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## Evolution of graphite structure under irradiation: A new scenario

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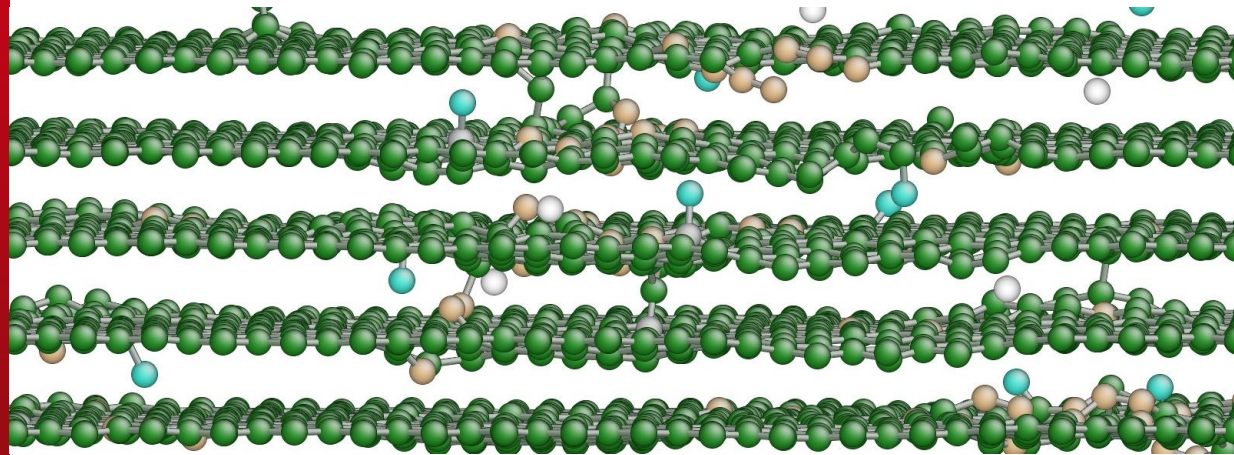
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# EVOLUTION OF GRAPHITE STRUCTURE UNDER IRRADIATION: A NEW SCENARIO

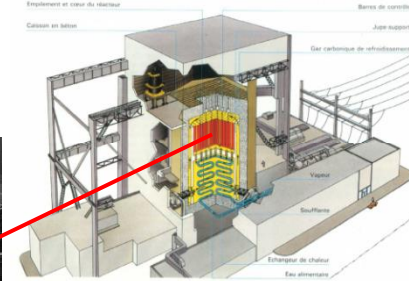


Alain Chartier, Laurent Van Brutzel

## Framework: decommissioning of graphite from "UNGG"

- Graphite = moderator in "UNGG" → neutrons, temperature
- In 11 years of exploitation 2.6 dpa
- Activation of some impurities

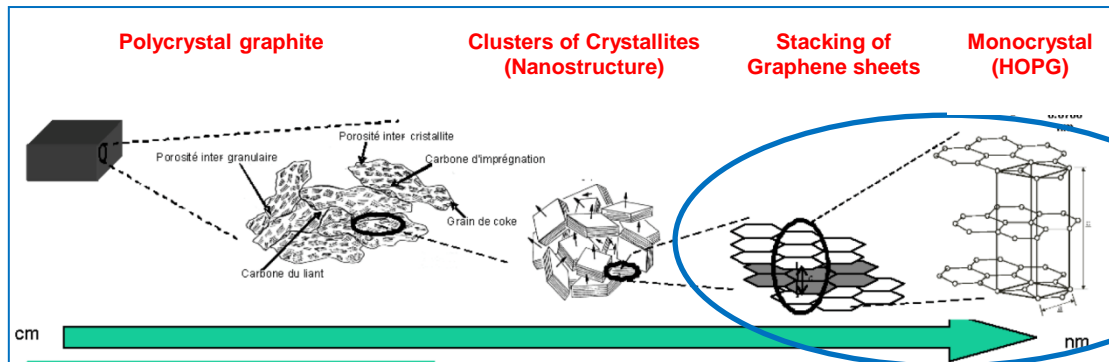
i-graphite contains  $^{14}\text{C}$  &  $^{36}\text{Cl}$  ( $\frac{1}{2}$  life 5 500 &  $3 \times 10^5$  years)



## Foreseen Solutions:

- Decommissioning under water
- Treatment to eliminate  $^{14}\text{C}$  &  $^{36}\text{Cl}$ , ( $^3\text{H}$ )
- Graphite microstructure evolution under irradiation?

interaction: graphite  $\leftrightarrow$   $\text{H}_2\text{O}$ ,  $\text{O}_2$ ,  $\text{CO}_2$ ...  
 depends on the localization of  $^{14}\text{C}$  &  $^{36}\text{Cl}$  after irradiation



Simulation of the primary damage with molecular dynamics simulations

# Scenarii of radiation damages of graphite

**Question:**

Neutron damages in nuclear graphite?

**Answers:**

- Some review articles

Heggie (2007)

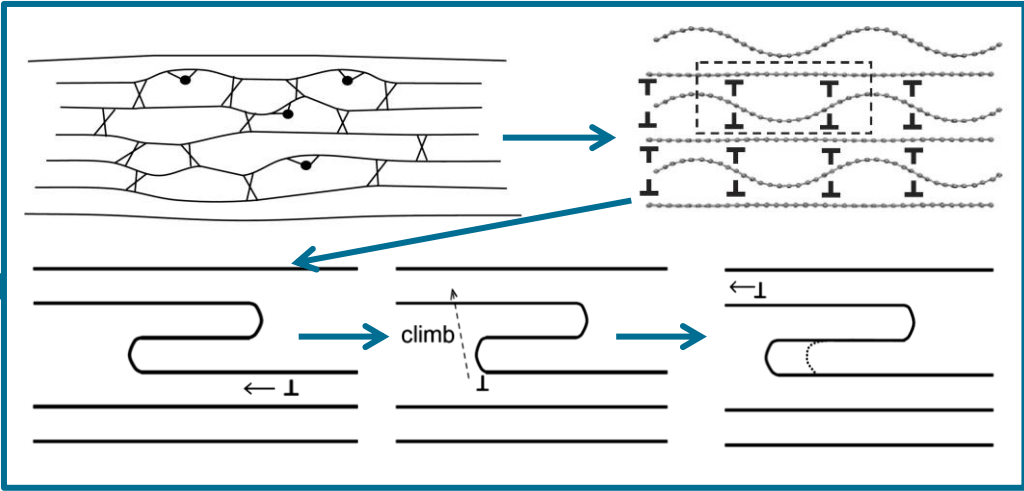
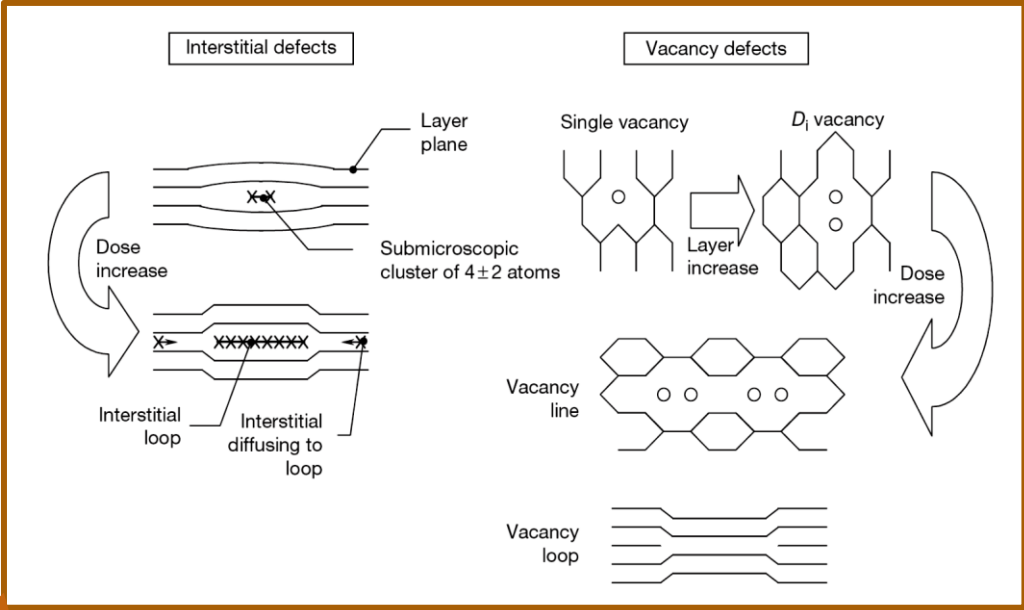
Marsden, Burchell and Fachinger (2012)

However, few data on  
Primary Damage State

- Two main scenarii proposed to describe radiation damages:

1. Creation of point defects, then clustering via diffusion and dislocation formation

2. Creation of point defects, then wrinkling, sliding, and dislocation formation (Heggie & Telling)



## Study of Primary Damage with Molecular Dynamics

Code: LAMMPS

Empirical potential: LCBOP (bond-order)



## Primary Damage: Displacement Cascades

Primary Knock-on Atom: C

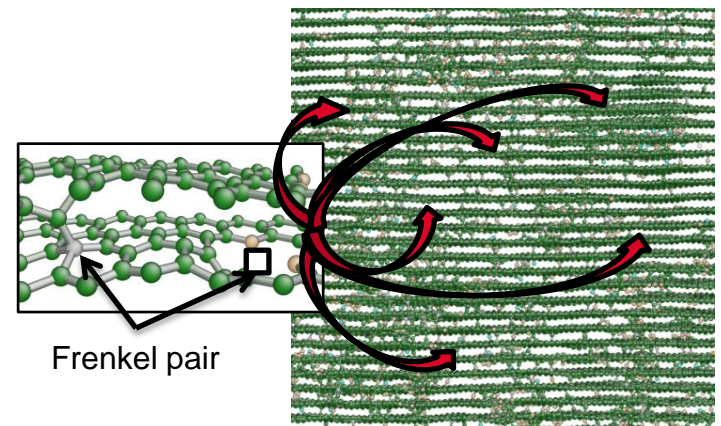
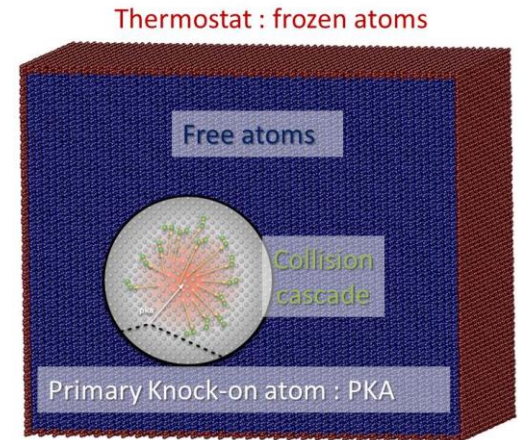
 $E_{PKA} = 0.5 \rightarrow 10 \text{ keV}$ 

T = 300 - 1000 K

Statistics: 16 cascades /  $E_{PKA}$ 

## Dose Effects: Point Defects Accumulation

Creation of random Frenkel pairs

Dose rate:  $10^{10} \text{ dpa/s}$ Dose: 0.1  $\rightarrow$  1 dpa300 - 1000 K (relaxation NPT)  $\rightarrow$  Swelling




Example: Cascade with 5 keV PKA

Projectile C - direction [100] – 300 K

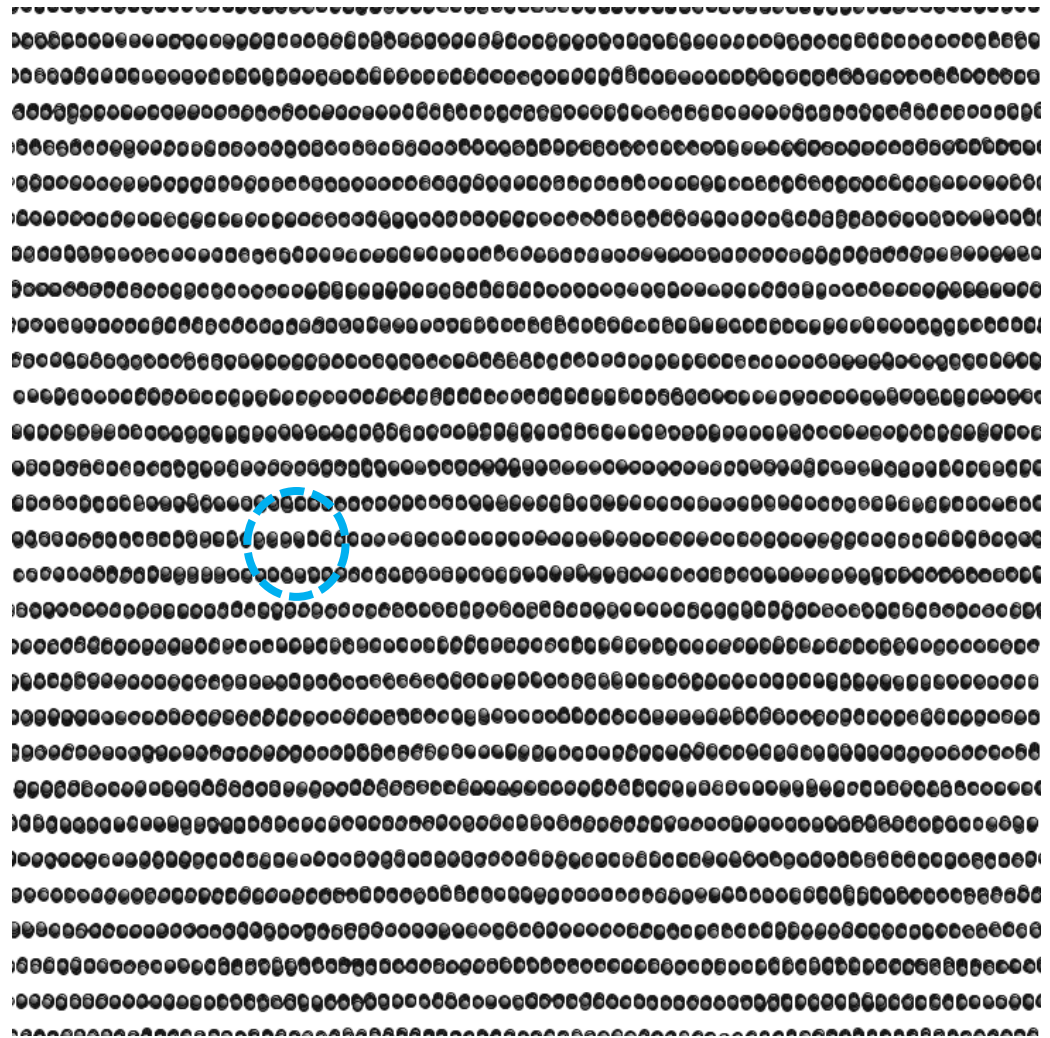
### Three Stages:

1. Collision Stage : 2 ps
2. Thermal Spike : 5 ps
3. Relaxation : 10 ps

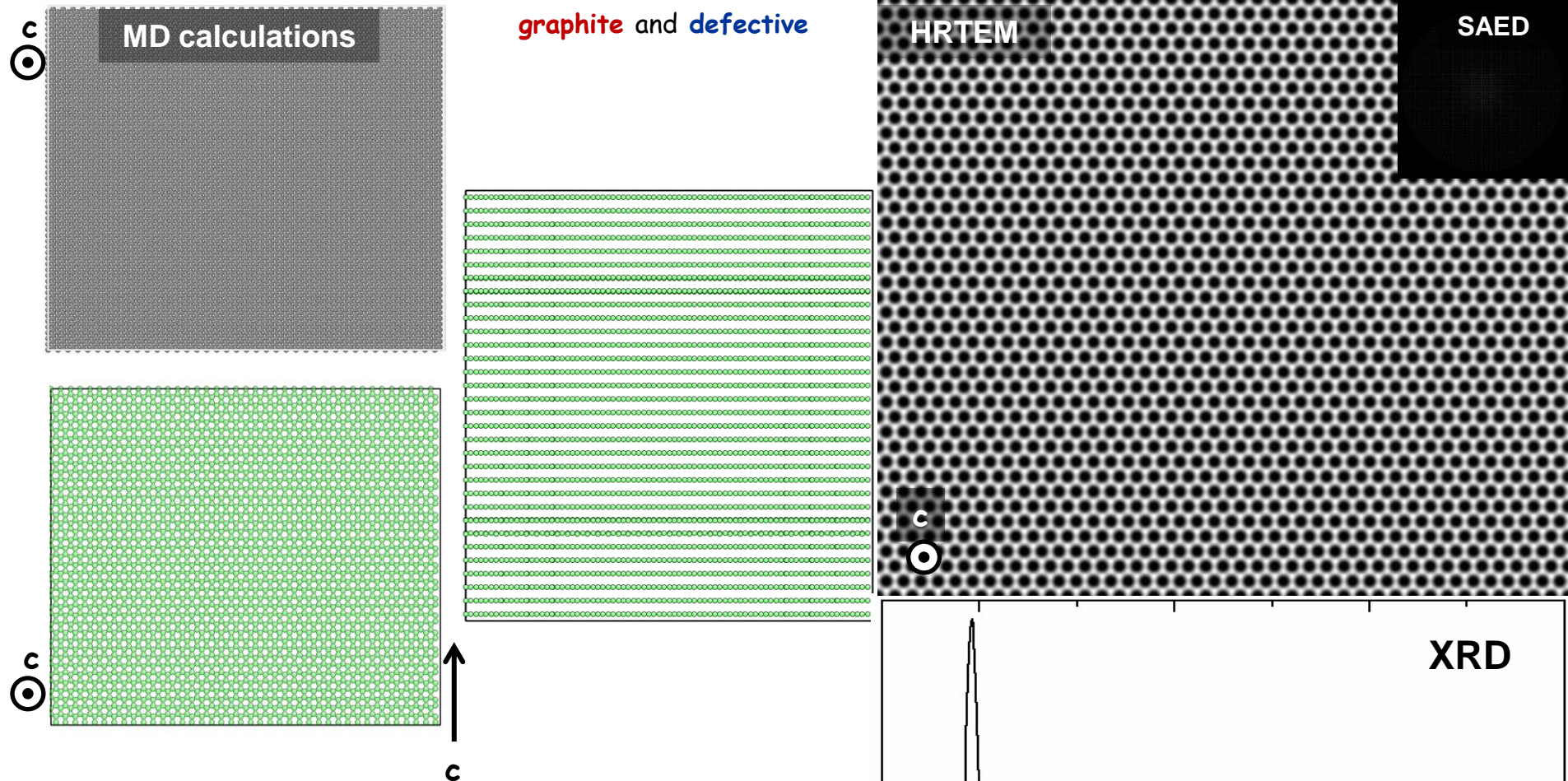
### Damage:

- No Amorphisation
- Numerous Point defects 
- Few Recombination
- No influence of the initial PKA orientation
- Number of vacancies  $\approx$  interstitials

→ Point Defect Accumulation  
method



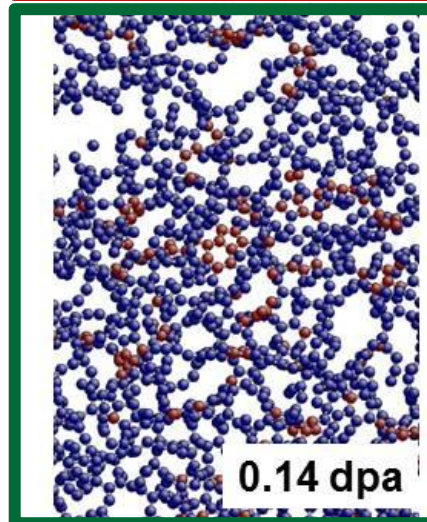
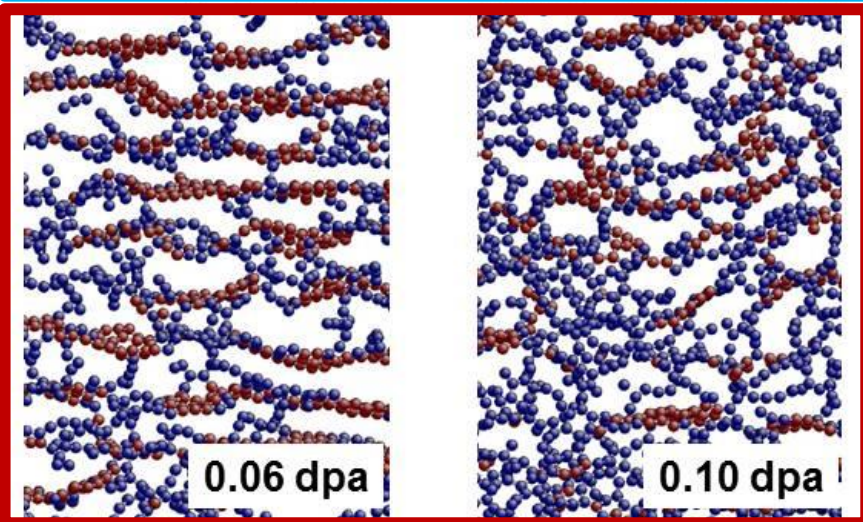
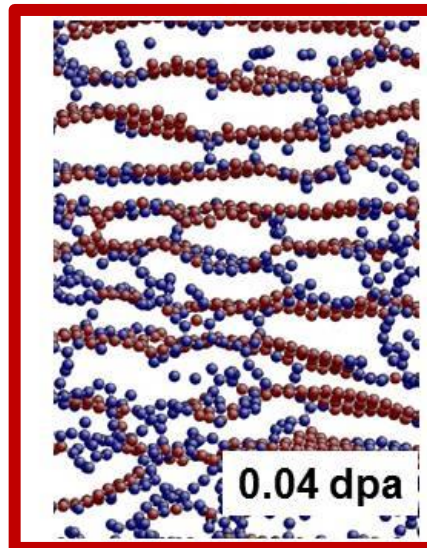
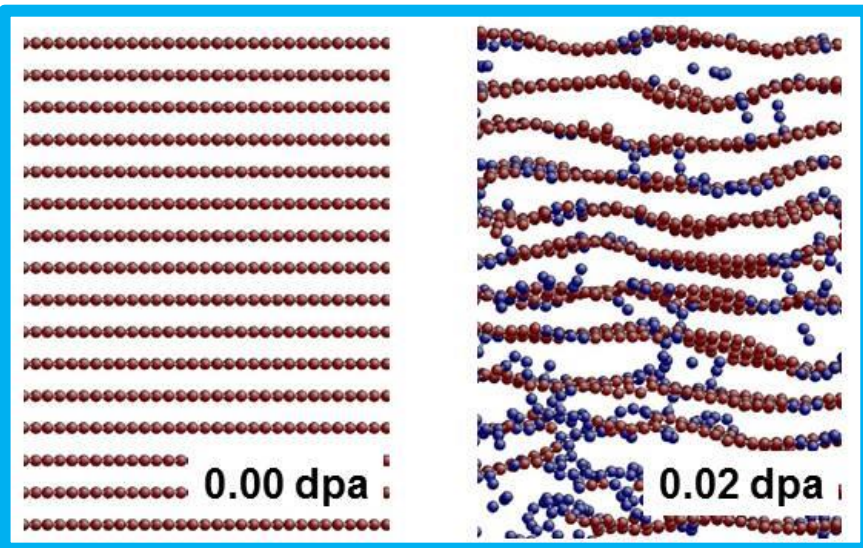
# Dose effect from MD – Analysis from curvature criterion, HRTEM, SAED and XRD calculations



- Visualization of defects in graphene planes (MD and HRTEM)
- Visualization of wrinkles (MD analysis)
- Swelling from size of box (not easy from XRD)
- amorphization at 0.10 dpa (SAED and XRD)



Perfect graphene sheets in red and point defects in blue



Three Steps:

1. Point Defects

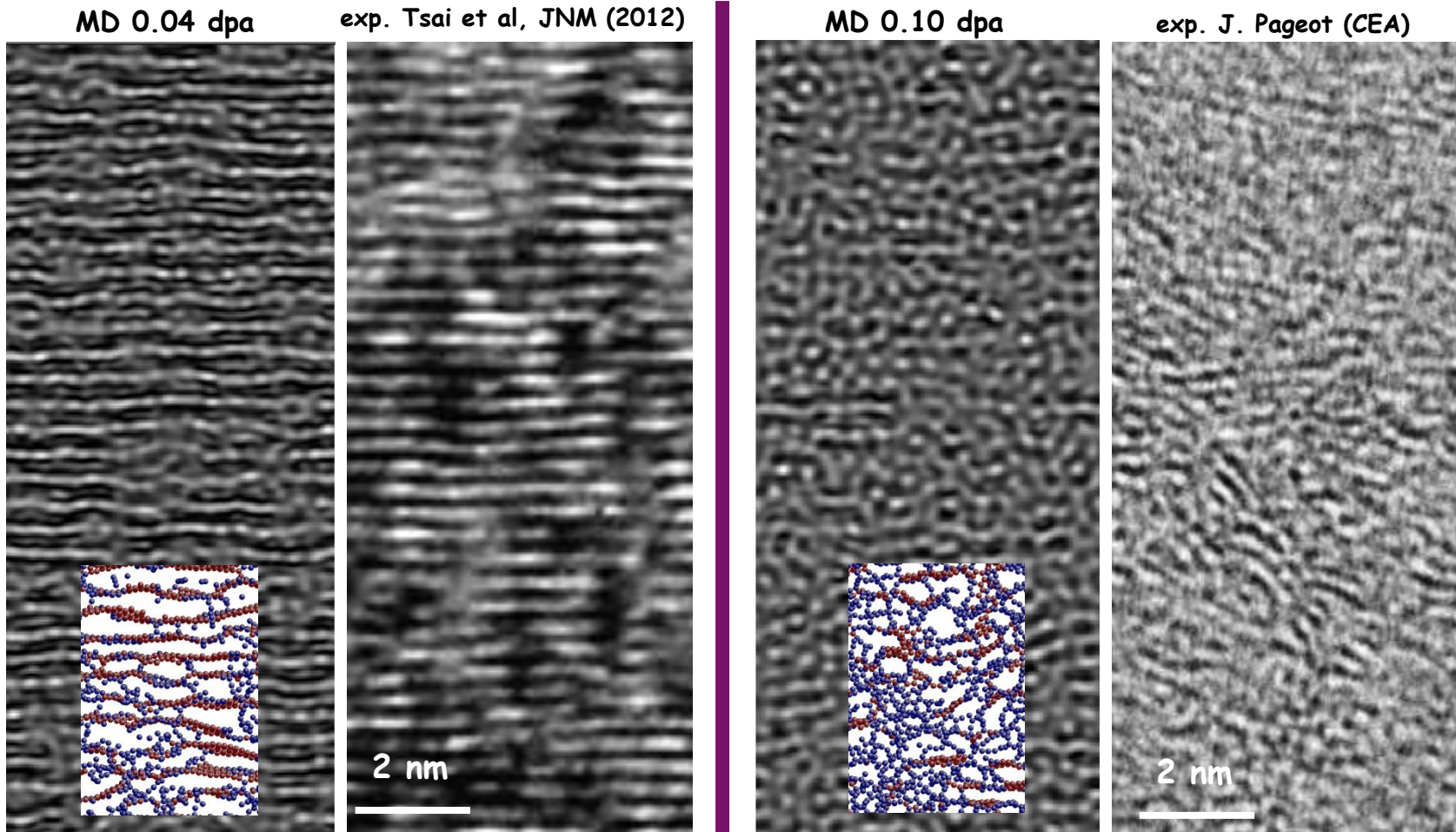
2. Pinning on small disordered cluster and Wrinkling of graphene sheets

3. Growth of amorphous pockets

→ Amorphisation



## HRTEM from atomic simulations



**Common explanation:** Decrease of graphene sheet' size with increasing dose

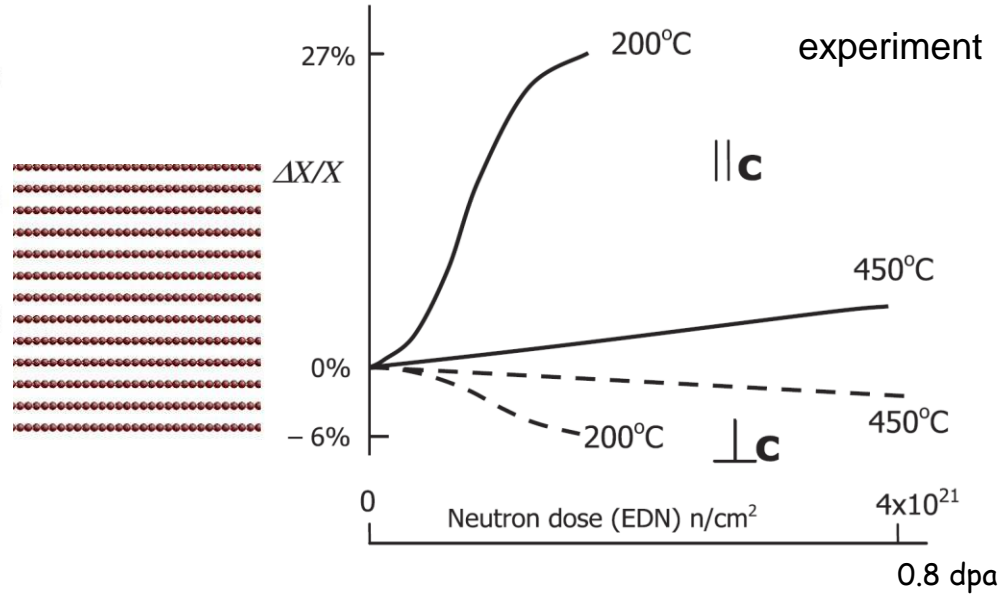
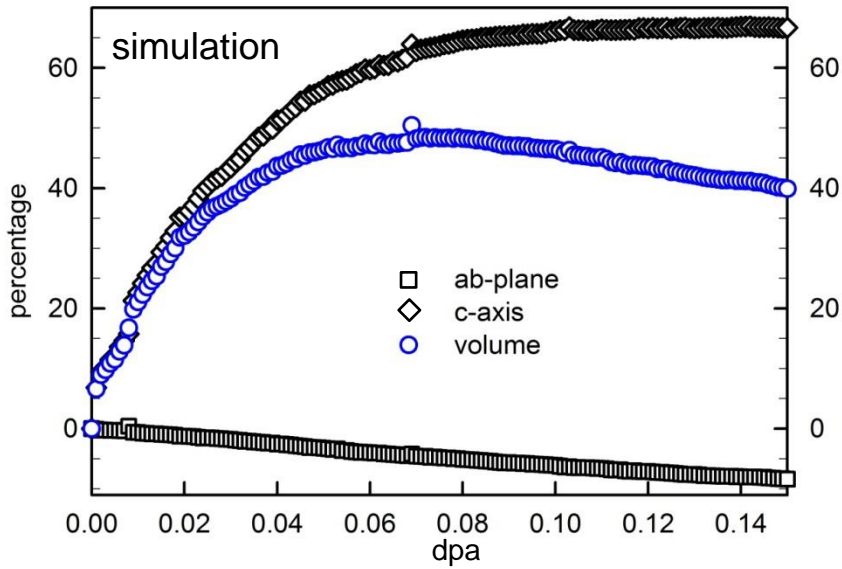
→ small graphene sheets in "noodles shape"

**What simulations show:** graphite amorphizes at 0.10 dpa

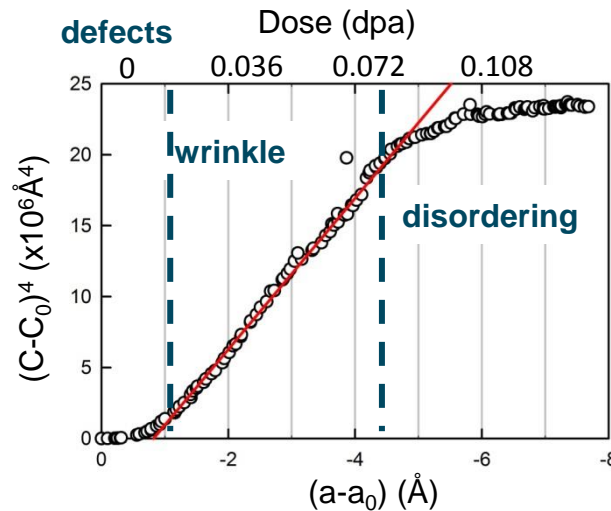
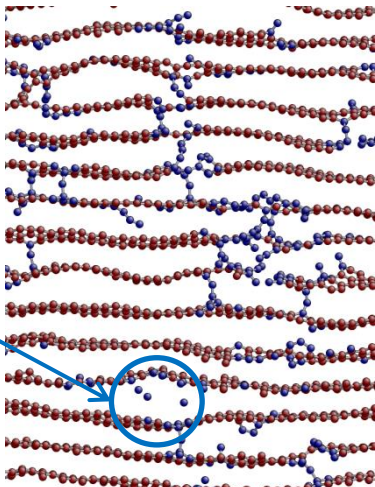


Graphene sheets in red, defects in blue

# Swelling under radiation



Expansion along the c-axis and shrinking of the graphene sheets



Wrinkling of graphene sheets:

$$c^4 \propto a$$



Tapasztó 2012 Nature Physics Letters1

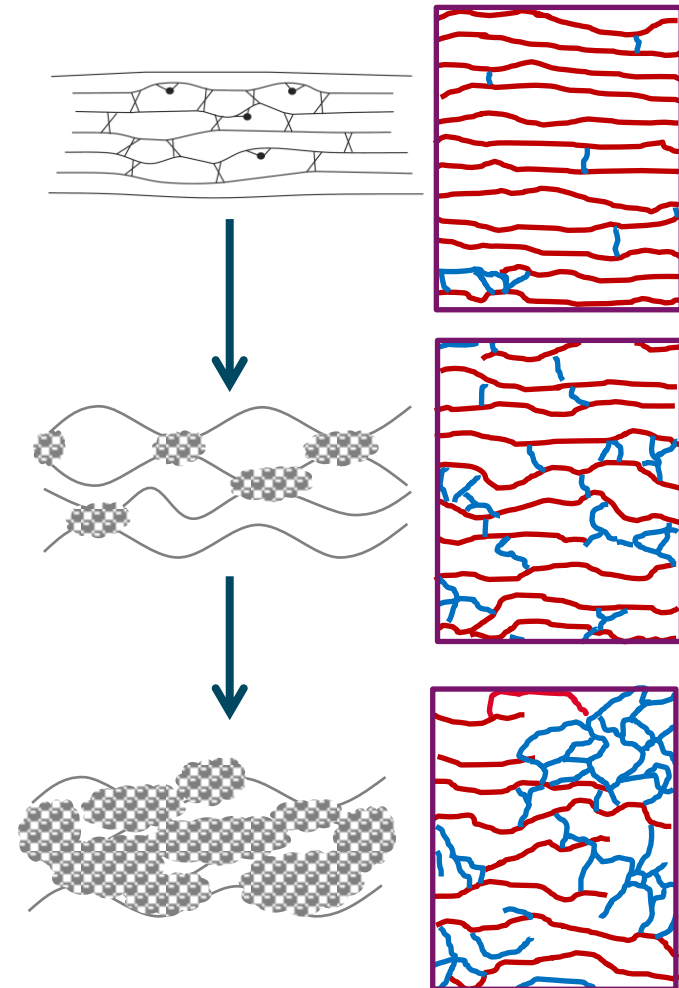
**Primary Damage:** Displacement Cascades

- Point Defects (large variety)
- Localized along PKA track
- # Vacancies  $\approx$  # Interstitials  $\rightarrow$  Frenkel pairs

**Dose effects:** Frenkel Pair Accumulation method

- New scenario for Amorphisation in 3 steps:
  1. Point Defects
  2. Pinning + Wrinkling of graphene sheets
  3. Growth of amorphous pockets  $\rightarrow$  Amorphisation

- Swelling due to both defects + wrinkling of graphene sheets







Challenge project – C097073



# Thank you for listening

## Questions ?

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