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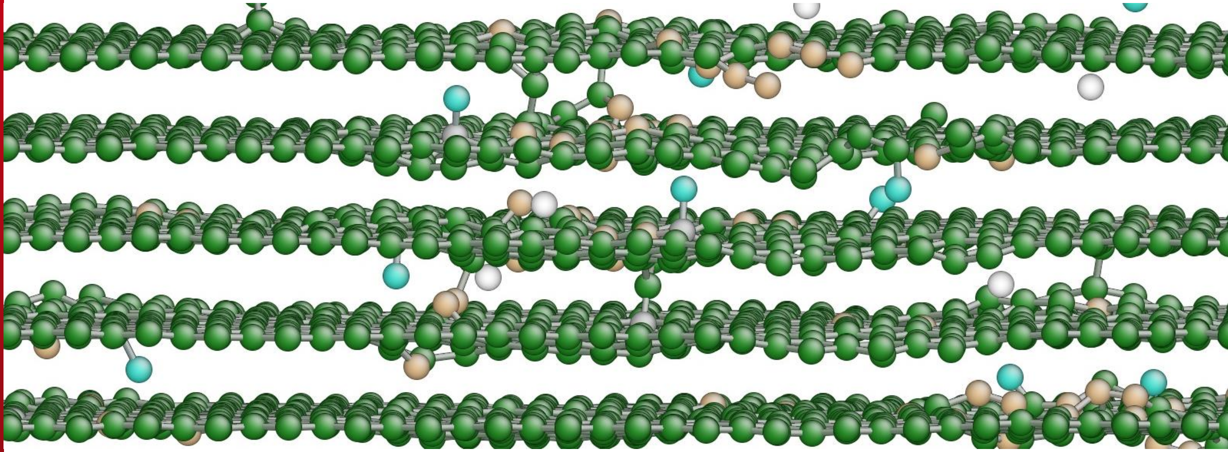
EVOLUTION OF GRAPHITE STRUCTURE UNDER IRRADIATION: A NEW SCENARIO



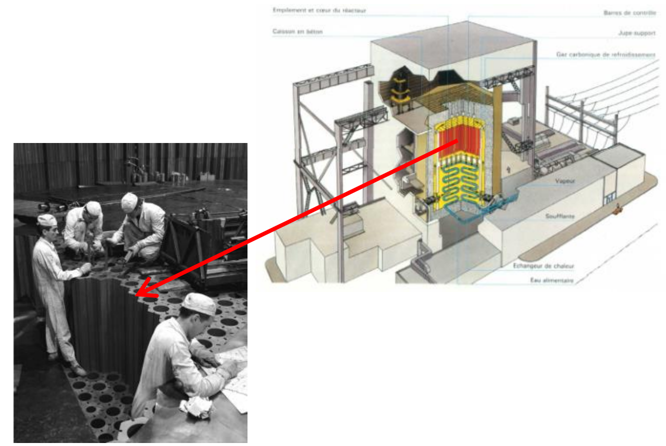
Alain Chartier, Laurent Van Brutzel

Irradiated graphite in graphite-gas nuclear reactors

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 (½ life 5 500 & 3×10^5 years)

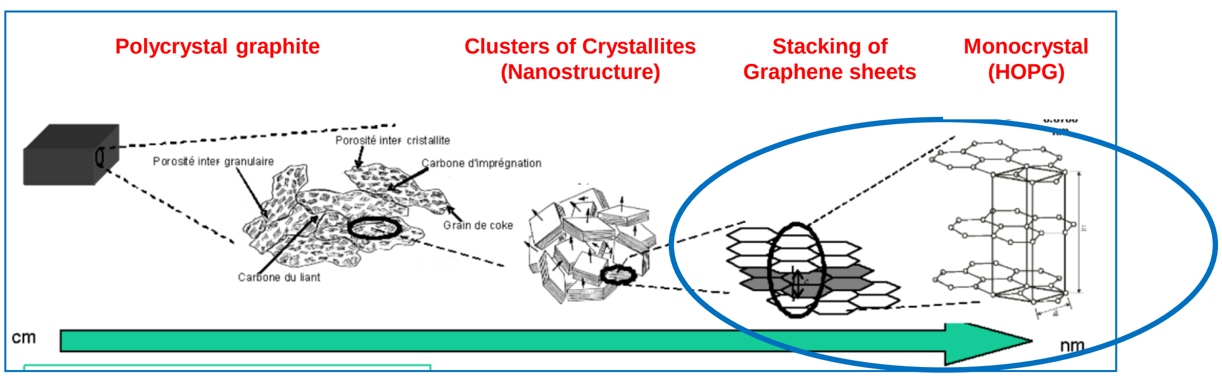


Foreseen Solutions:

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

interaction: graphite ↔ H_2O, O_2, CO_2…
depends on the localization of ^{14}C & ^{36}Cl after irradiation

- Graphite microstructure evolution under 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)

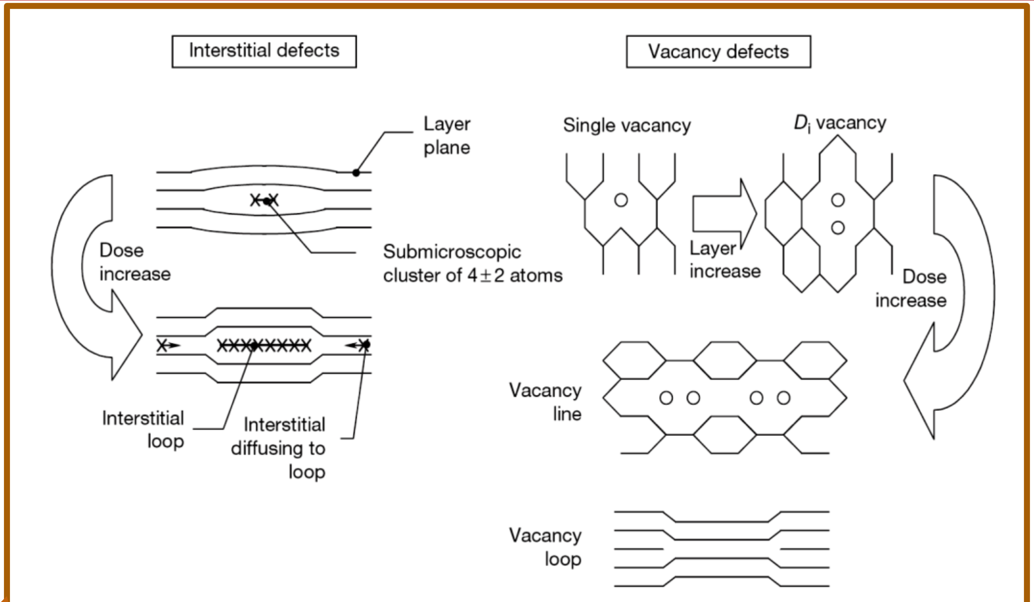
Marsden, Burchell and Fachinger (2012)

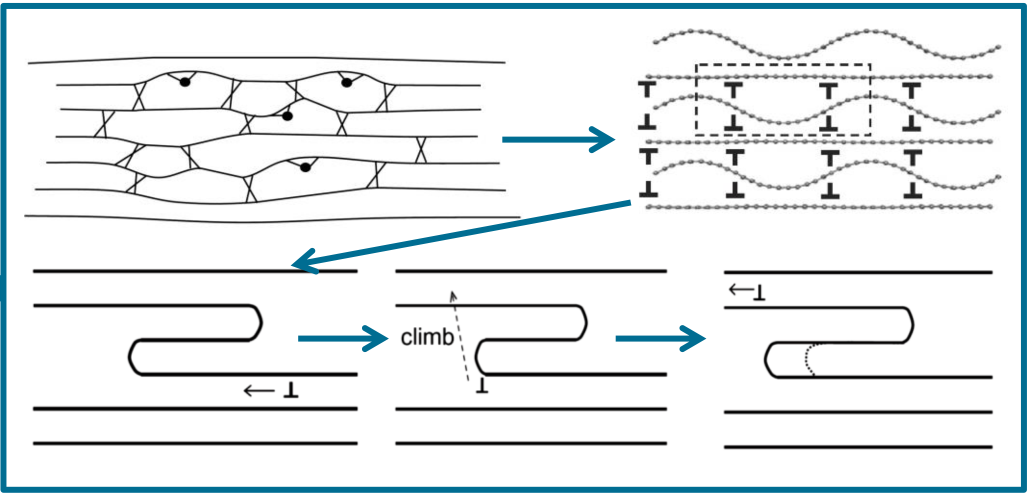
However, few data on Primary Damage State

- 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)

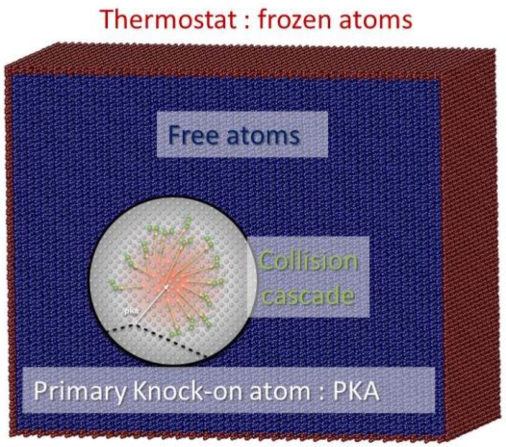




Modeling of irradiations

Study of Primary Damage with Molecular Dynamics

Code: LAMMPS
Empirical potential: LCBOP (bond-order)

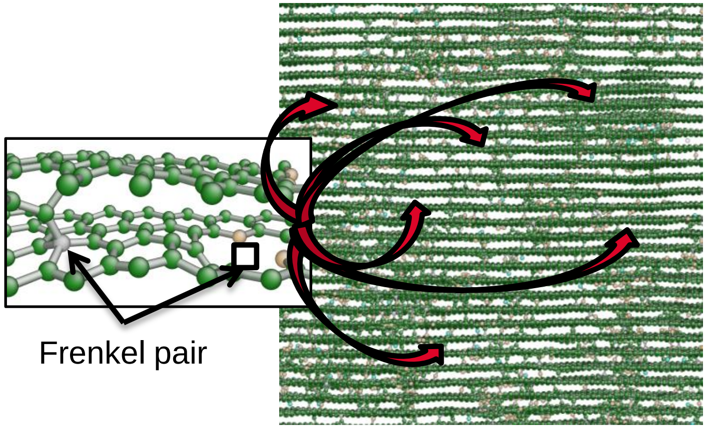


Primary Damage: **Displacement Cascades**

- Primary Knock-on Atom: C
- E_{PKA} = 0.5 → 10 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 → 1 dpa
- 300 – 1000 K (relaxation NPT) → Swelling



Primary damage in graphite

Example: Cascade with 5 keV PKA

Projectile C - direction [100] – 300 K

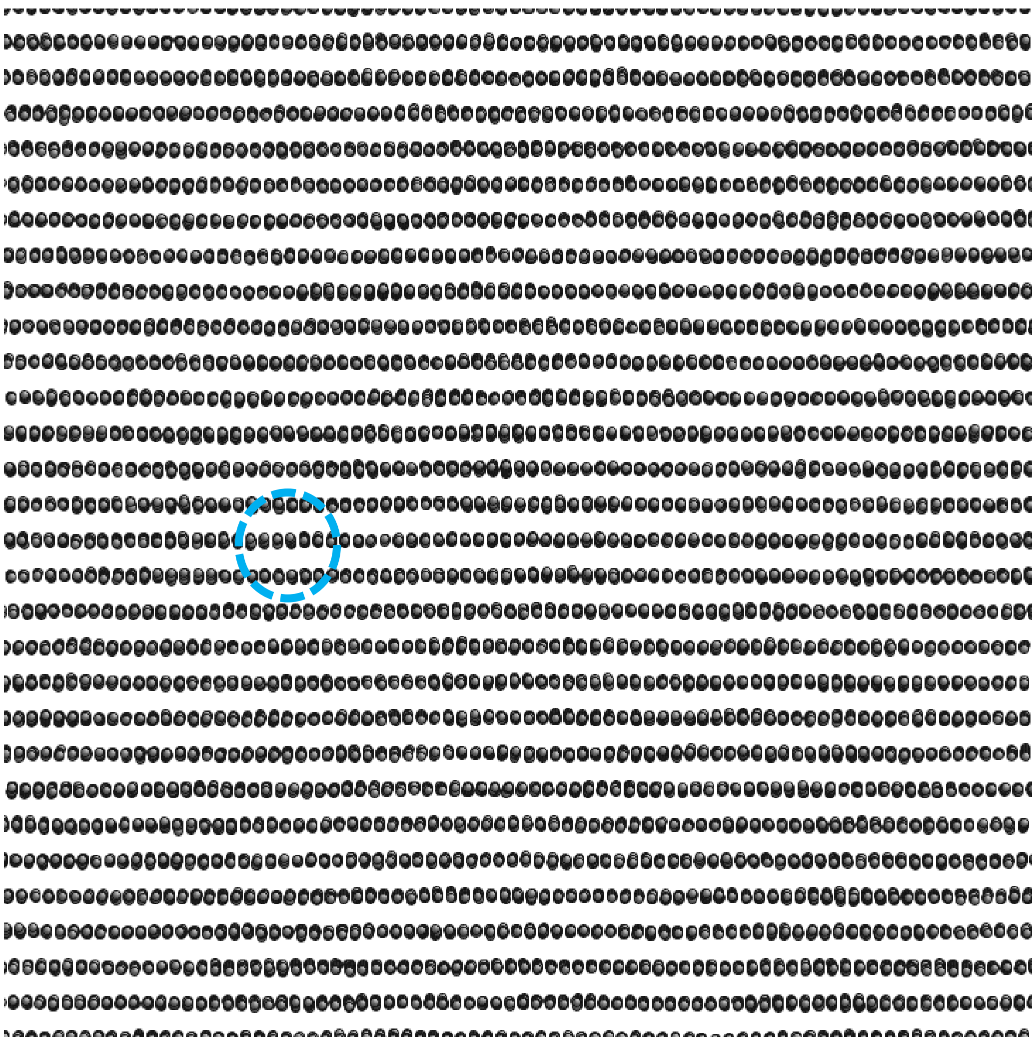
Three Stages:

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

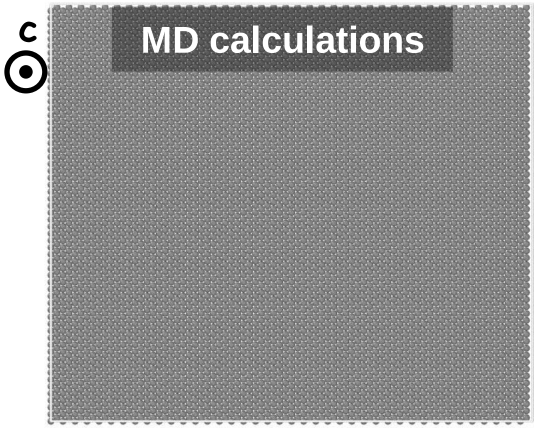
Damage:

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

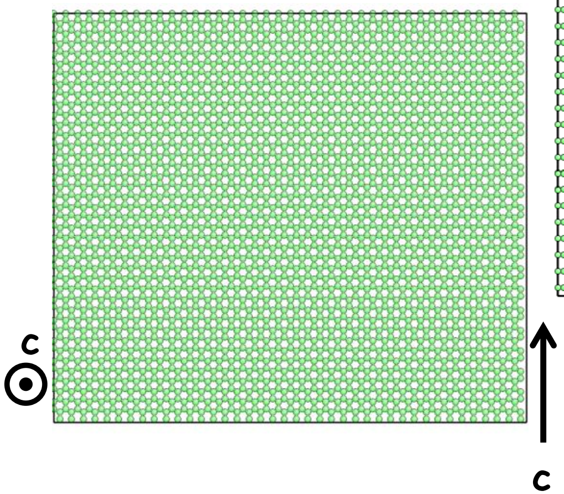
→ Point Defect Accumulation method

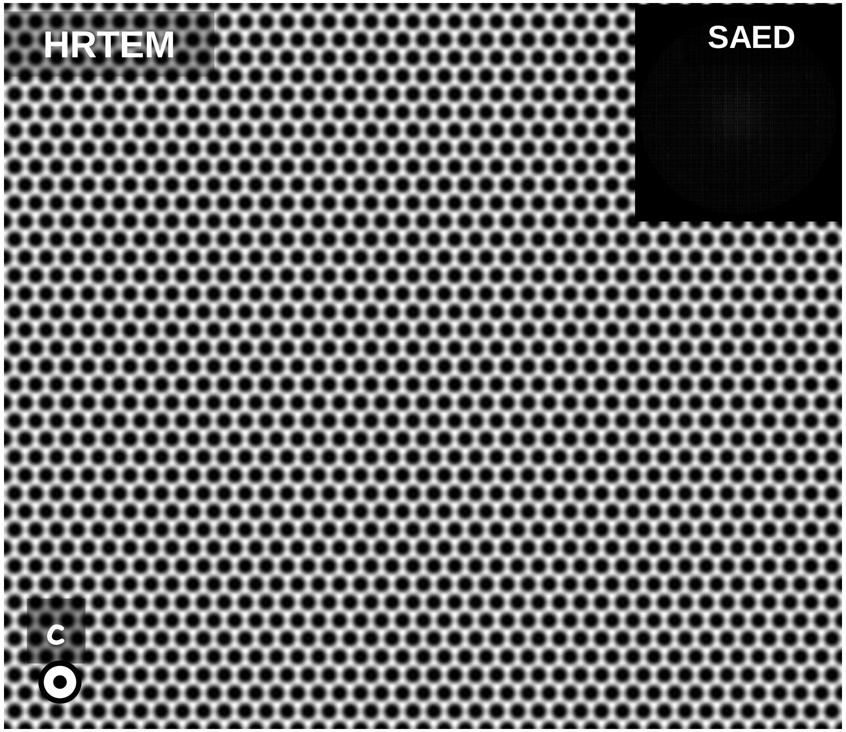


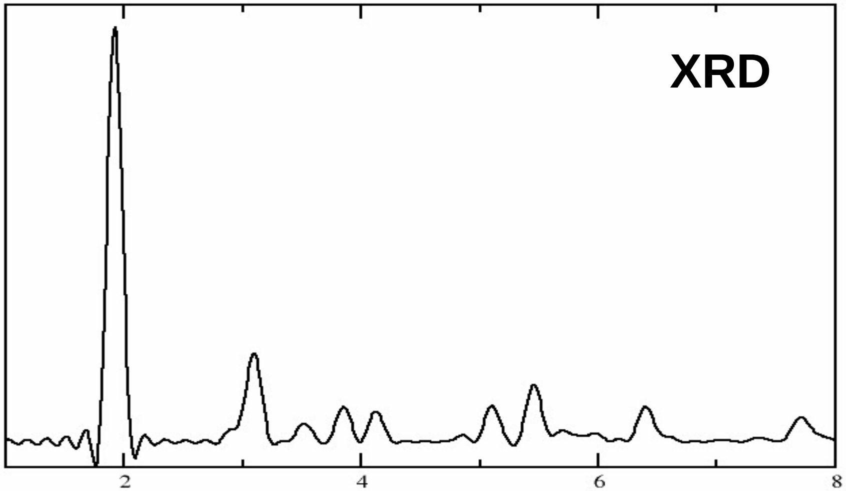
Dose effect from MD – Analysis from curvature criterion, HRTEM, SAED and XRD calculations



graphite and defective







→ Vizualization of defects in graphene planes (MD and HRTEM)

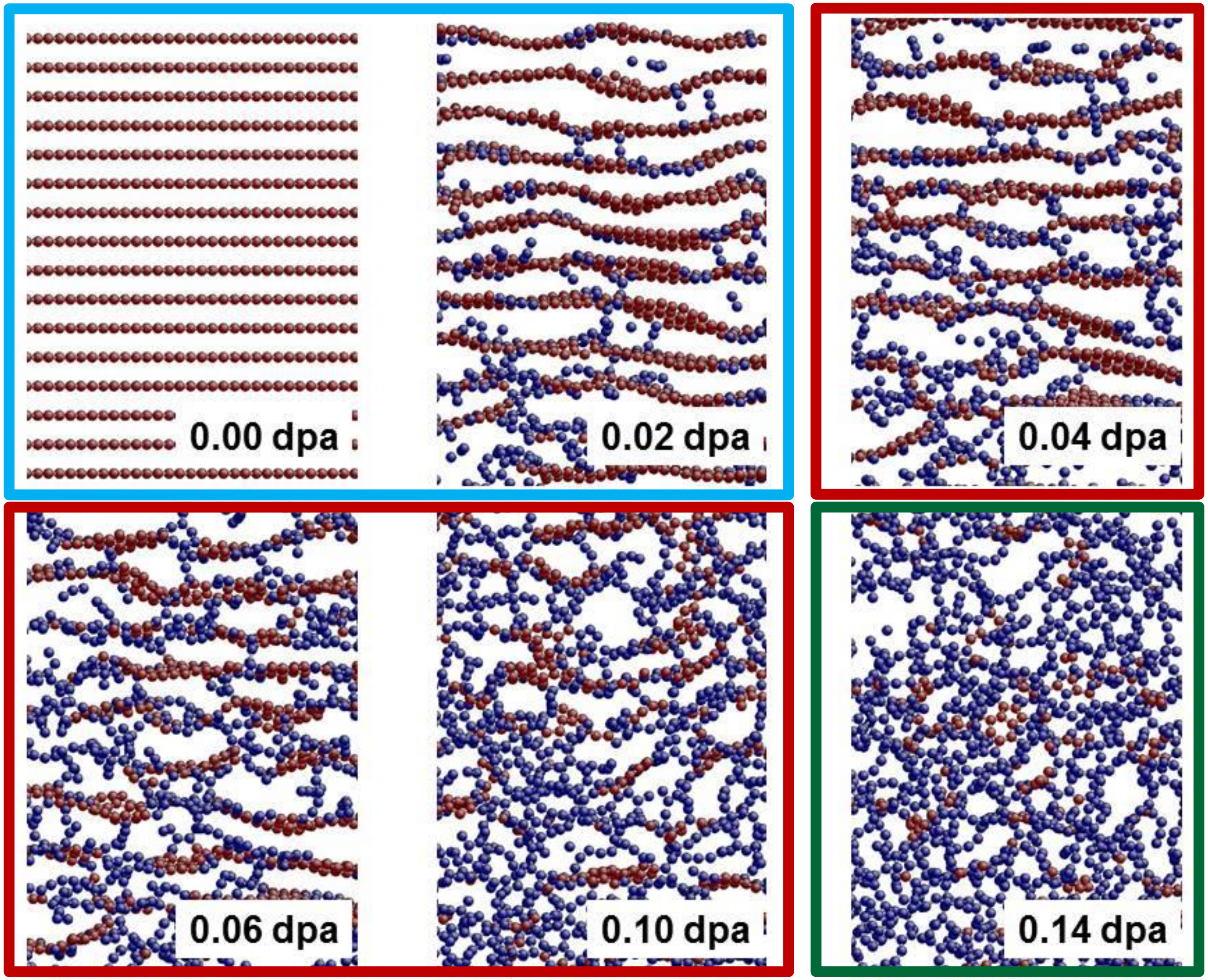
→ Vizualization of wrinkles (MD analysis)

→ Swelling from size of box (not easy from XRD)

→ amorphization at 0.10 dpa (SAED and XRD)

Dose effect modeling

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

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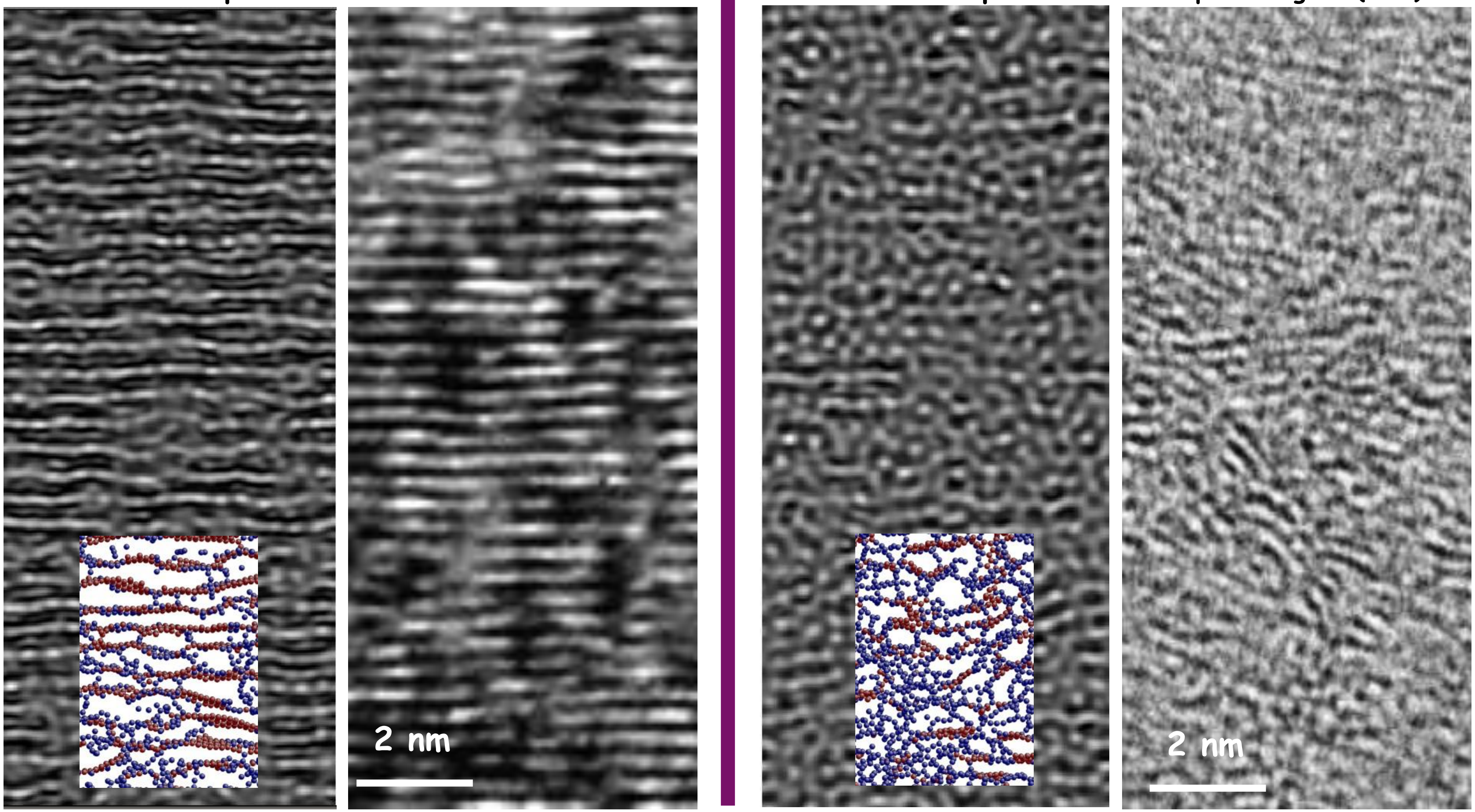
HRTEM from atomic simulations

MD 0.04 dpa | exp. Tsai et al, JNM (2012) | MD 0.10 dpa | exp. J. Pageot (CEA)



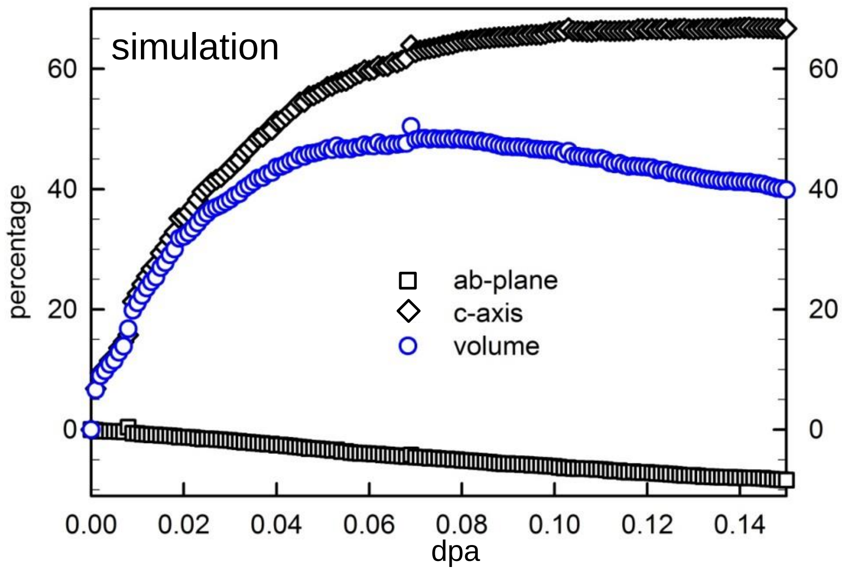
Graphene sheets in red, defects in blue

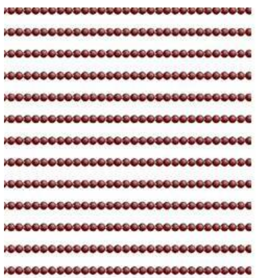
Common explanation: Decrease of graphene sheet' size with increasing dose

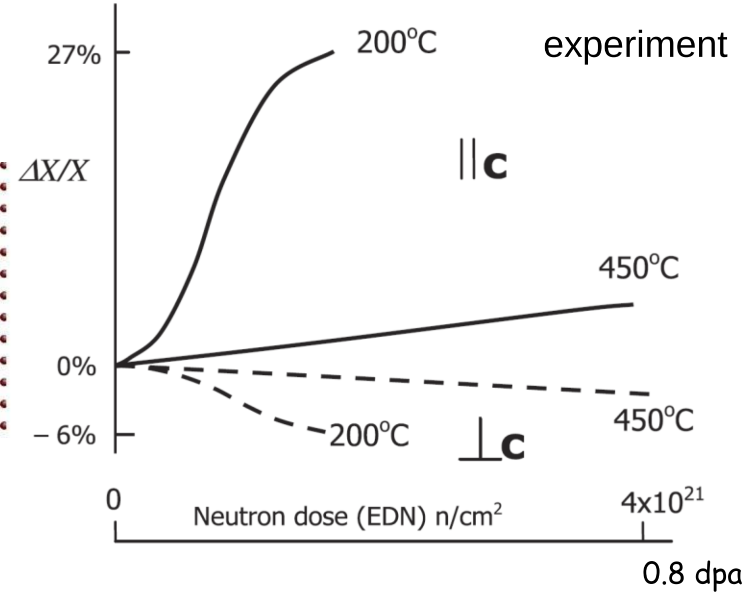
→ small graphene sheets in "noodles shape"

What simulations show: graphite amorphizes at 0.10 dpa

Swelling under radiation

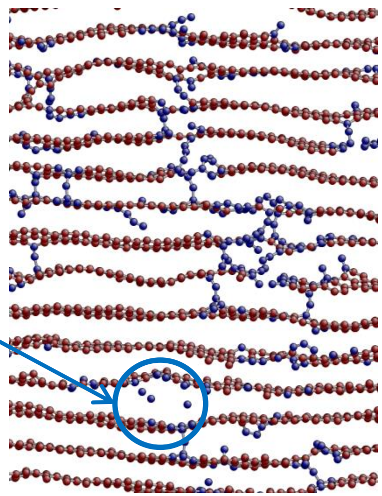


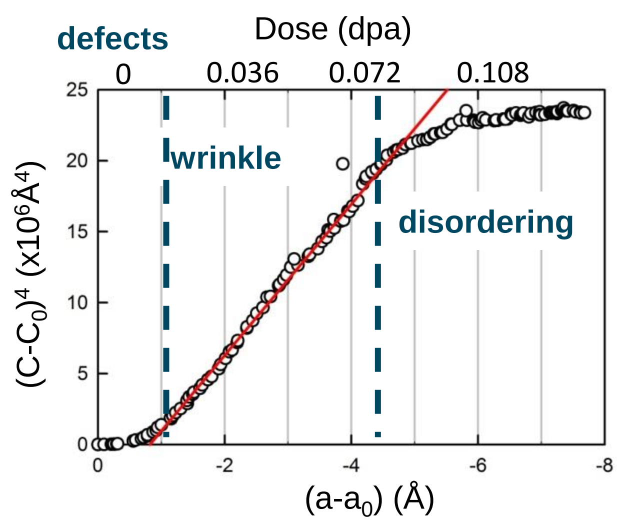




Expansion along the c-axis and shrinking of the graphene sheets

Interstitials pushing graphene sheets





Wrinkling of graphene sheets:

$c^4 \propto a$

Tapaszto 2012 Nature Physics Letters1

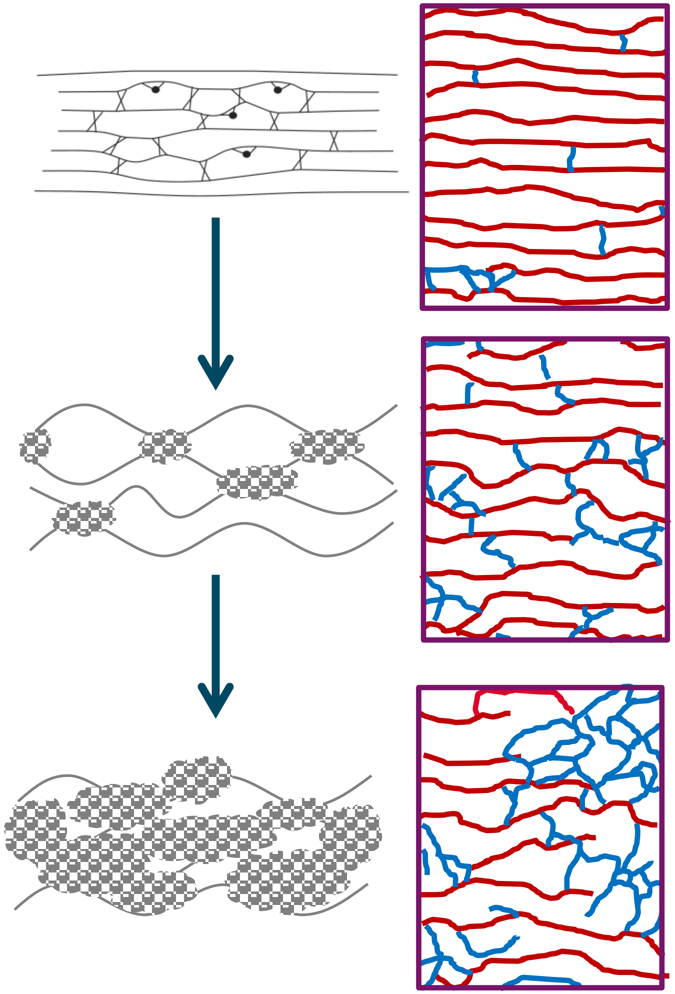
Summary - Conclusion

Primary Damage: Displacement Cascades

- Point Defects (large variety)
- Localized along PKA track
- # Vacancies ≈ # Interstitials → 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 → Amorphisation
- Swelling due to both defects + wrinkling of graphene sheets



A. Chartier, L. Van Brutzel, B. Pannier, and Ph. Baranek, Carbon 91 (2015) 395.

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Challenge project – C097073

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Thank you for listening

Questions ?

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