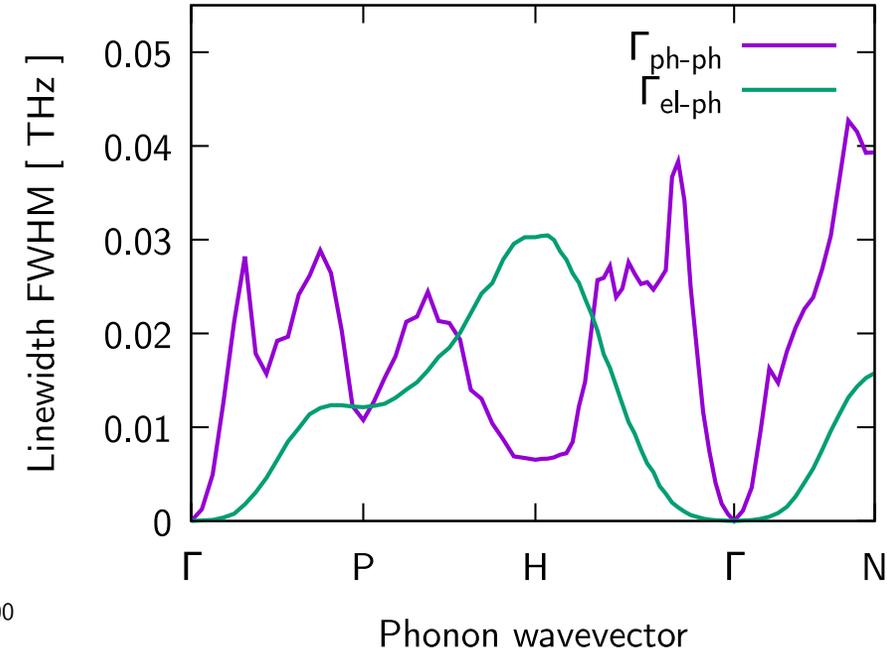
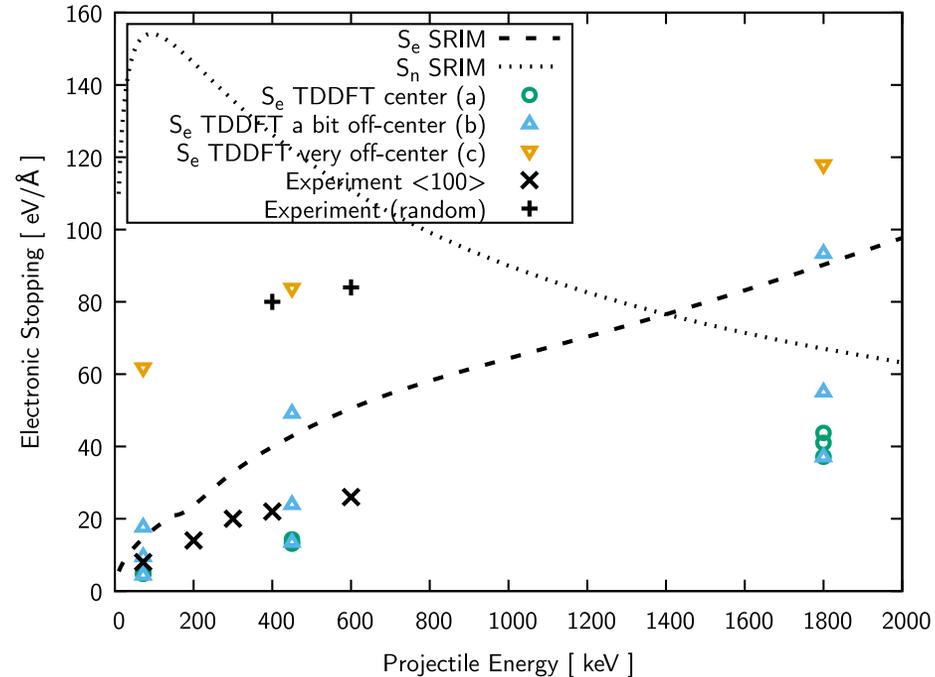
A. Ghorbani *et al.* in preparation

# Electron-ion coupling

Electron-ion coupling manifests in primary damage in two ways

- Electronic stopping – responsible for transferring energy from fast moving ions to electrons
- Electron-phonon coupling – mechanism that drives the material towards a thermal state

Radiation damage is a non-equilibrium process



M. Mo *et al.* Sci. Adv. 10, adk9051 (2024)  
A. Tamm *et al.* in preparation

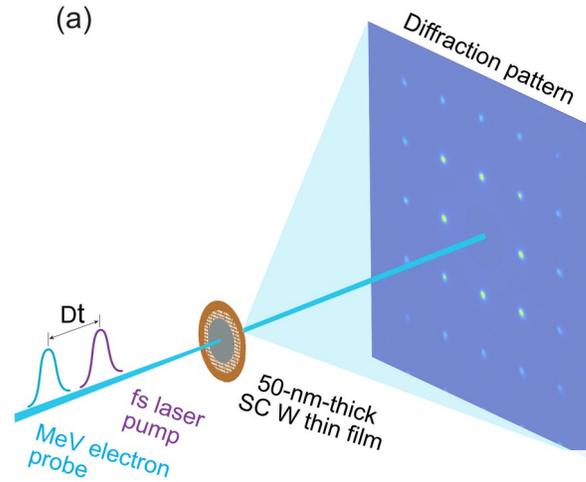
# Electron-phonon coupling from UED

UED pump-probe experiments can be used for MD model validation

Material requirements:

- Single crystal
- No defects or other impurities
- No phase change

- 1) Excite the material
- 2) Measure the dynamics
- 3) Extract el-ph and ph-ph coupling



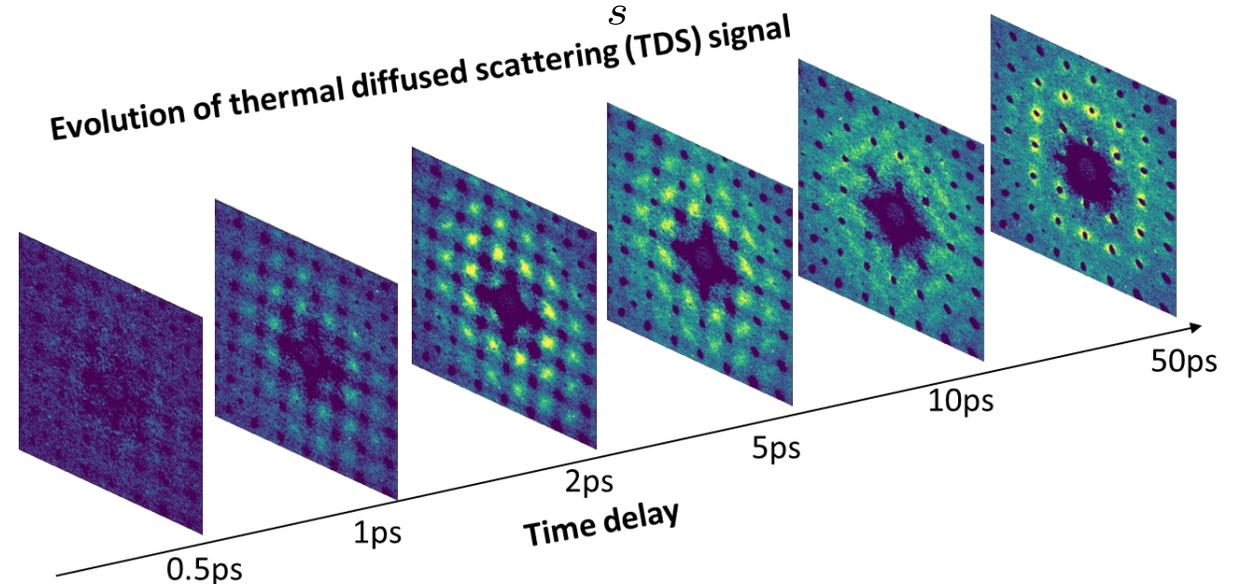
From measurements

$$I(\mathbf{Q}) = I_0(\mathbf{Q}) + I_1(\mathbf{Q}) + \dots$$

$$I_1(\mathbf{Q}) \propto \sum_j \frac{n_j + 1/2}{\omega_j} |F_{1,j}(\mathbf{Q})|^2$$

From simulation

$$I(\mathbf{Q}) \propto \sum_s |f_s(\mathbf{Q}) \exp(-i\mathbf{Q} \cdot \mathbf{r}_s)|^2$$





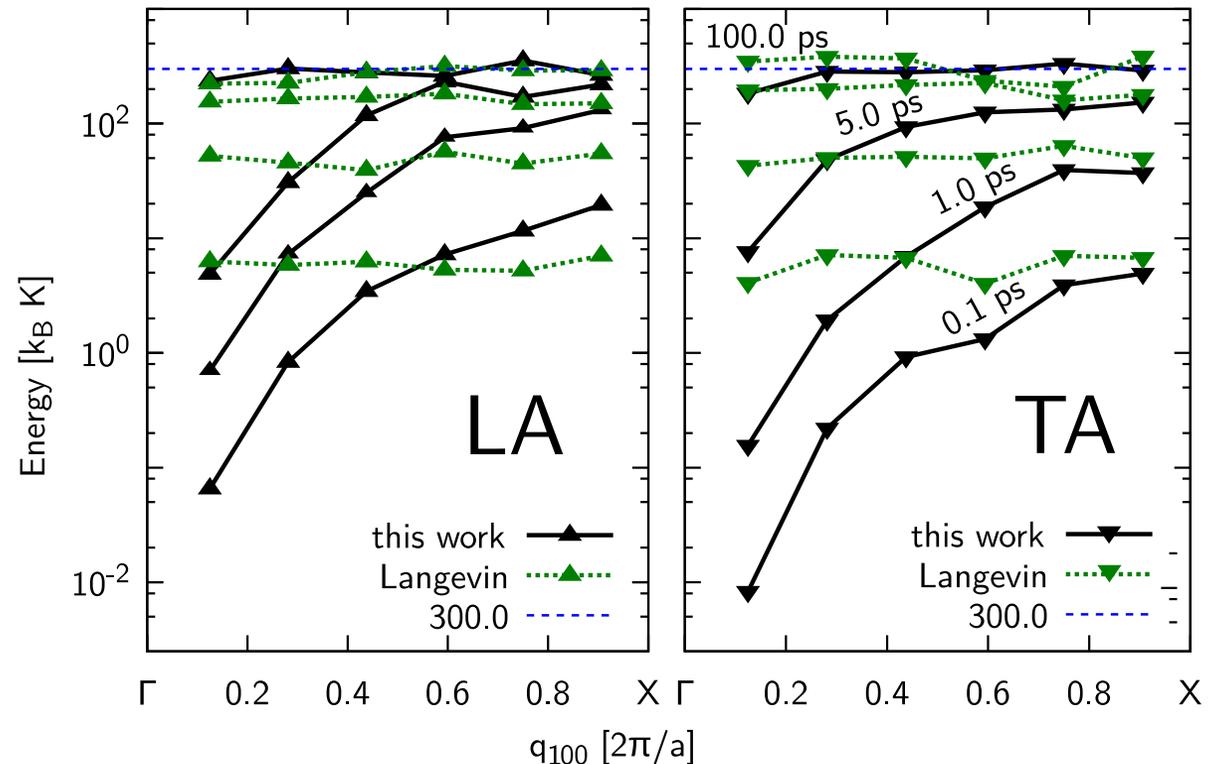
# Model for MD simulations

$$\mathbf{f}_i = -\nabla_i U - \underbrace{\sum_j B_{ij} \mathbf{v}_j}_{\sigma_i} + \underbrace{\sum_j W_{ij} \boldsymbol{\xi}_j}_{\eta_i}$$

We developed a model based on Langevin dynamics to introduce electron-ion coupling into MD simulations

Spatial correlations of the stochastic (and friction) forces is necessary for capturing both q and polarisation dependent coupling

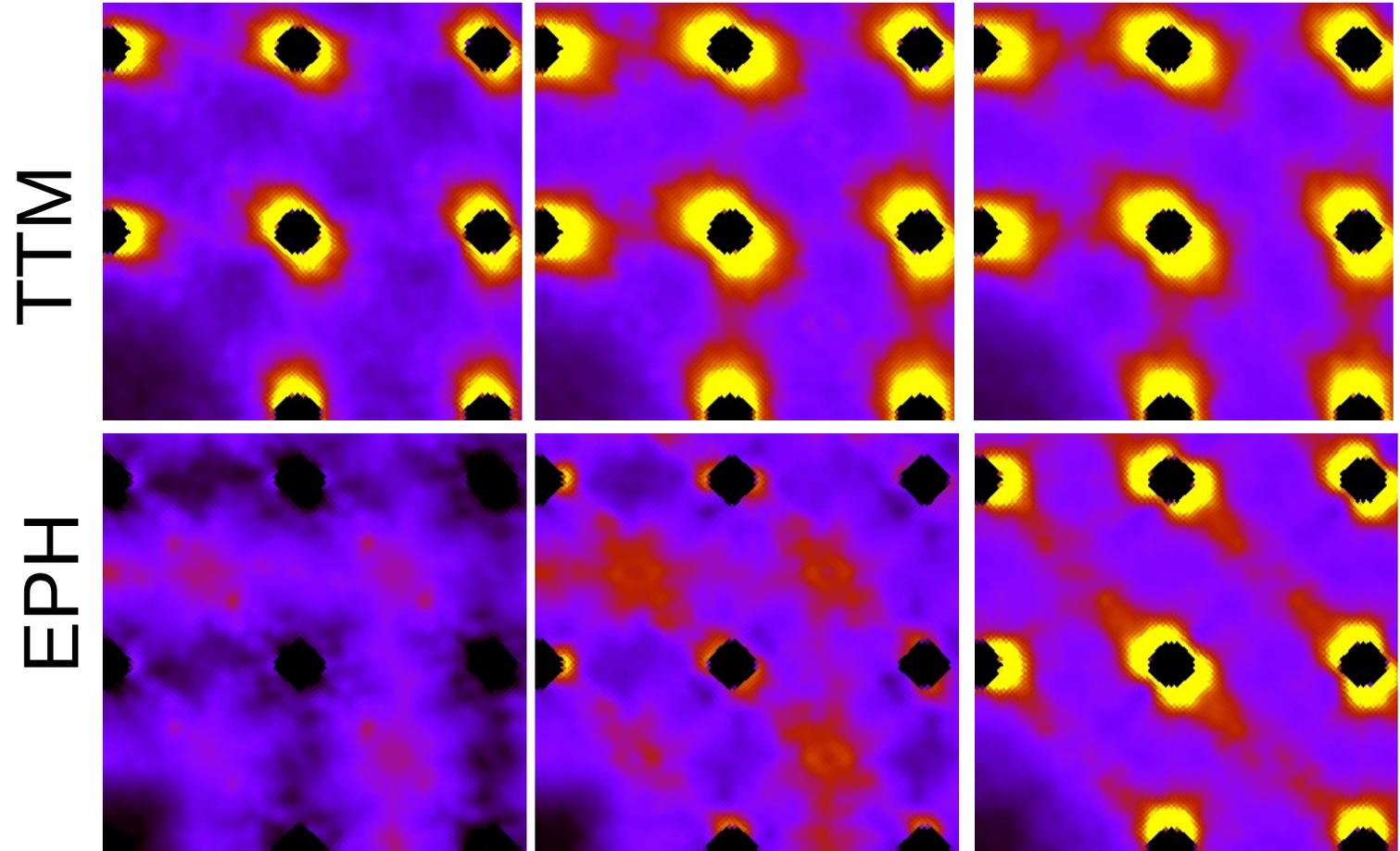
q-vector dependent coupling is crucial for simulating non-equilibrium dynamics of laser excited metals



A. Tamm *et al.* PRL 120, 185501 (2018)

# Importance of electron-phonon coupling model in MD

- Electron-ion coupling model directly affects the dynamics
  - TTM excites all modes at the same rate
  - This causes “thermal like” distribution for every timestep
  - EPH model has momentum resolved mode excitations
  - The dynamics of the non-equilibrium process is more realistic

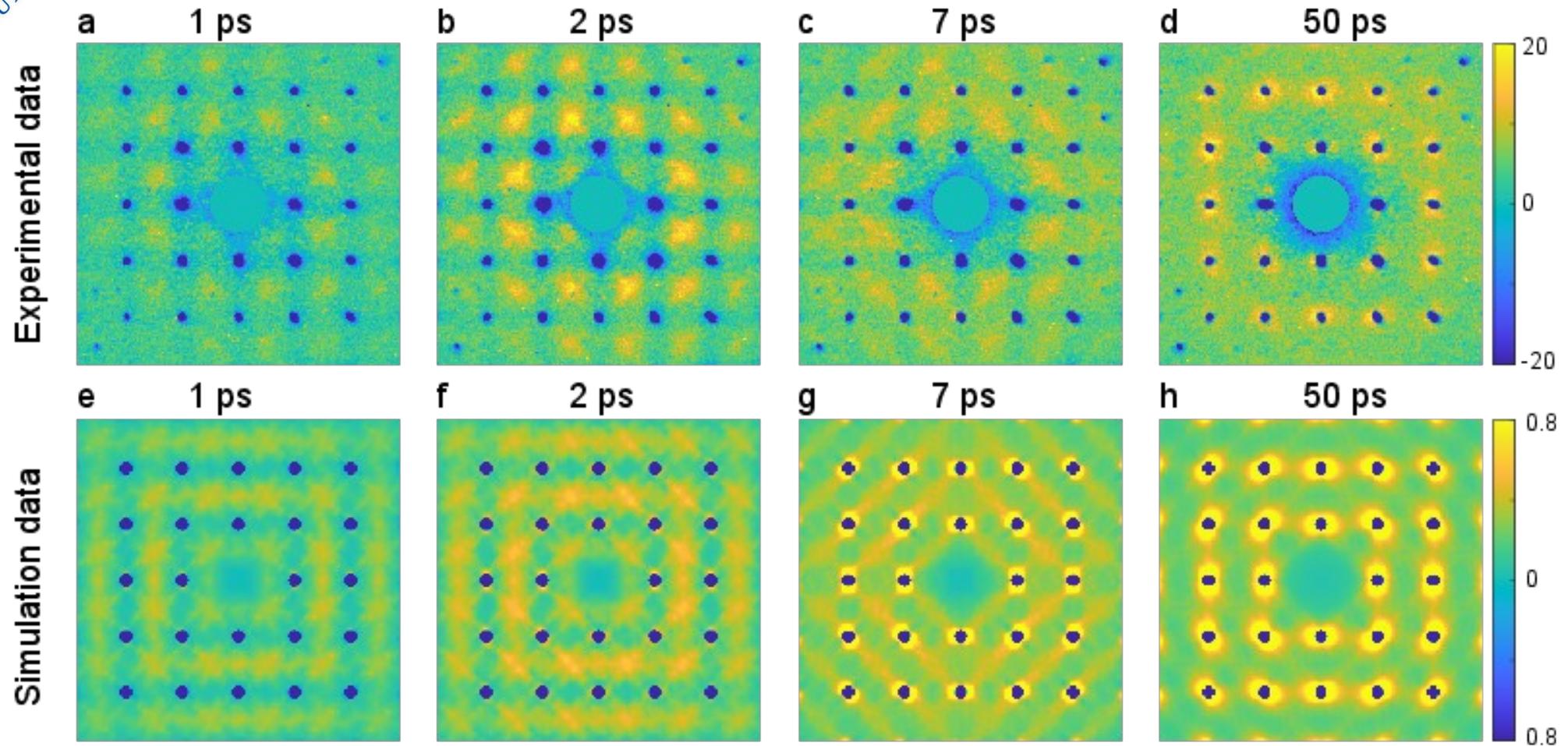




# Non-equilibrium dynamics in $W$

! Show the movie !

# UED experiment vs simulation

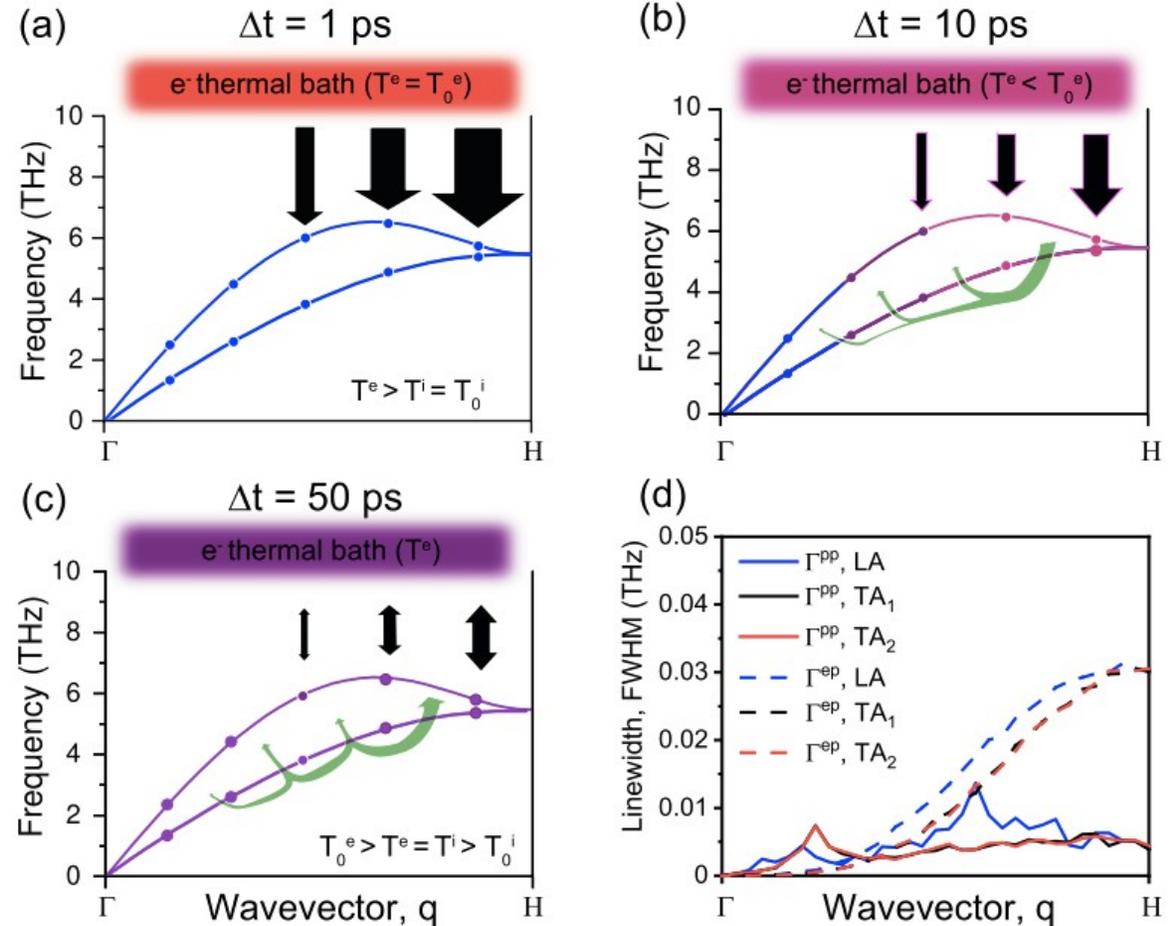


# Non-equilibrium dynamics of laser heated tungsten

The path towards equilibrium in laser excited tungsten is following:

- First, the hot electrons couple strongly to modes near the edge of the Brillouin zone
- Next, energy from strongly excited modes near the border edge is transferred to other modes due to phonon-phonon scattering
- Finally, all modes have the same energy and the system equilibrates

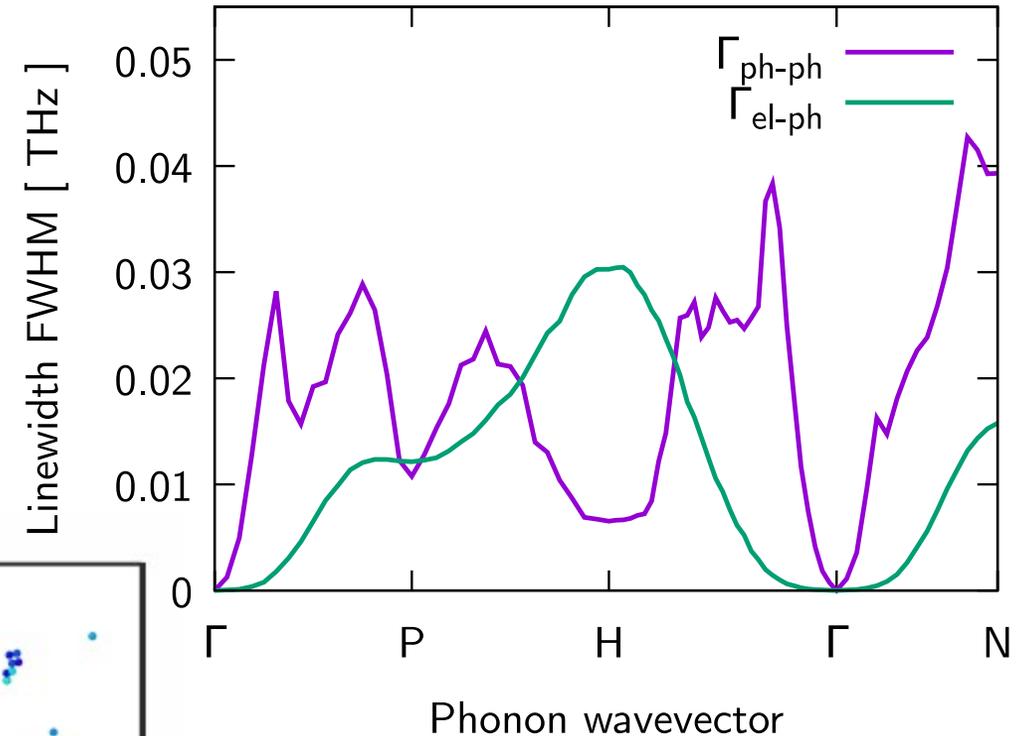
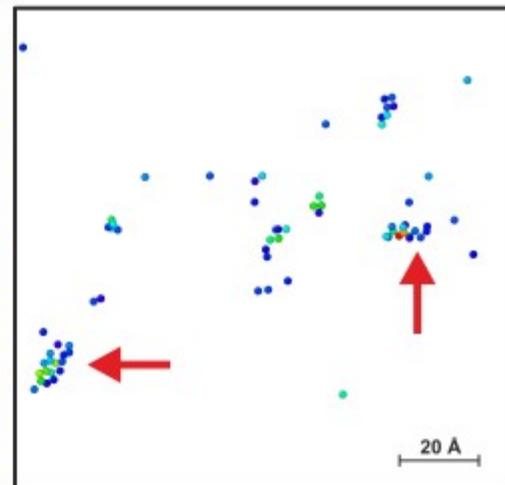
The rates of el-ph and ph-ph excitations are  $q$ -dependent



# Effect of radiation damage on electron-phonon coupling

Will defects affect the el-ph and ph-ph scattering?

- Point defects act as scattering centres
- ph-ph interaction should drive the dynamics towards equilibrium faster
- el-ph coupling coupling might excite strongly localised modes
- What are phonons in disordered system?
- What kind of defects do we have and where are they?





# W-He UED and simulation results

**REDACTED**

# Conclusions

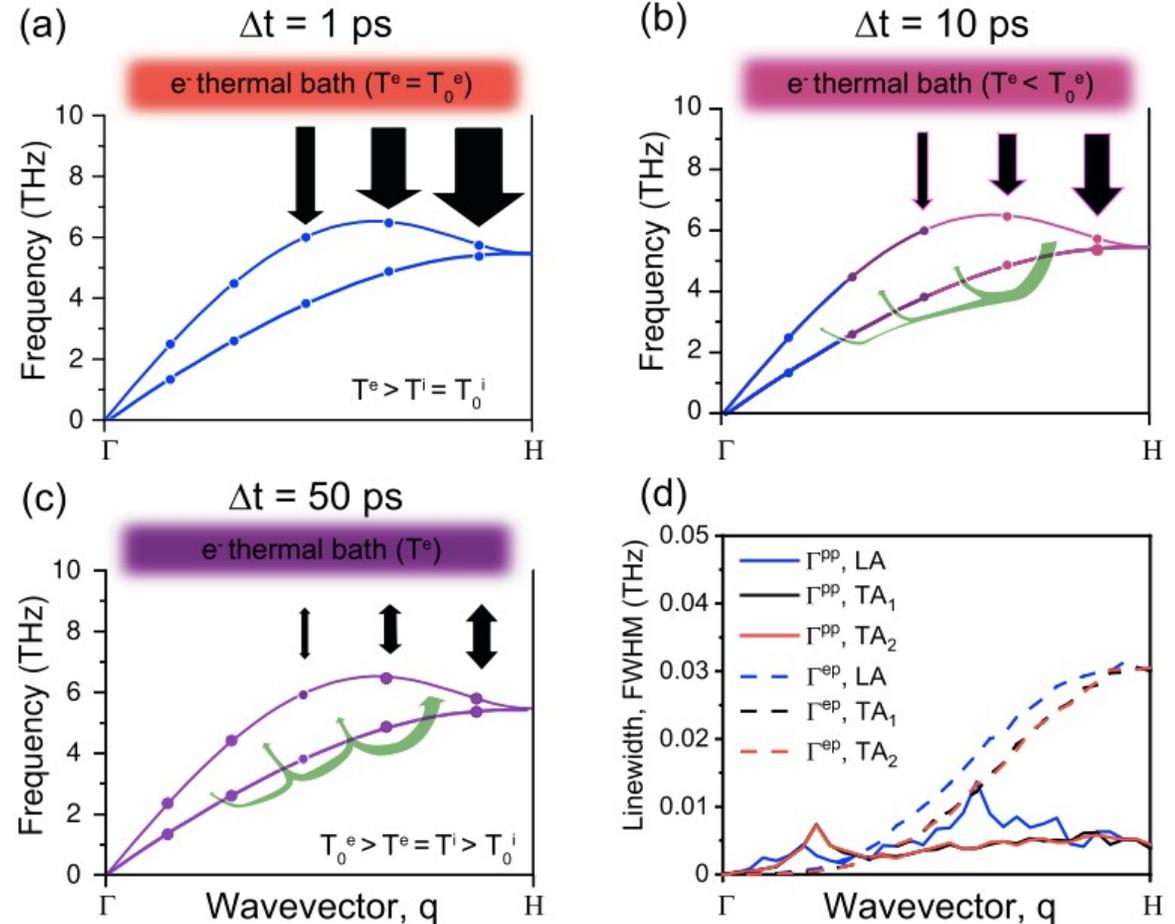
UED is excellent for studying non-equilibrium processes in materials

Combining experiments with modelling allows to explain the dynamics in detail

UED signal could be used to estimate amount of damage in the material

Challenges:

- Material characterisation not detailed enough for modelling
- Unknowns in the experiment make it difficult to directly compare results





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Thank you for  
your attention!

Questions?

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