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Evolution of graphite structure under irradiation: A new scenario

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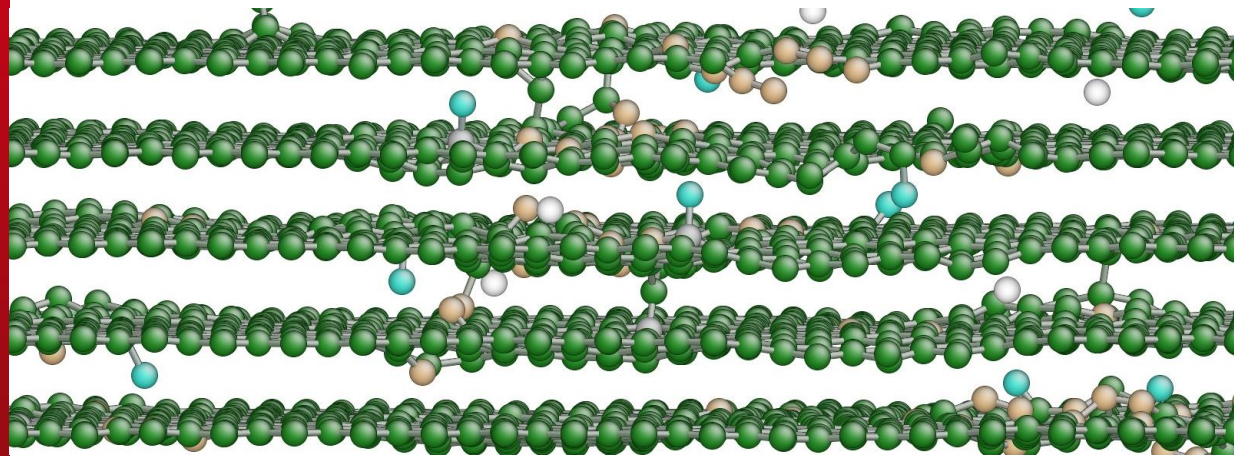
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EVOLUTION OF GRAPHITE STRUCTURE UNDER IRRADIATION: A NEW SCENARIO

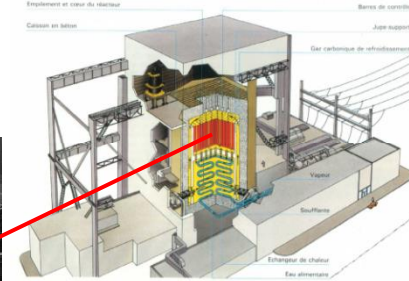


Alain Chartier, Laurent Van Brutzel

Framework: decommissioning of graphite from "UNGG"

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

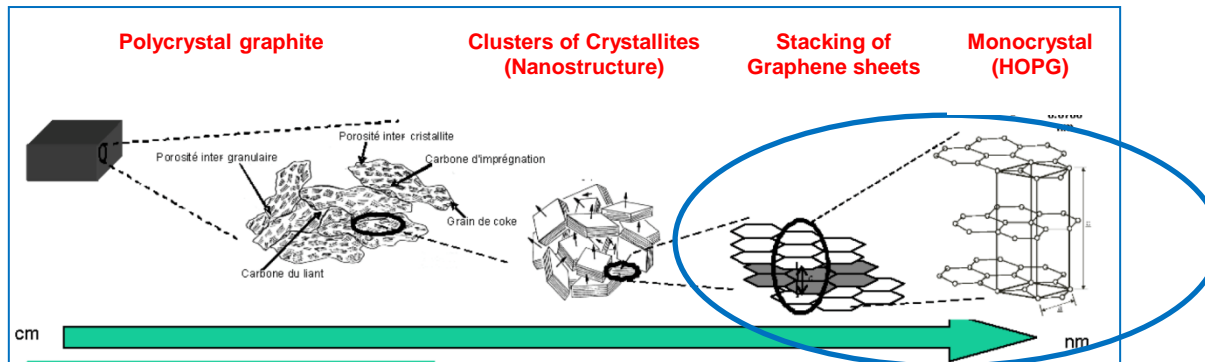
i-graphite contains ^{14}C & ^{36}Cl ($\frac{1}{2}$ life 5 500 & 3×10^5 years)



Foreseen Solutions:

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

interaction: graphite \leftrightarrow H_2O , O_2 , CO_2 ...
 depends on the localization of ^{14}C & ^{36}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)

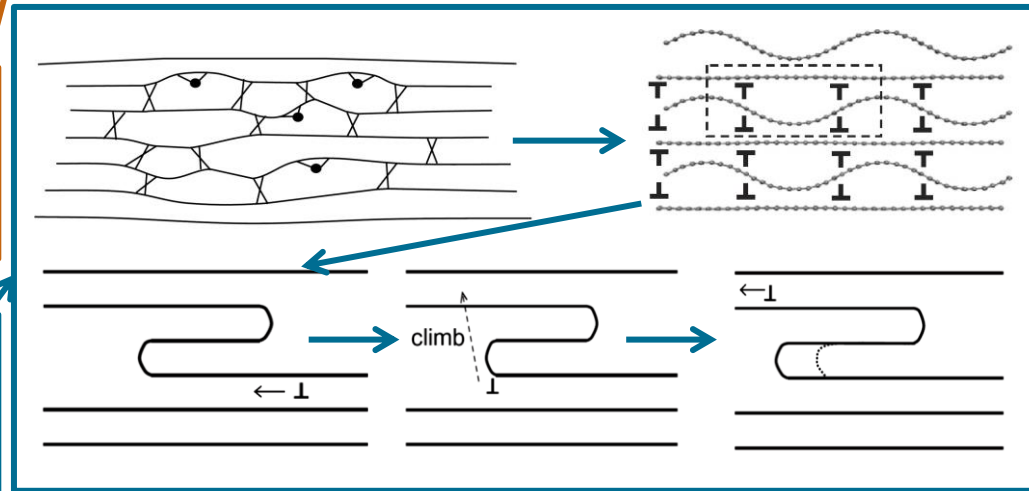
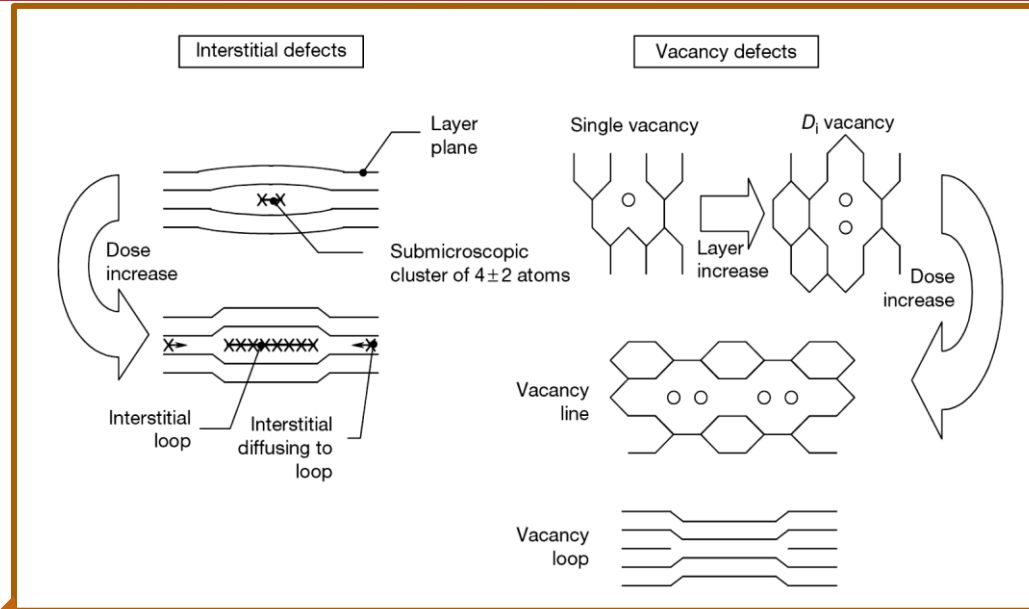
Marsden, Burchell and Fachinger (2012)

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

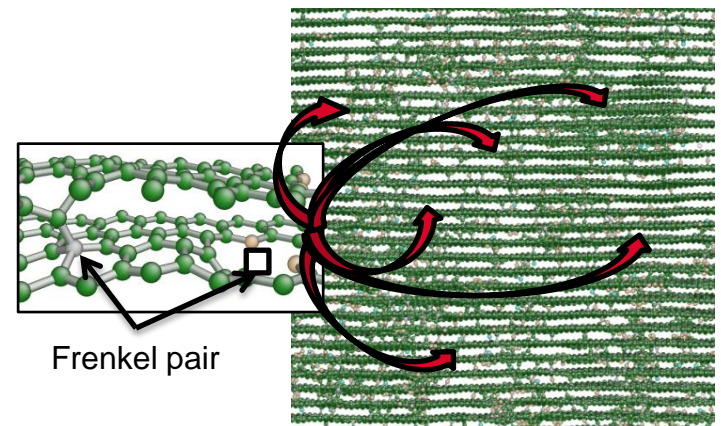
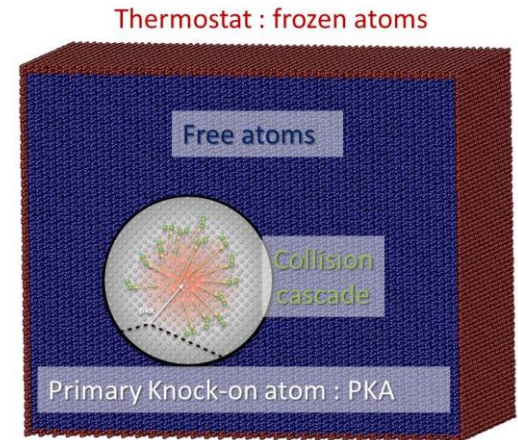
 $E_{PKA} = 0.5 \rightarrow 10 \text{ keV}$

T = 300 - 1000 K

Statistics: 16 cascades / E_{PKA}

Dose Effects: Point Defects Accumulation

Creation of random Frenkel pairs

Dose rate: 10^{10} 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

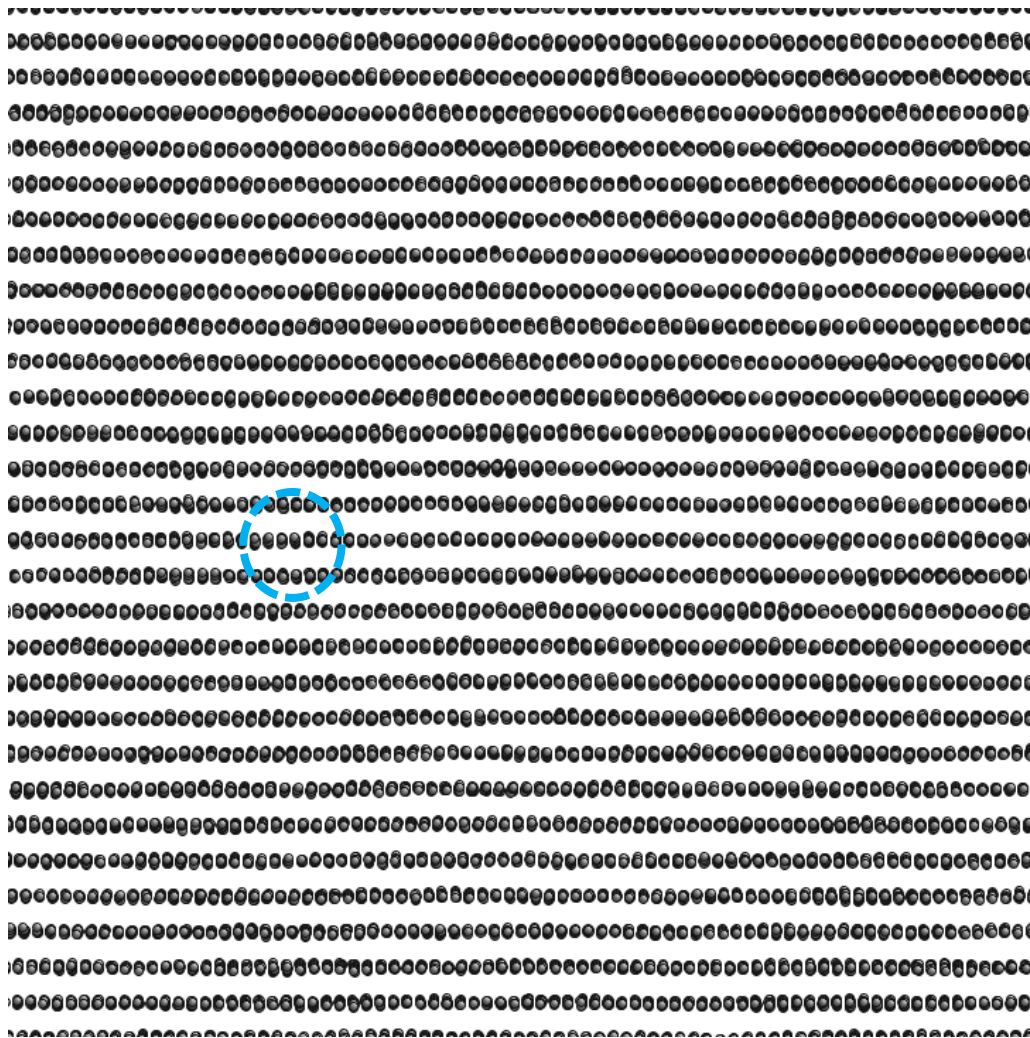
Three Stages:

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

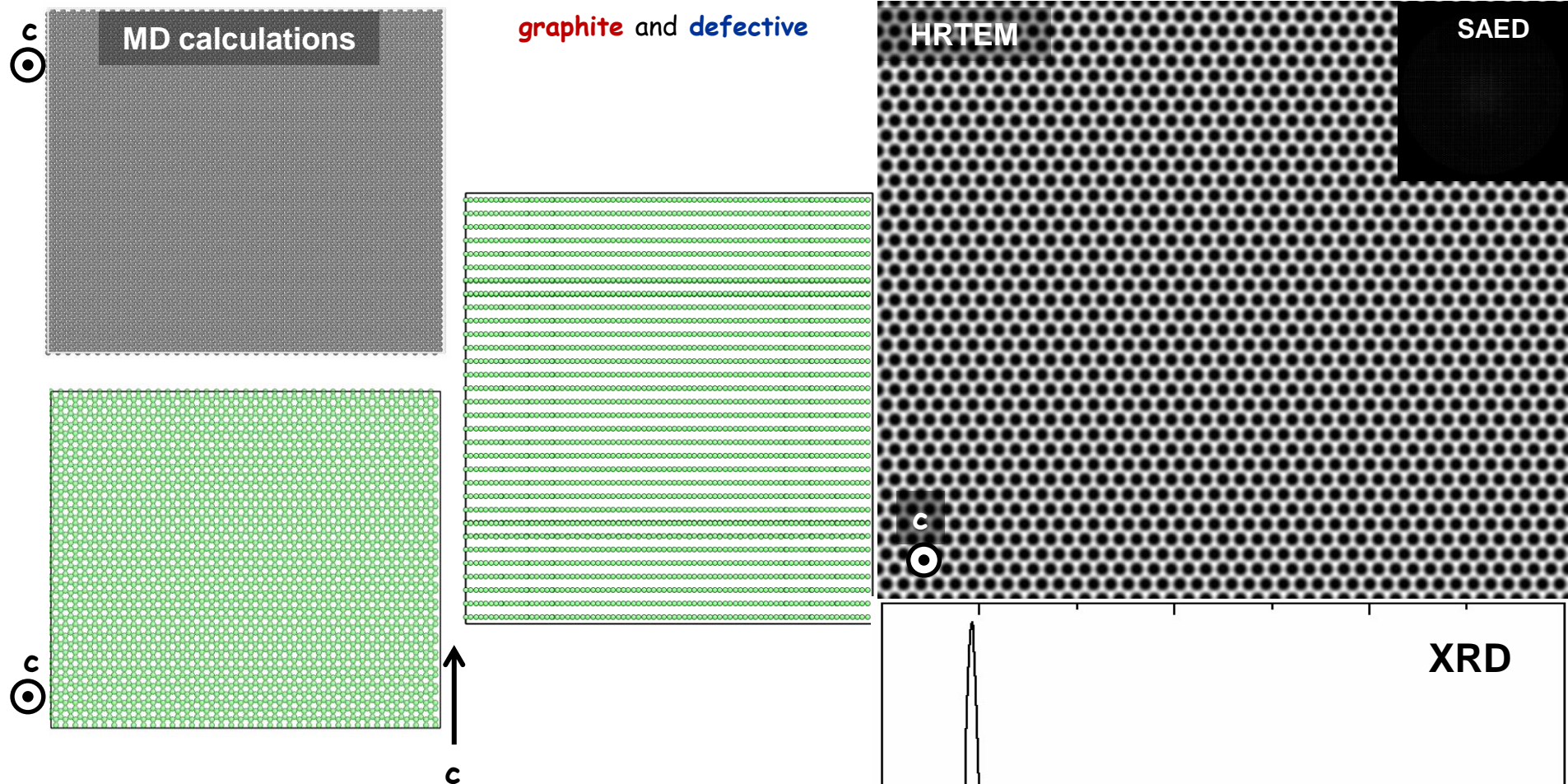
Damage:

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

→ Point Defect Accumulation
method

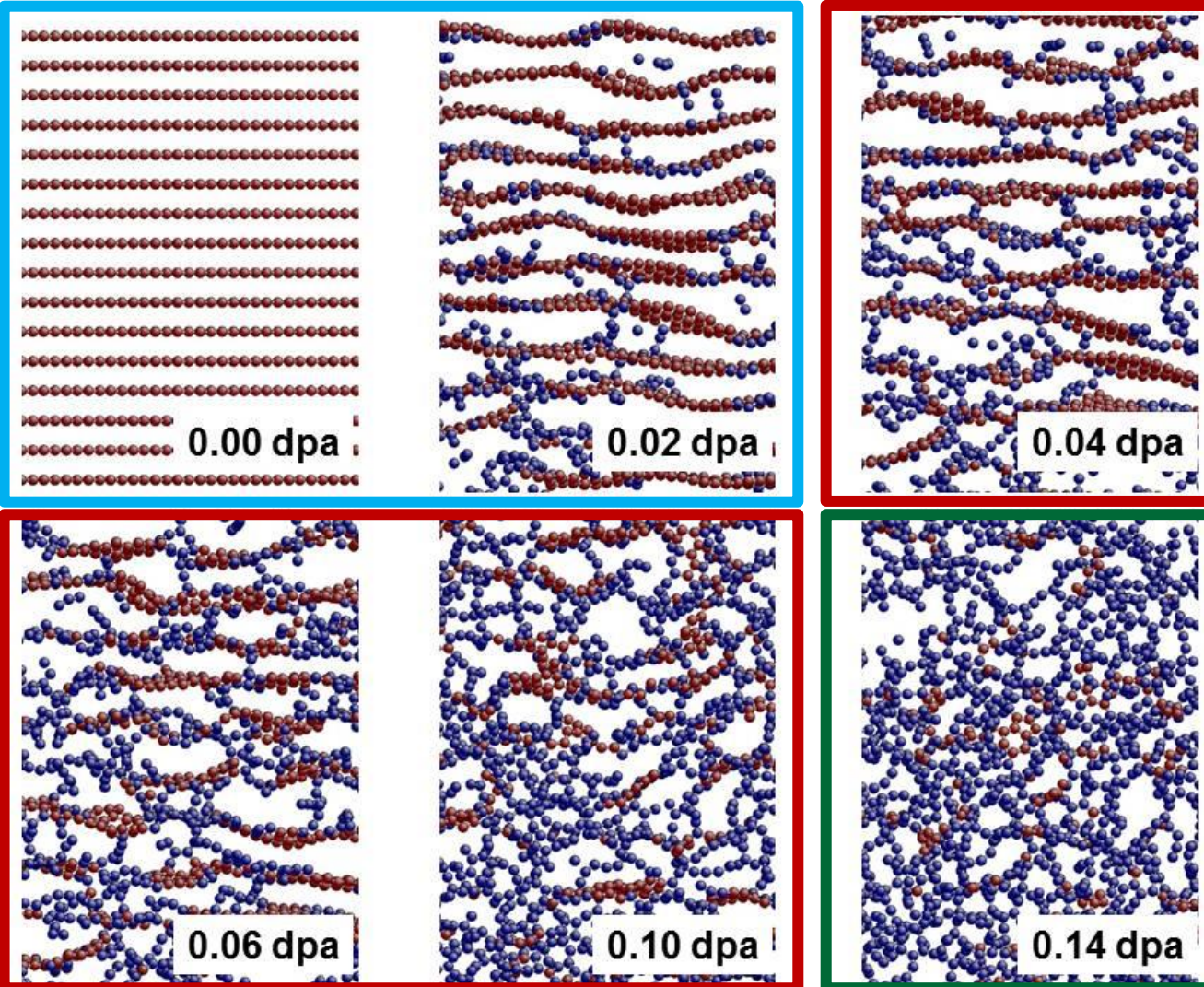


Dose effect from MD – Analysis from curvature criterion, HRTEM, SAED and XRD calculations



- 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)

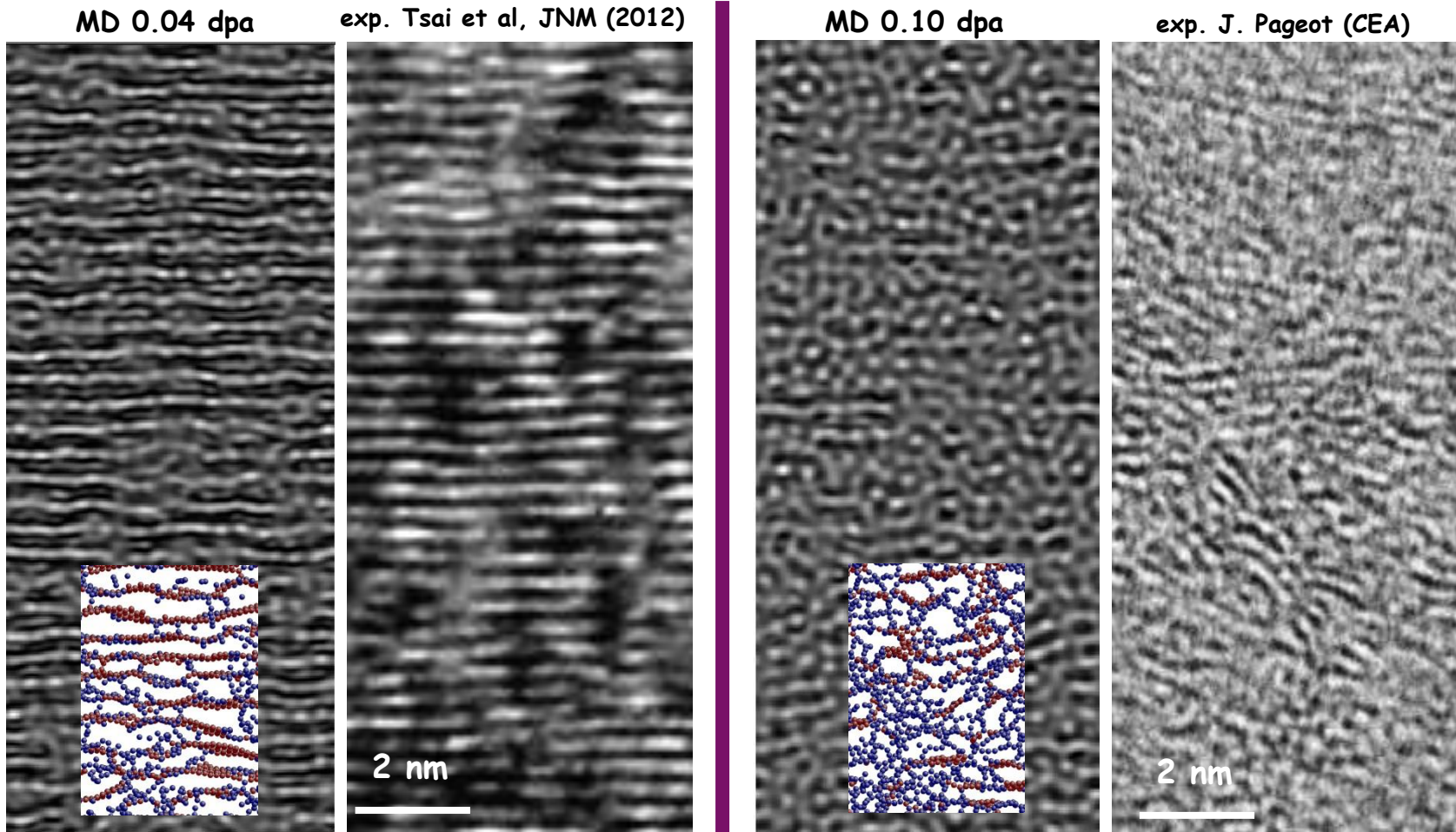
Perfect graphene sheets in red and point defects in blue



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



Graphene sheets in red, defects in blue

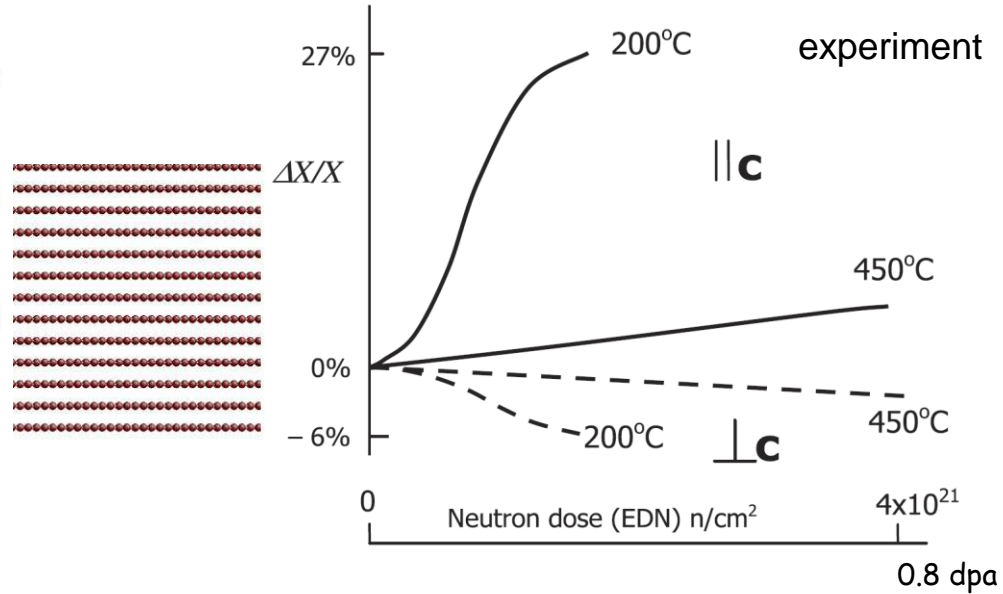
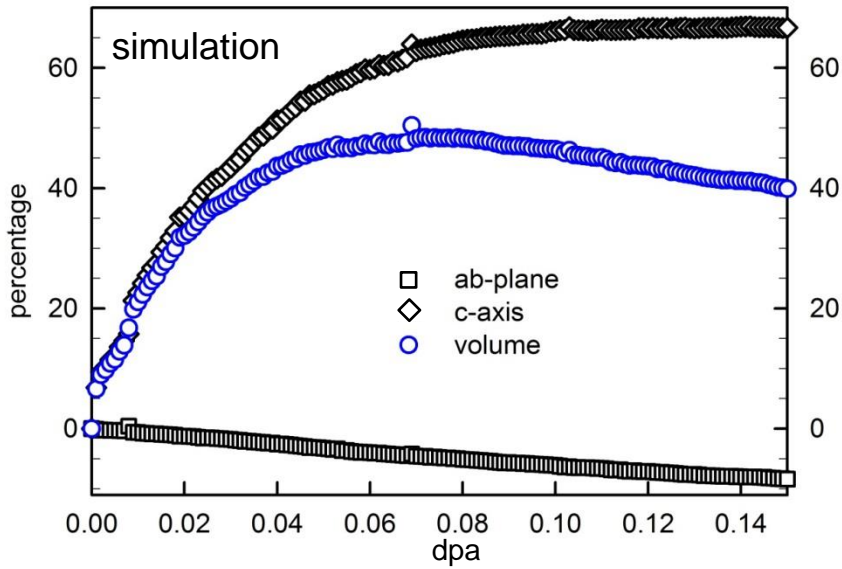
Common explanation: Decrease of graphene sheet' size with increasing dose

→ small graphene sheets in "noodles shape"

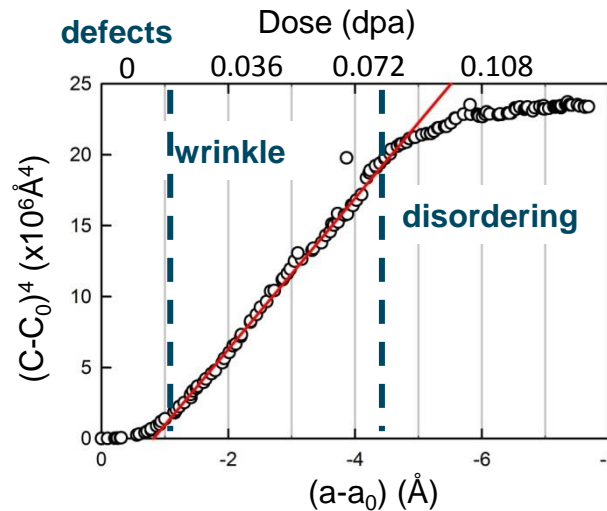
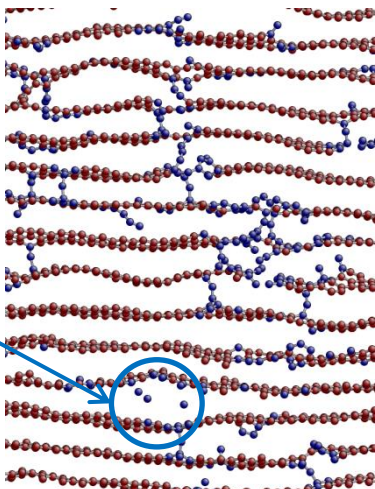
What simulations show: graphite amorphizes at 0.10 dpa



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

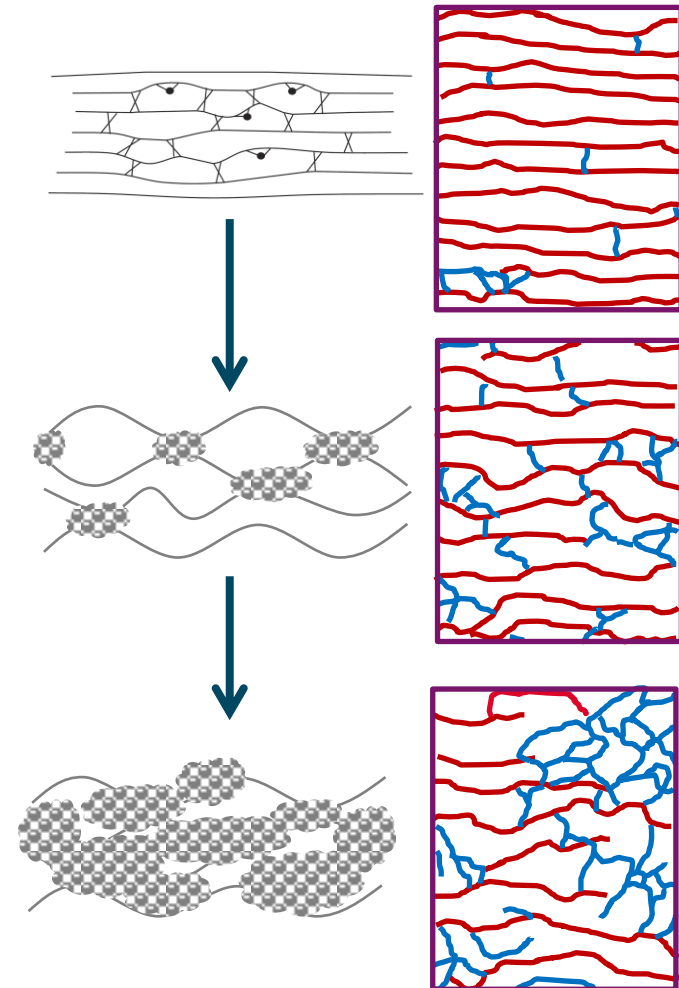
Primary Damage: Displacement Cascades

- 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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Commissariat à l'énergie atomique et aux énergies alternatives

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