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University of BRISTOL

UNIVERSITY OF OXFORD

UNIGRAF
Understanding and Improving Graphite for Nuclear Fission

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Oxford: James Marrow

SINOSTEEL

GSI Helmholtzzentrum für Schwerionenforschung GmbH

OAK RIDGE National Laboratory

清華大學 Tsinghua University

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HTR-PM Commercial Demo Reactor Update

- 14. 09. 2016: Second pressuriser installed.

- 19.06. 2017: Successfully commissioned 220kV electrical transmission for HTR-PM

- 08.06.2017: All iso-graphite components had been installed for the 2nd reactor.
  - Core diameter: 3m
  - Height: 11.8m

- 30.07.2017: successfully commissioned turbine generators

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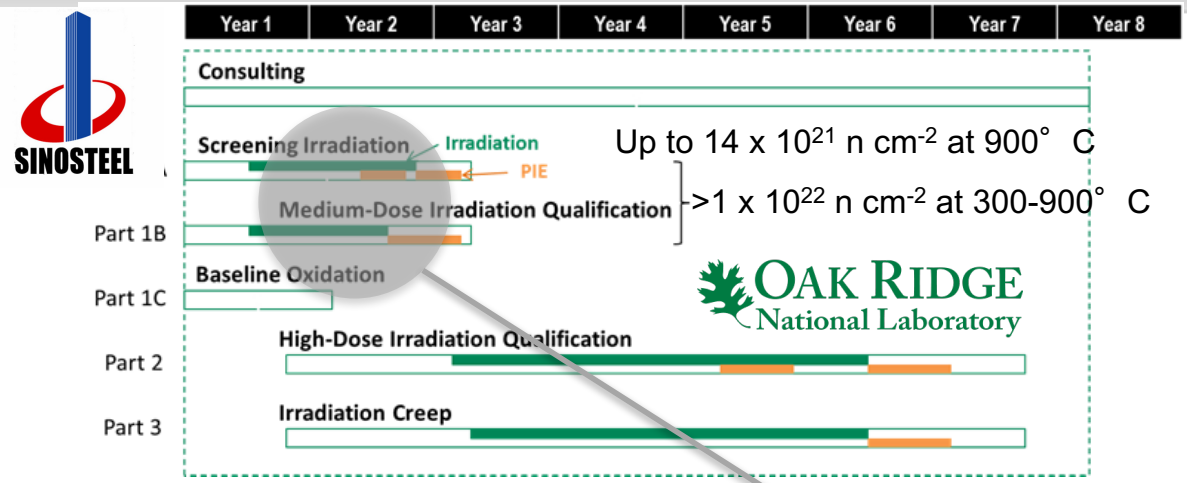
Opportunity and Methodology



Sinosteel/ORNL Irradiation Programme (Year 1 = 2015)

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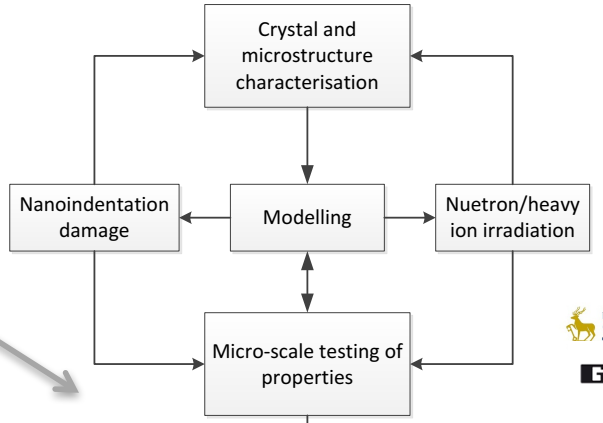
SINOSTEEL
- Producer of graphite for the Chinese HTR-PM programme,
- Funding the irradiations at ORNL to select graphites



Eight Graphites (different Filler and Binder)

- Characterization over length scales:
  - Dimensional change, Young's modulus, thermal expansion, tensile strength, toughness
  - HRTEM, nano-indentation, Raman, EELS
- Modelling at the meso-scale
  - MD atomistic simulations (up to ~50 nm^3) to predict physical and mechanical properties
- Testing at the meso-scale
  - In situ nano-indentation, pillar compression and Nano-XCT
  - In situ TEM testing with DIC and diffraction strain measurement

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Experimental nuclear graphite grades

Experimental nuclear graphite grades included in Sinosteel-ORNL irradiation programme.

- SNG342, SNG623, SNG742, SNG722, SNG7420, SNG3420, SNG545, SNG220.
- All iso-moulded; main difference in coke size, amount of binder, sources of raw materials, impregnation/graphitisation conditions, density, porosity.
- Most grades aim for HTGRs; a couple of grades for TMSR.

Typical graphite billets

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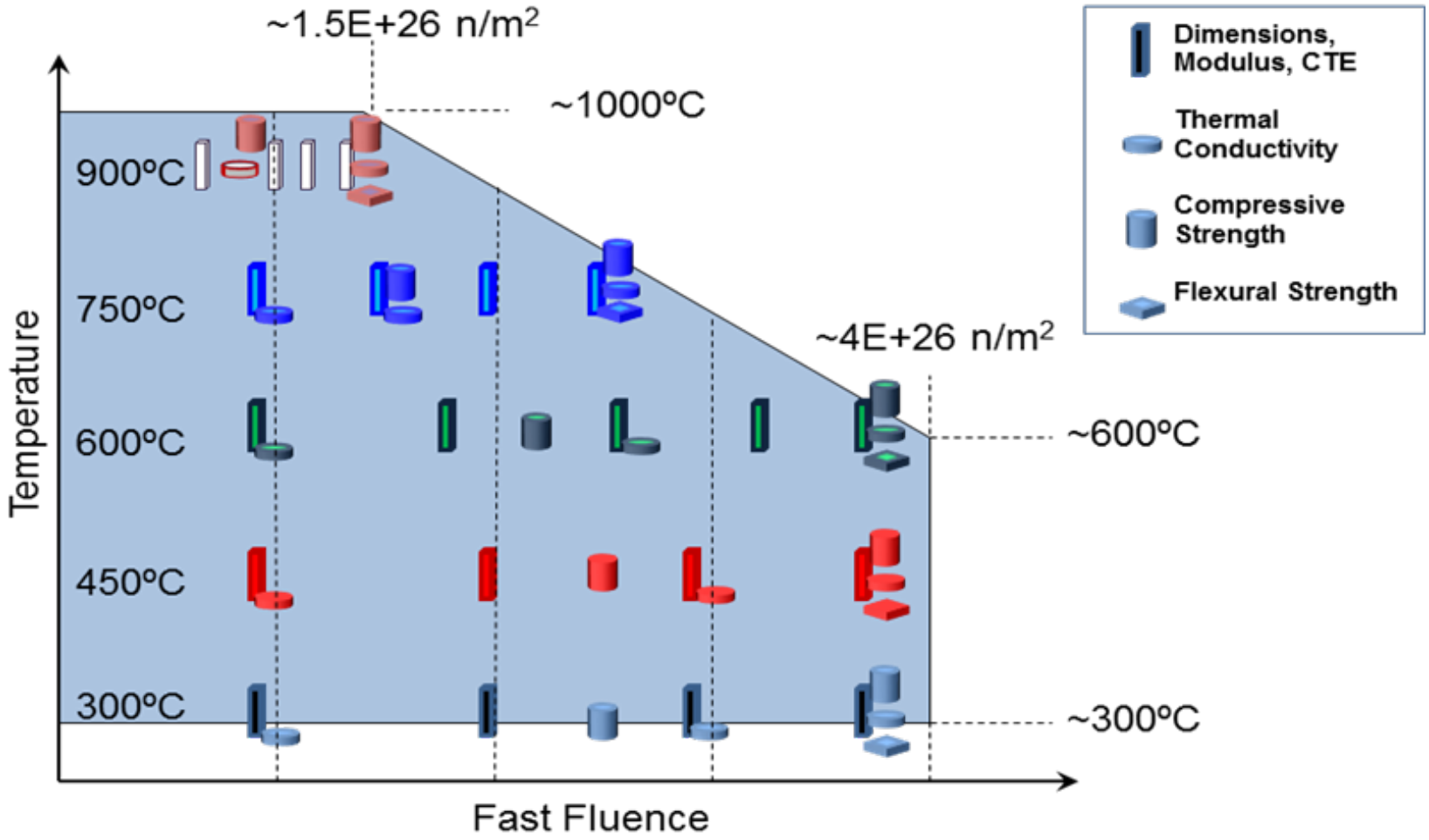
Neutron irradiation programme



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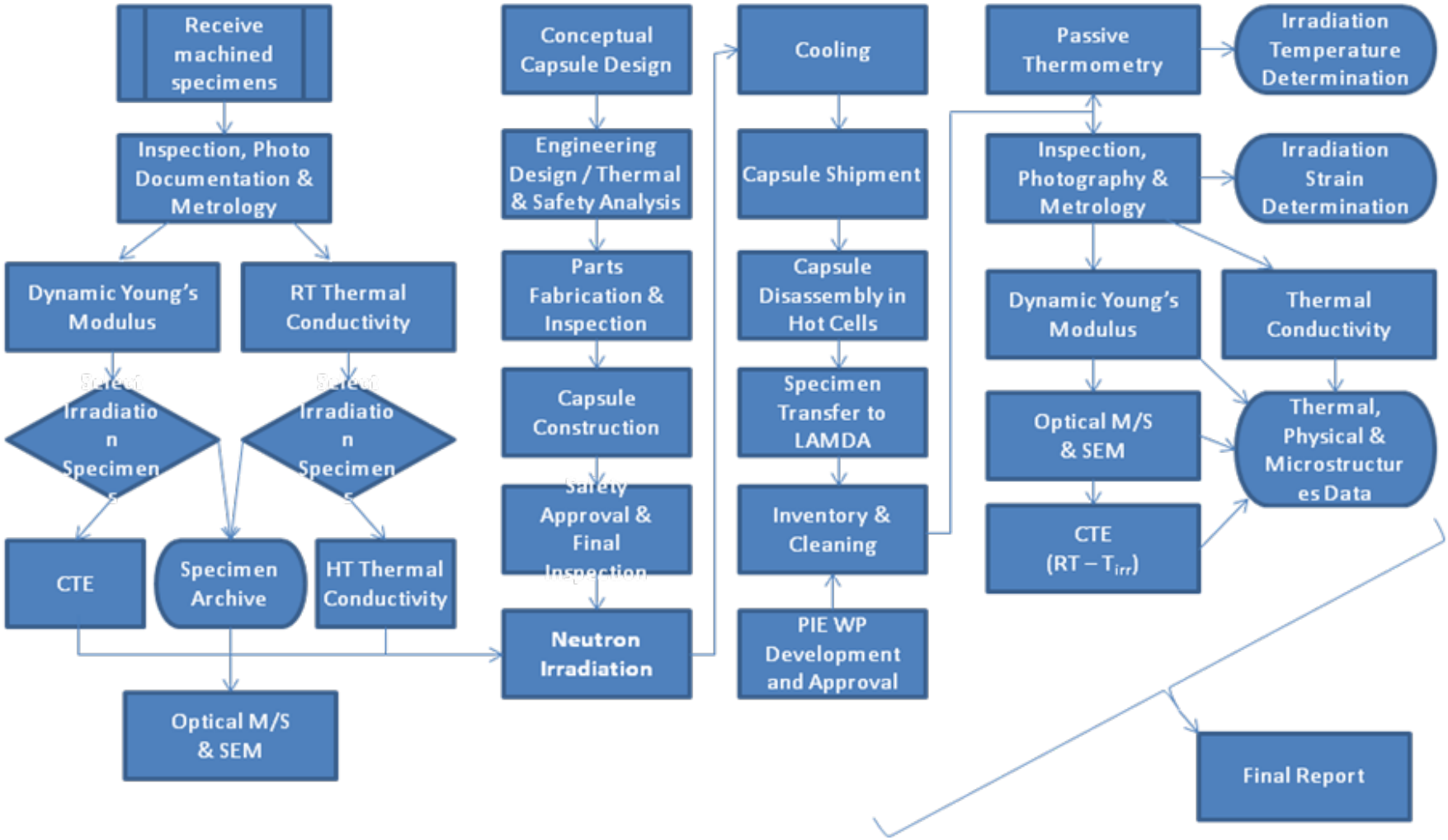
Neutron irradiation programme (cont.)



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Neutron irradiation timeline

- **Screening irradiation Phase – focus of UNIGRAF**
  - Irradiation completed (Irradiation at 900 ^{o}C with neutron fluence: 4.4, 4.5 & 8.1 X 10^{25} n/$m^{2)}$
  - PIE completed and report in preparation
  - Irradiated samples now accessible for UNIGRAF researchers
- **Medium dose irradiation phase 1B**
  - Most irradiation completed
  - Most PIE completed and data analysis in progress
  - Some irradiated samples accessible from 2018
- **Other samples will be available from 2019 and beyond**
  - High dose
  - creep

Heavy ion irradiation completed

Graphite grades	Au 5.9MeV/u	Ca 4.8MeV/u	C 5.9MeV/u	Sm 4.8MeV/u
	Fluence (i/cm^2)			
SNG342 SNG 623 SNG742	1e11	1e11	1e11	
	1e12	1e12	1e12	1e12
	1e13	1e13	1e13	
	5e13	5e13	5e13	5e13

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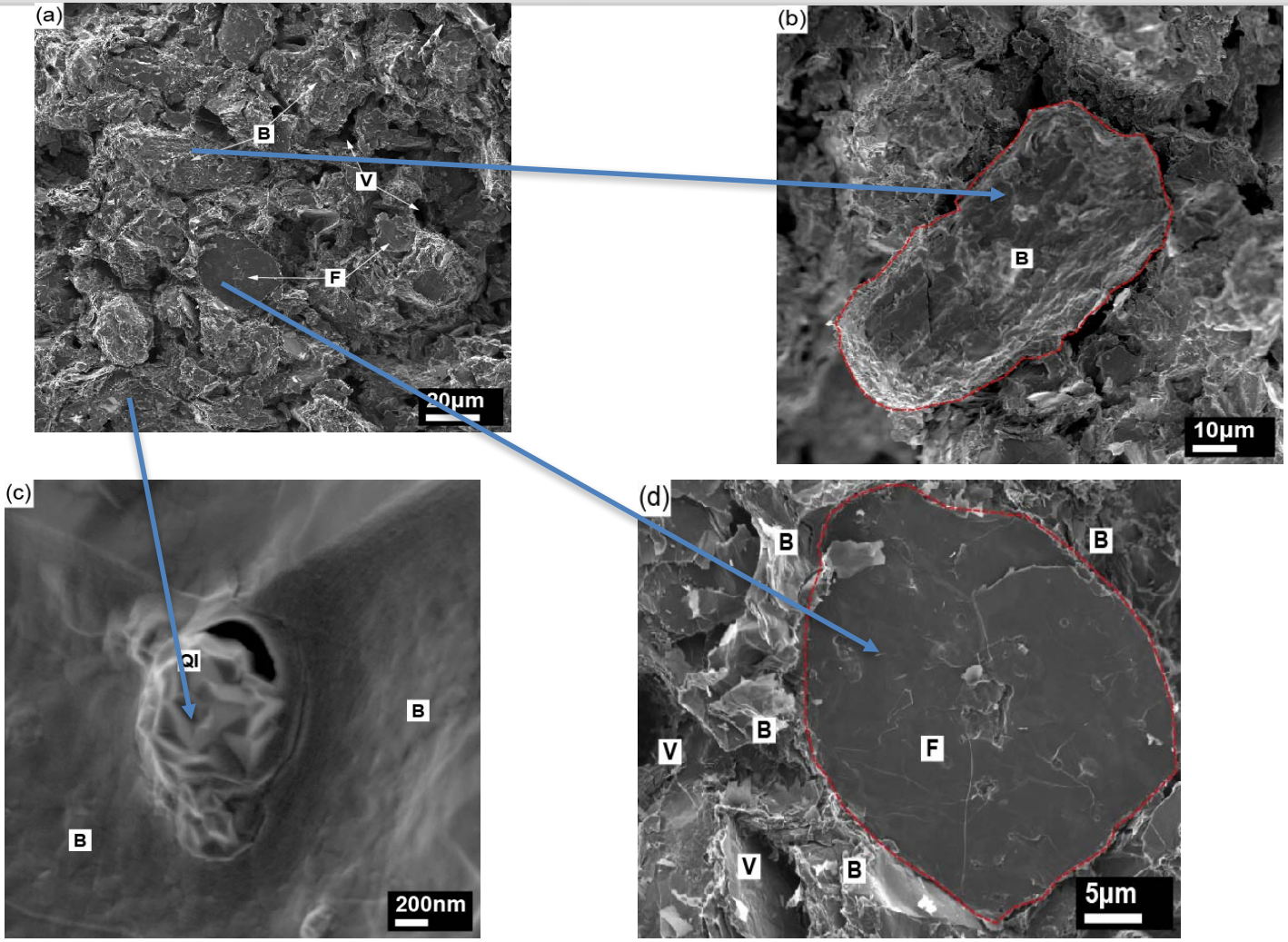
Ion irradiation in Surry

- Not started yet
- To be done in later part of UNIGRAF

Progress

- **Research on non-irradiated samples – on going, SNG623 completed**
  - Microstructure
  - Pore structure
  - Micro-scale testing
- **Research on ion irradiated samples – on going**
  - Microstructure
  - Micro-scale testing
- **Research on neutron irradiated samples - start in Oct 2017 at ORNL**
  - Microstructure
  - Micro-scale testing
- **Modelling – on going**
  - Atomic structure of mesoscopic structure in graphite
  - Nanoindentation damage

Microstructre & mesoscopic structure in iso-graphite (SNG623)



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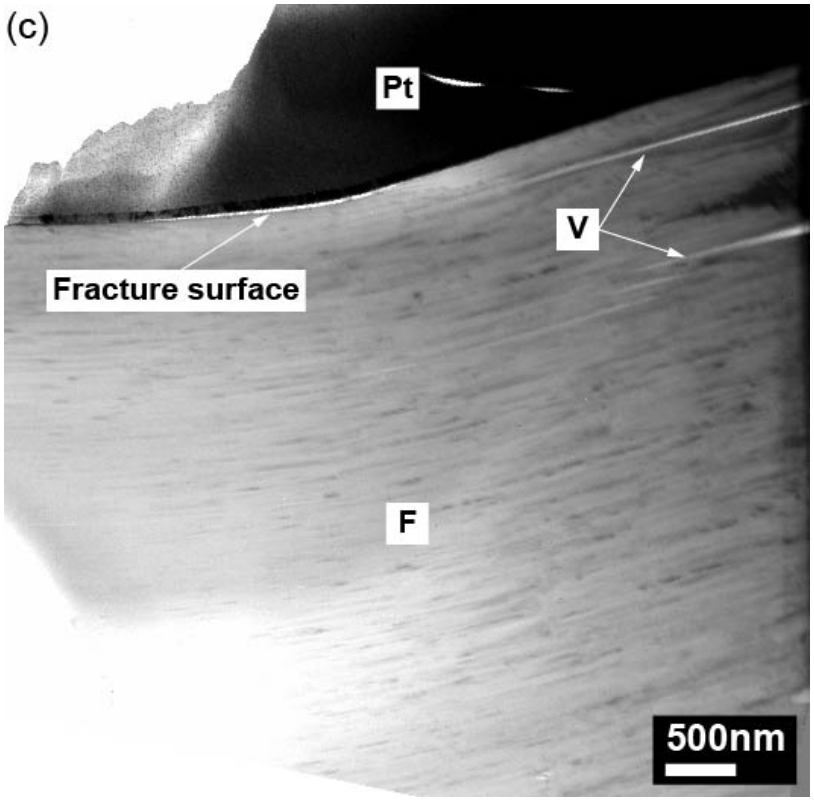
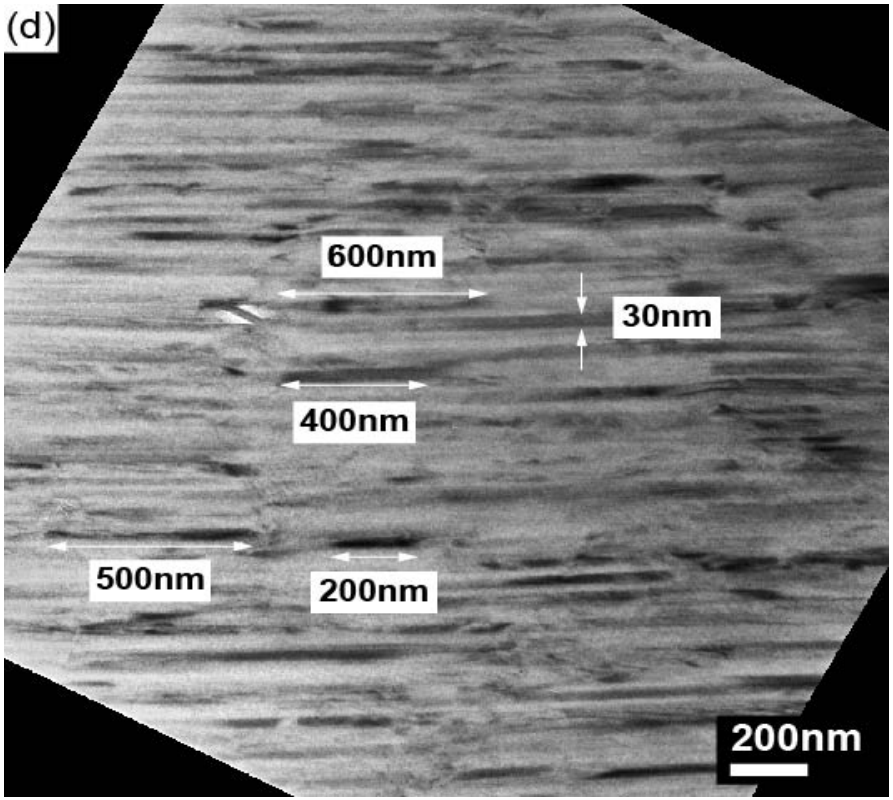
Mesoscopic structure inside coke

View along (0001) plane:





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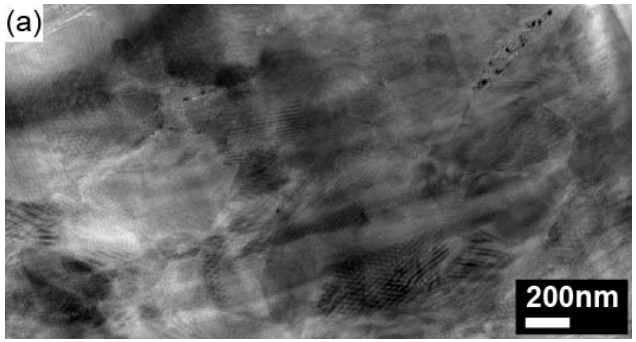
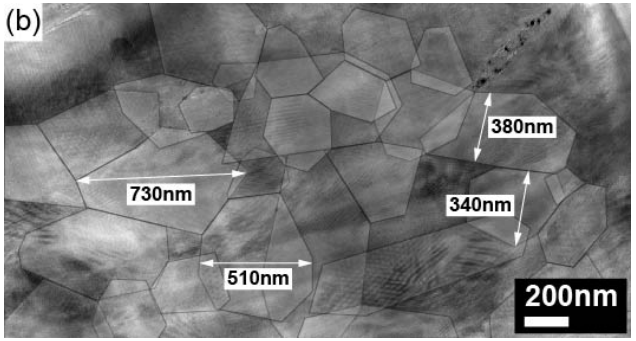
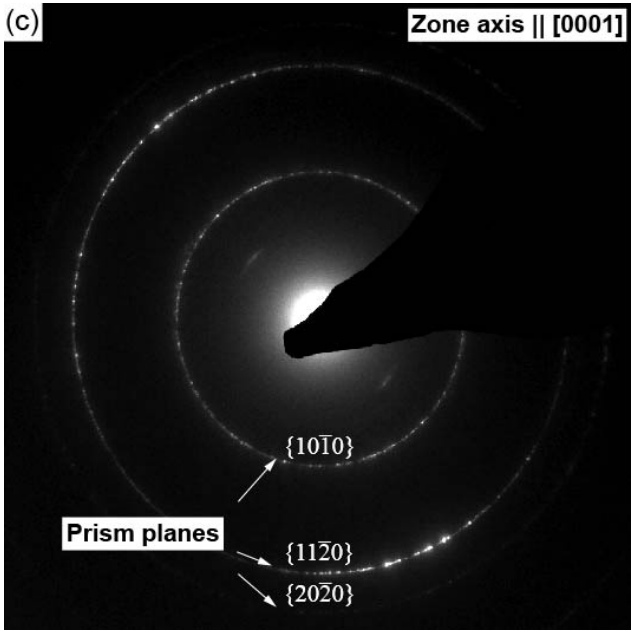
Mesoscopic structure inside coke

View perpendicular to (0001) plane:







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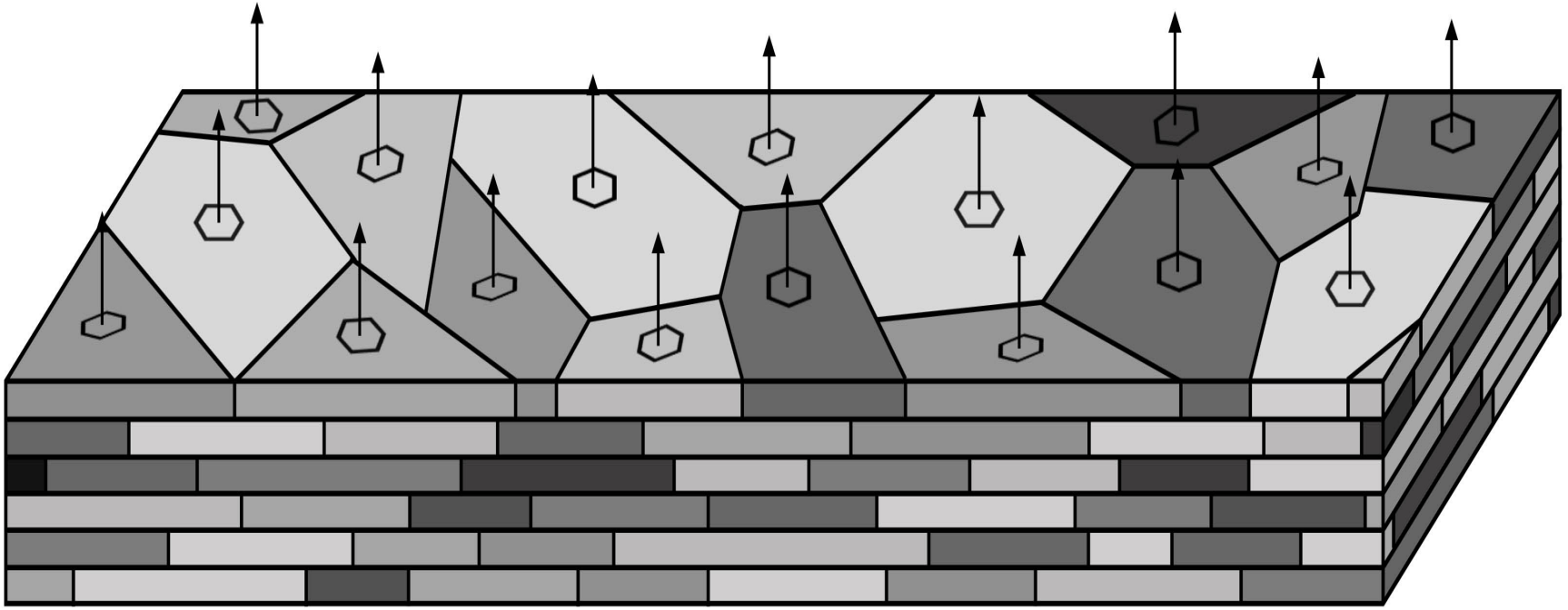
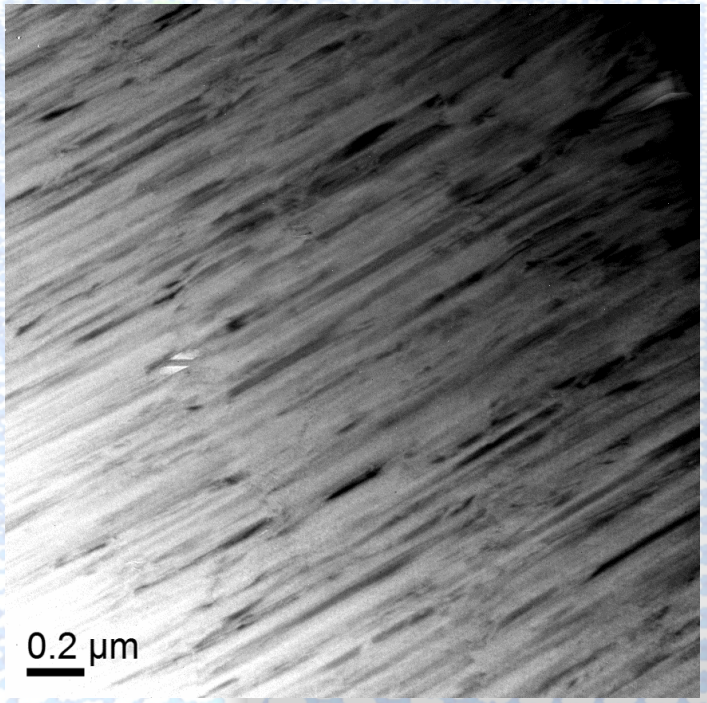
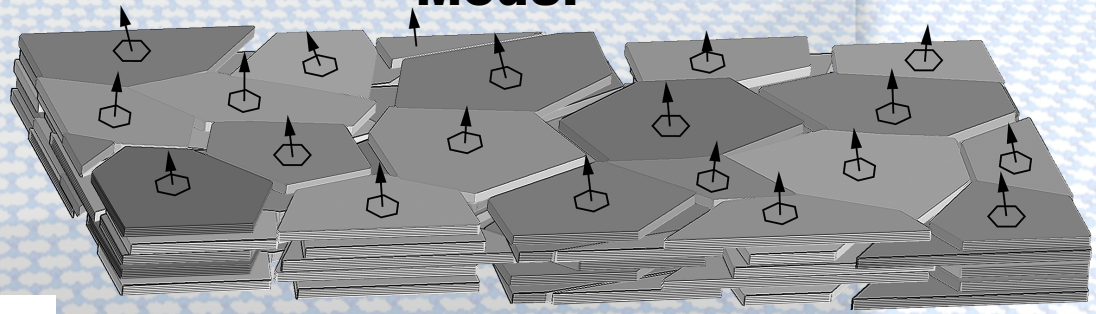
“crazy paving” mesoscopic structure proposed

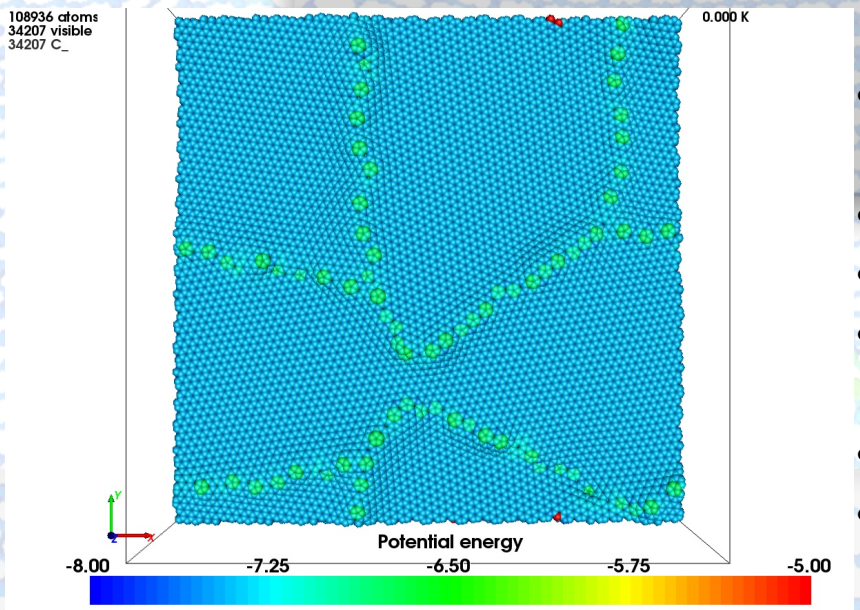


Nano crystalline graphite slabs



- **Experimental result:**
  - **Layers of 'crazy paving' slabs.**
  - **Layers thickness: 20-30 nm**
  - **Slab diameter: 100-150 nm**
- **Variation of the c-axis over long range**
- **Model**





- **Build small system for MD simulation**
- **150 Å x 150 Å x 30 Å**
- **(12 graphene layers)**
- **Generate grain boundaries with a geometric relaxation method.**
- **108,936 atoms**
- **3 voronoi cells**

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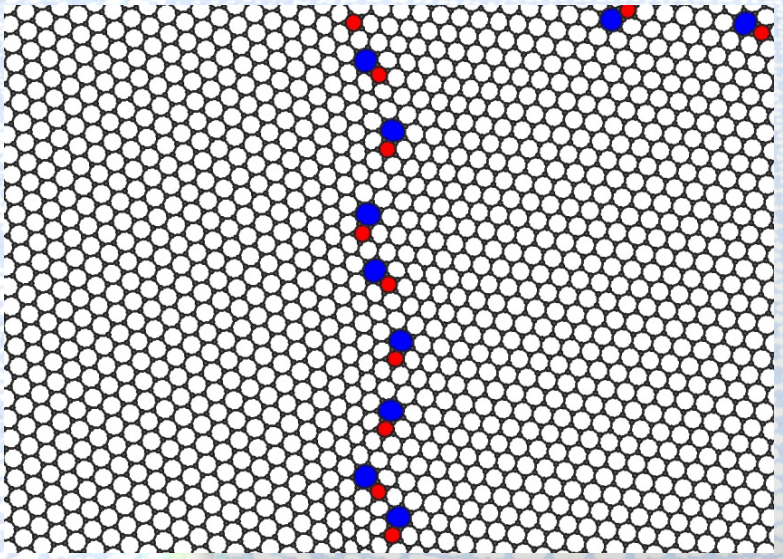
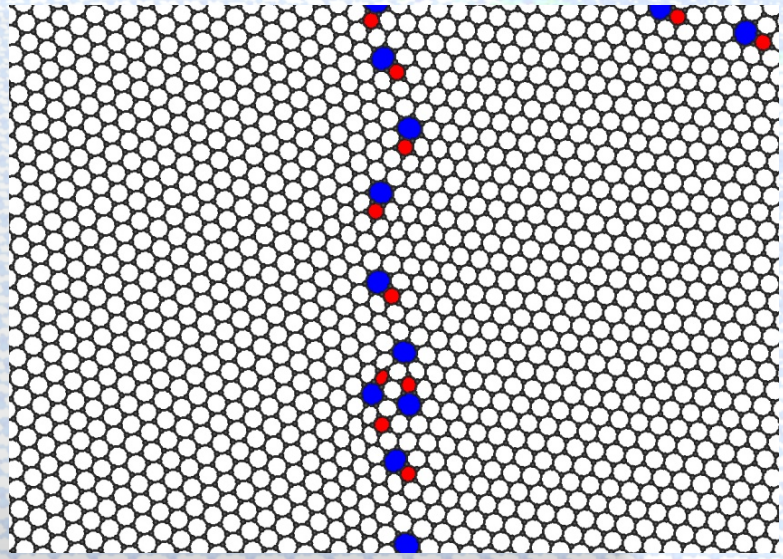
Nano crystalline graphite slabs

15° grain boundary

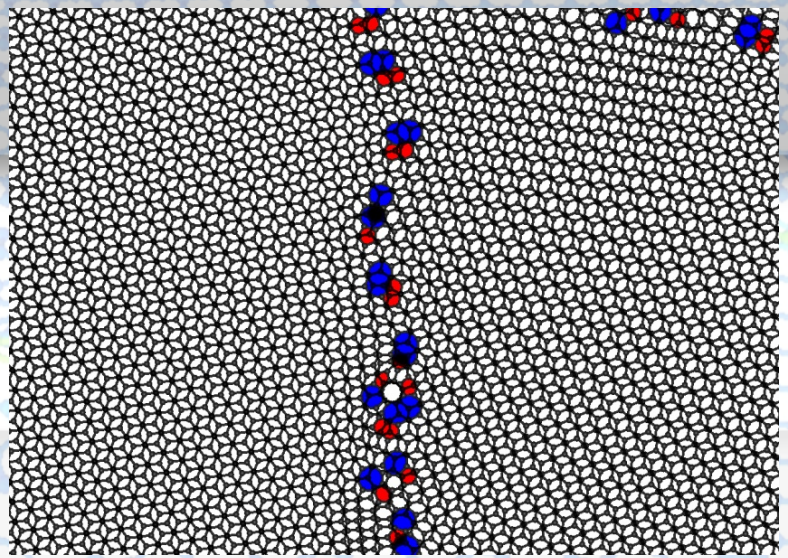
Top layer



Second layer



Composite of two layers



Key:

5

6

7

- **Each unique layer is prepared and geometrically relaxed separately.**
- **Layers assembled into large graphite structure.**
- **Final relaxation in MD.**

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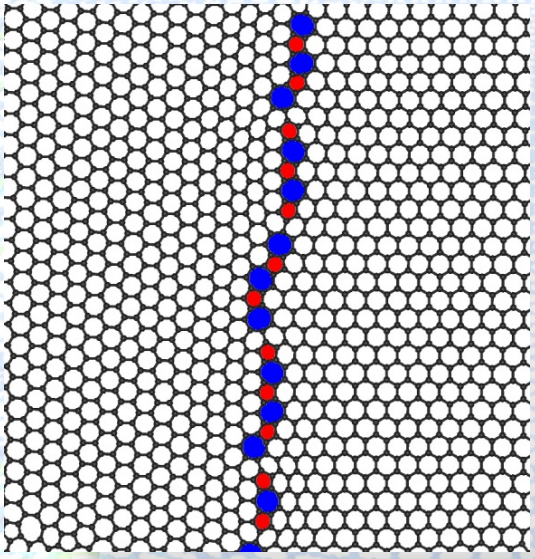
Nano crystalline graphite slabs

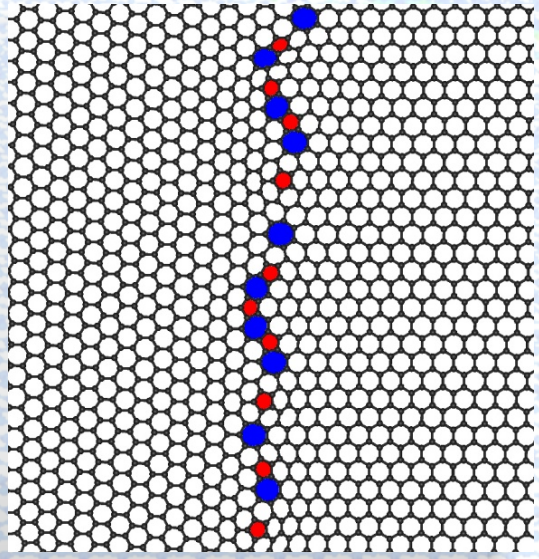
32° grain boundary

Top layer

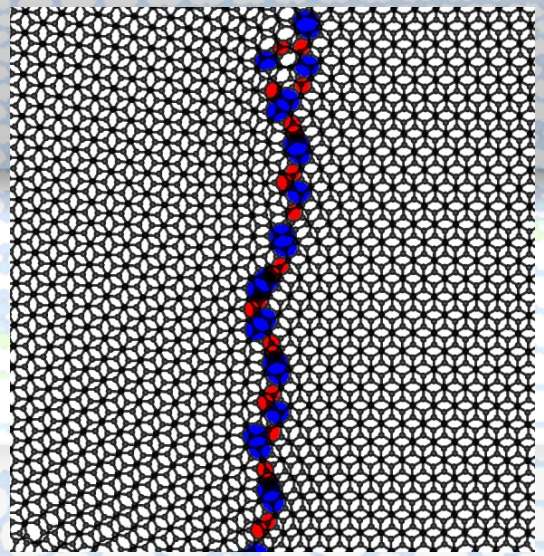


- **High angle boundary.**
- **Armchair meets zigzag edge.**

Second layer



Composite of two layers



Key:

5

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7

- **Each unique layer is prepared and geometrically relaxed separately.**
- **Layers assembled into large graphite structure.**
- **Final relaxation in MD.**

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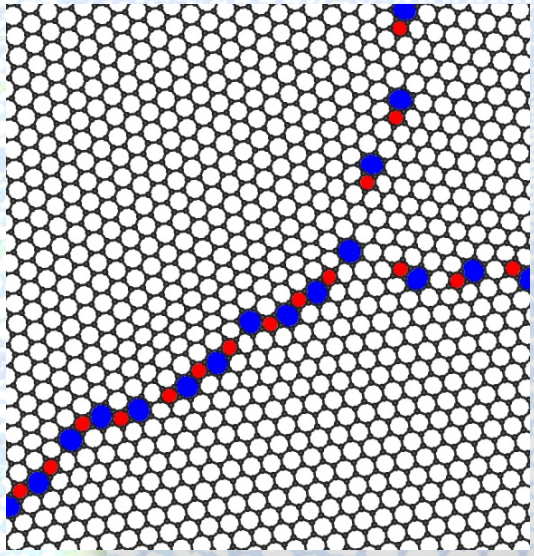
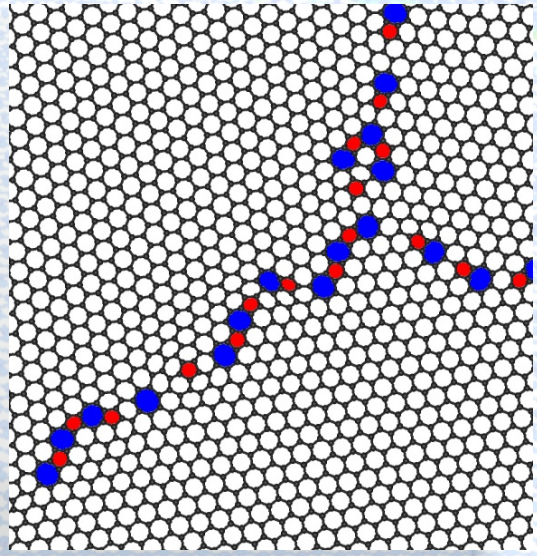
Nano crystalline graphite slabs

Triple junction grain boundary

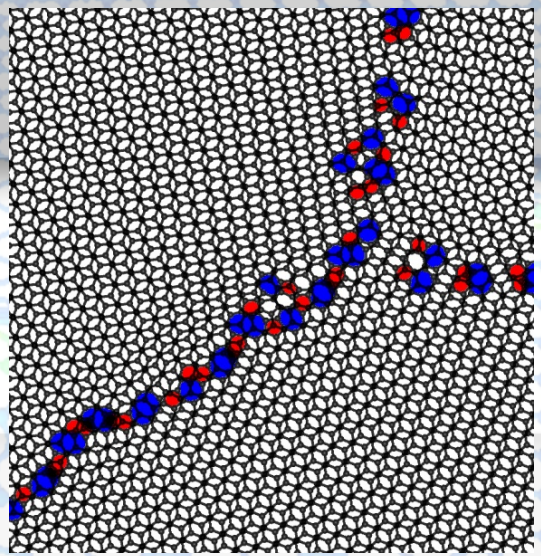
Top layer



Second layer



Composite of two layers



Key:

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- Each unique layer is prepared and geometrically relaxed separately.
- Layers assembled into large graphite structure.
- Final relaxation in MD.

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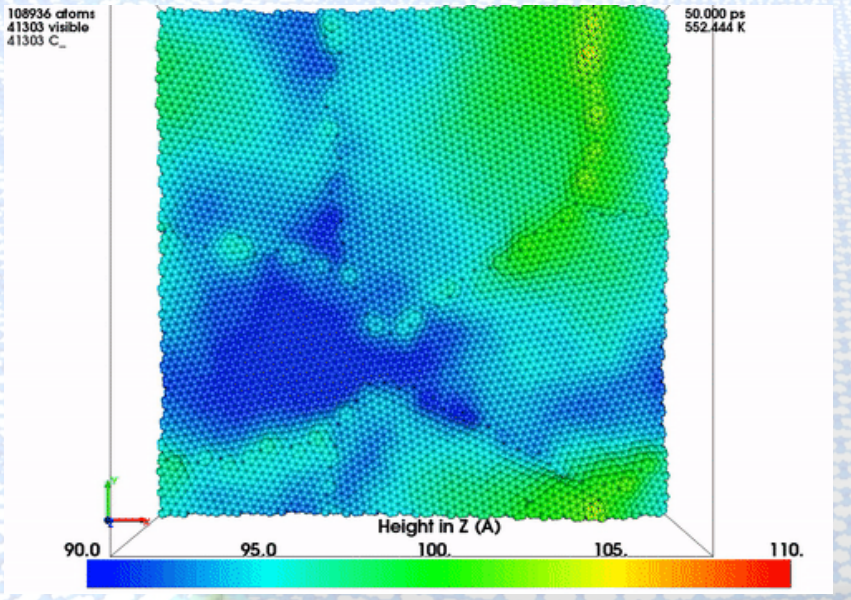
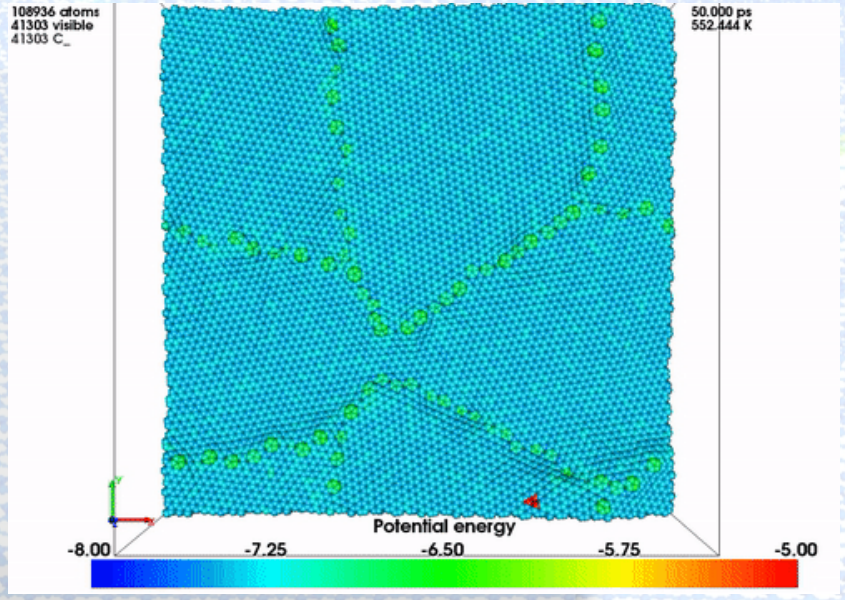
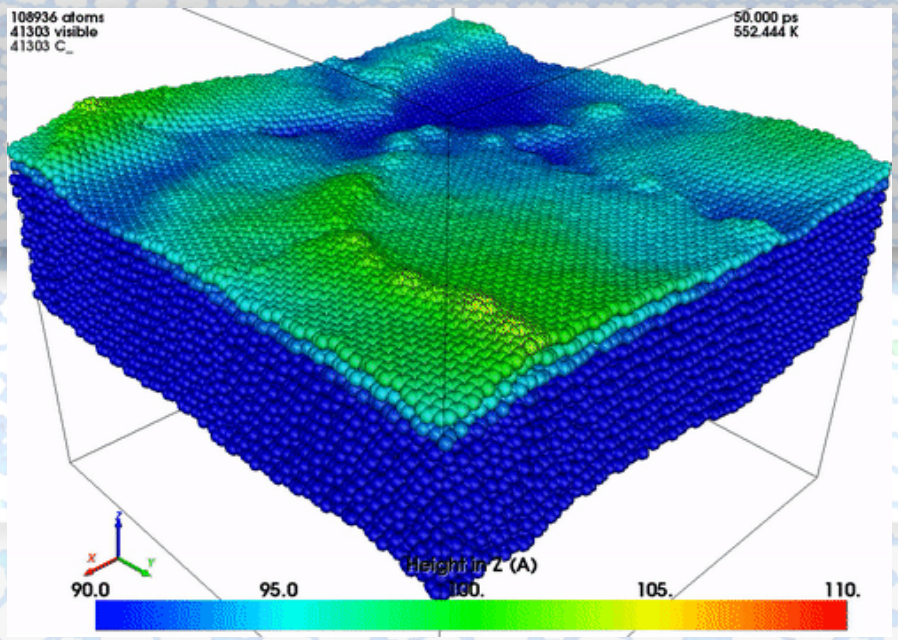
Nano crystalline graphite slabs

AIREBO: heated to 1000 K (npt) over 300 ps







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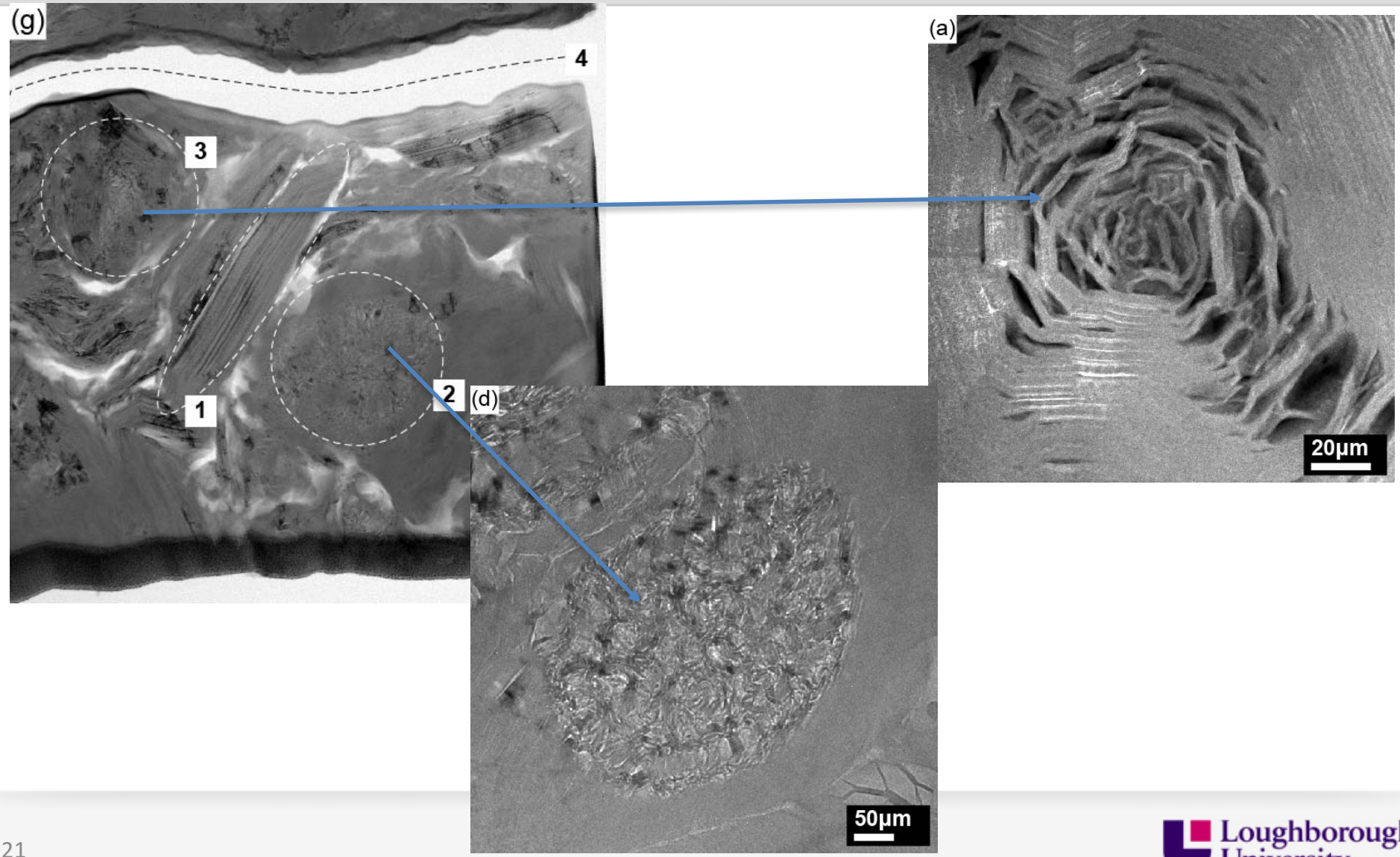
Graphite in binding matrix



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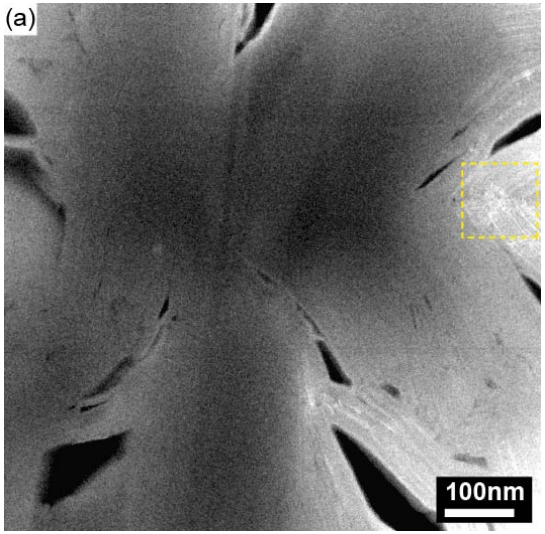

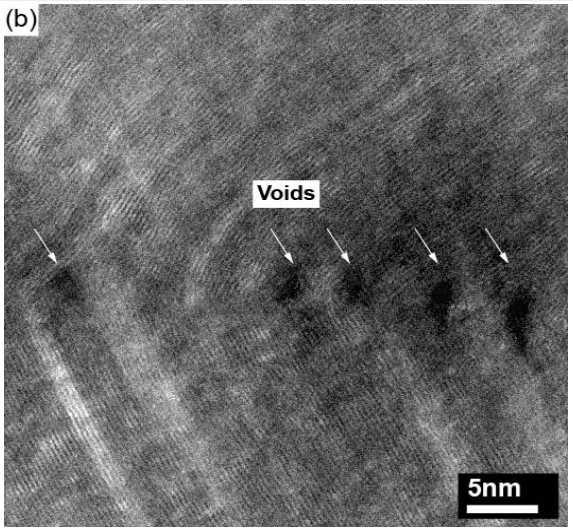

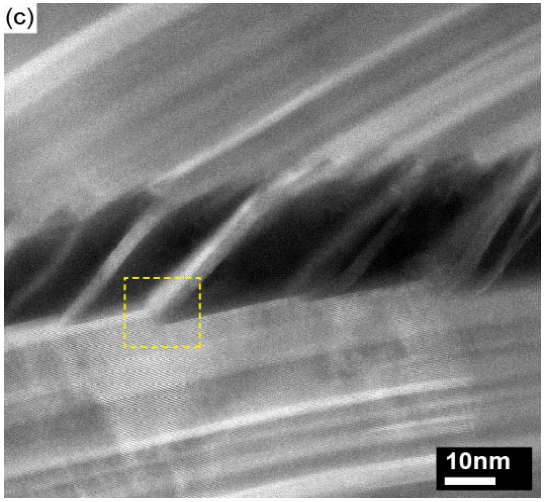

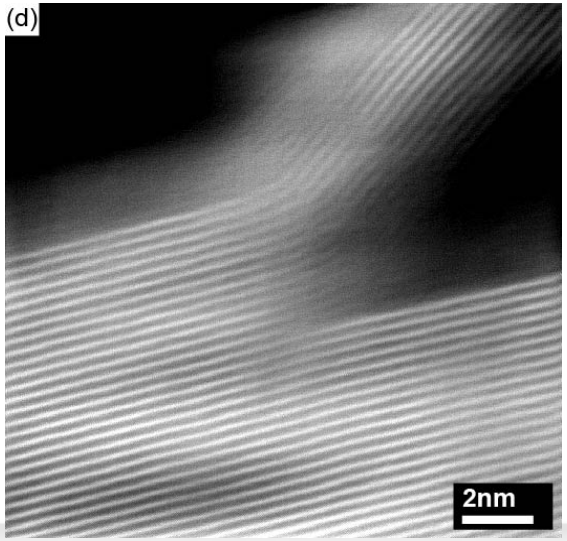

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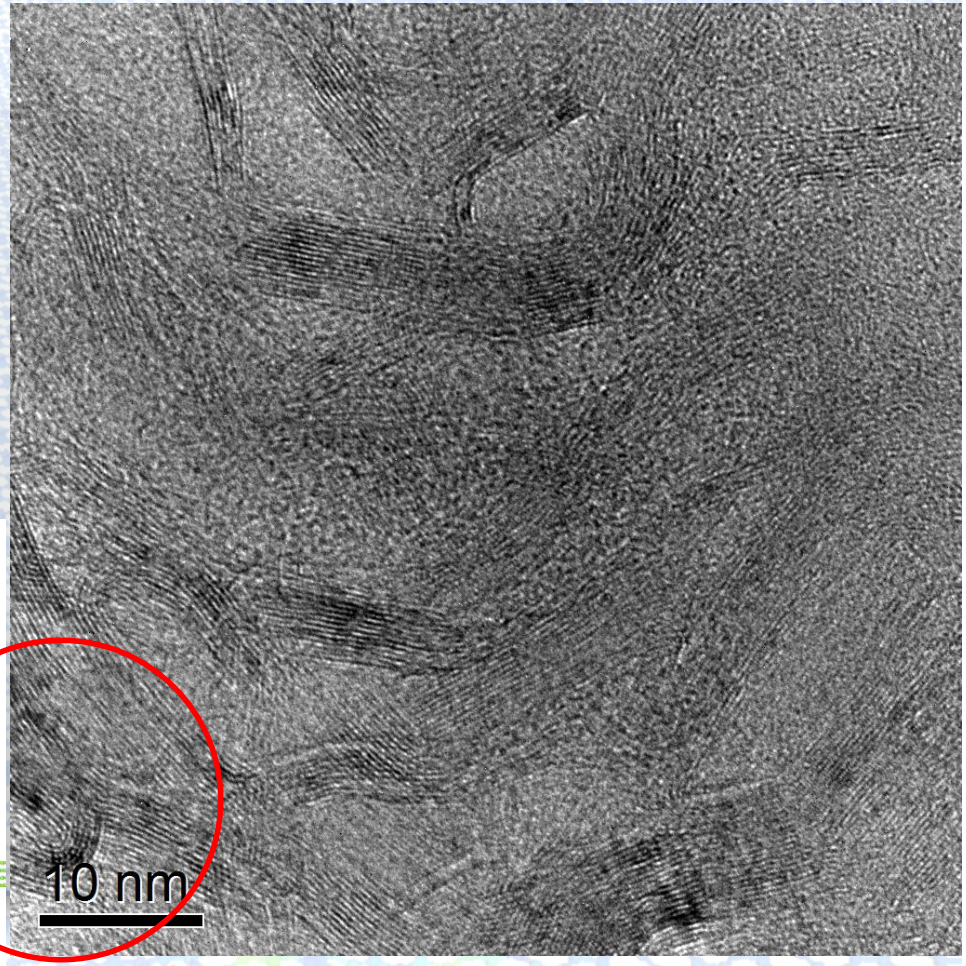
Machined surface

- Experimental image shows a machined surface.
- The mechanical stress causes the graphite units to bend in various angles.
- Graphene layers bent into a U shape, are observed.



- MD simulation: compression of a 400 Å periodic slab.

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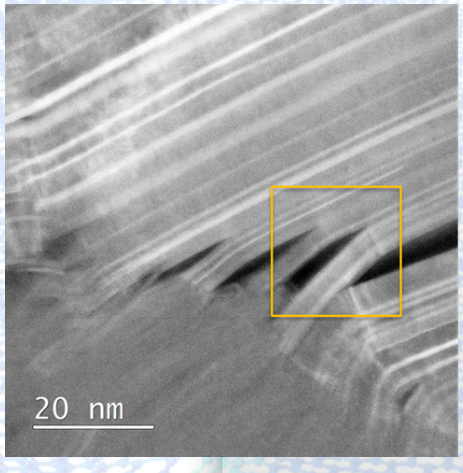
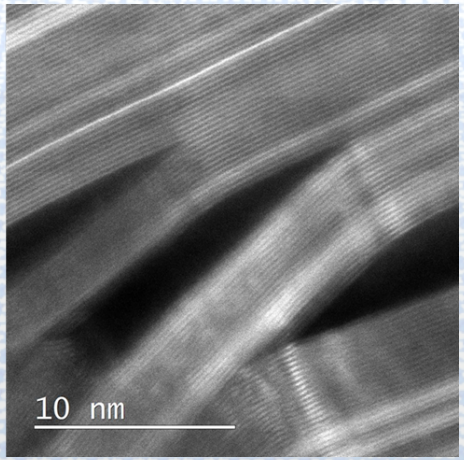
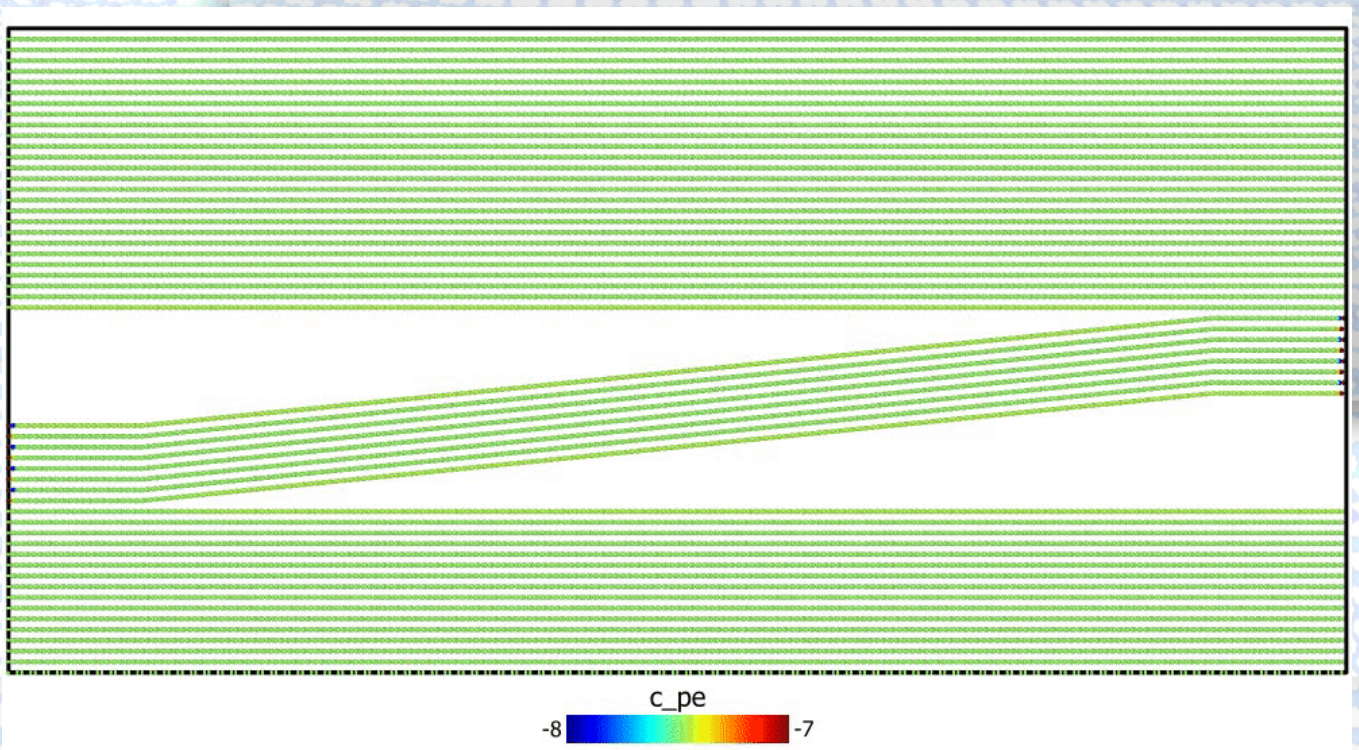
Crack with bridge





- On the left, the bridging graphite layers near the tip of a microcrack appear sharp.
- But at higher magnification reaching to atomistic level, smooth transition is seen, as shown in right hand side



- Relax a simple bridge model in MD.
- Observe similar smooth bends of the basal planes.

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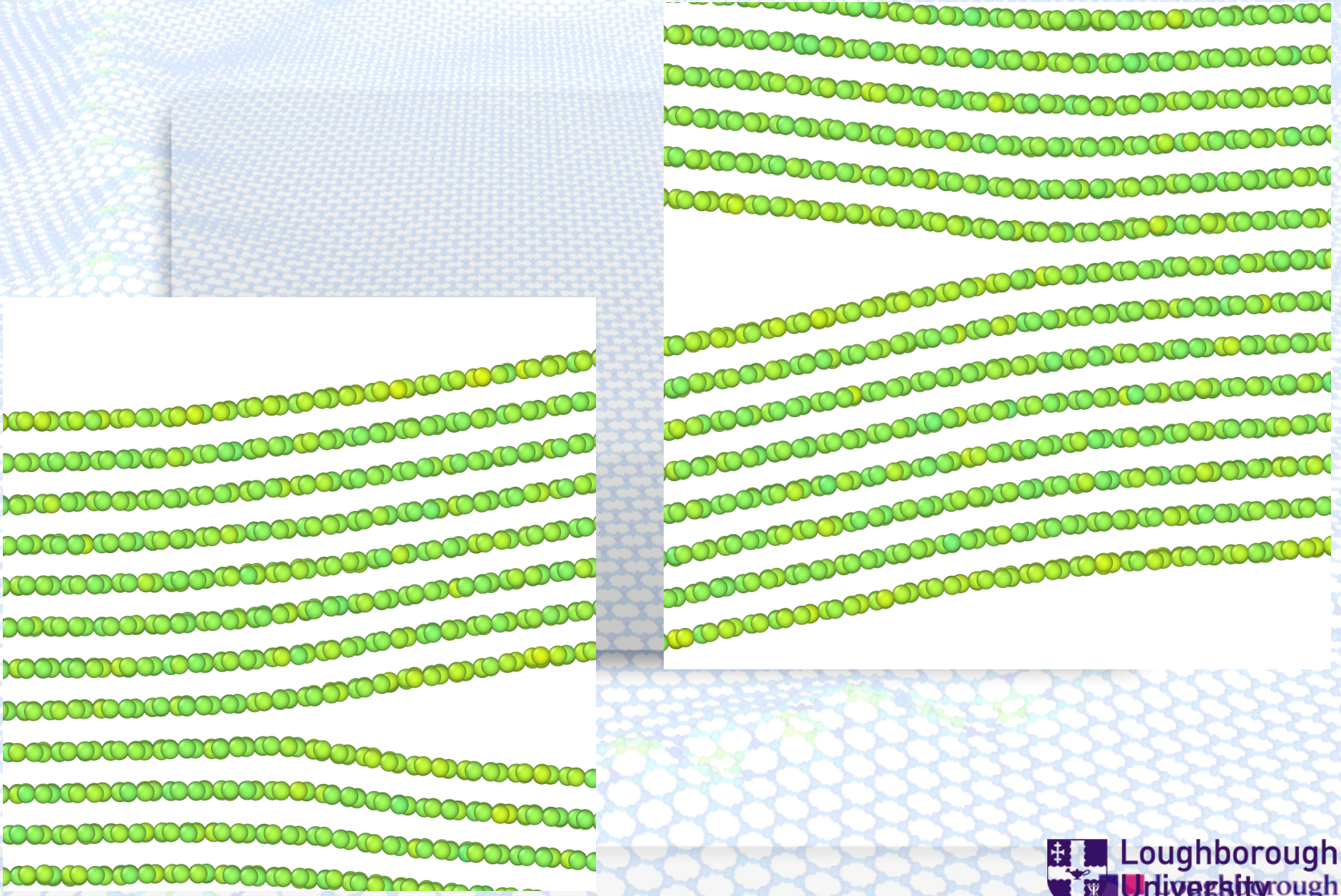
Crack with bridge



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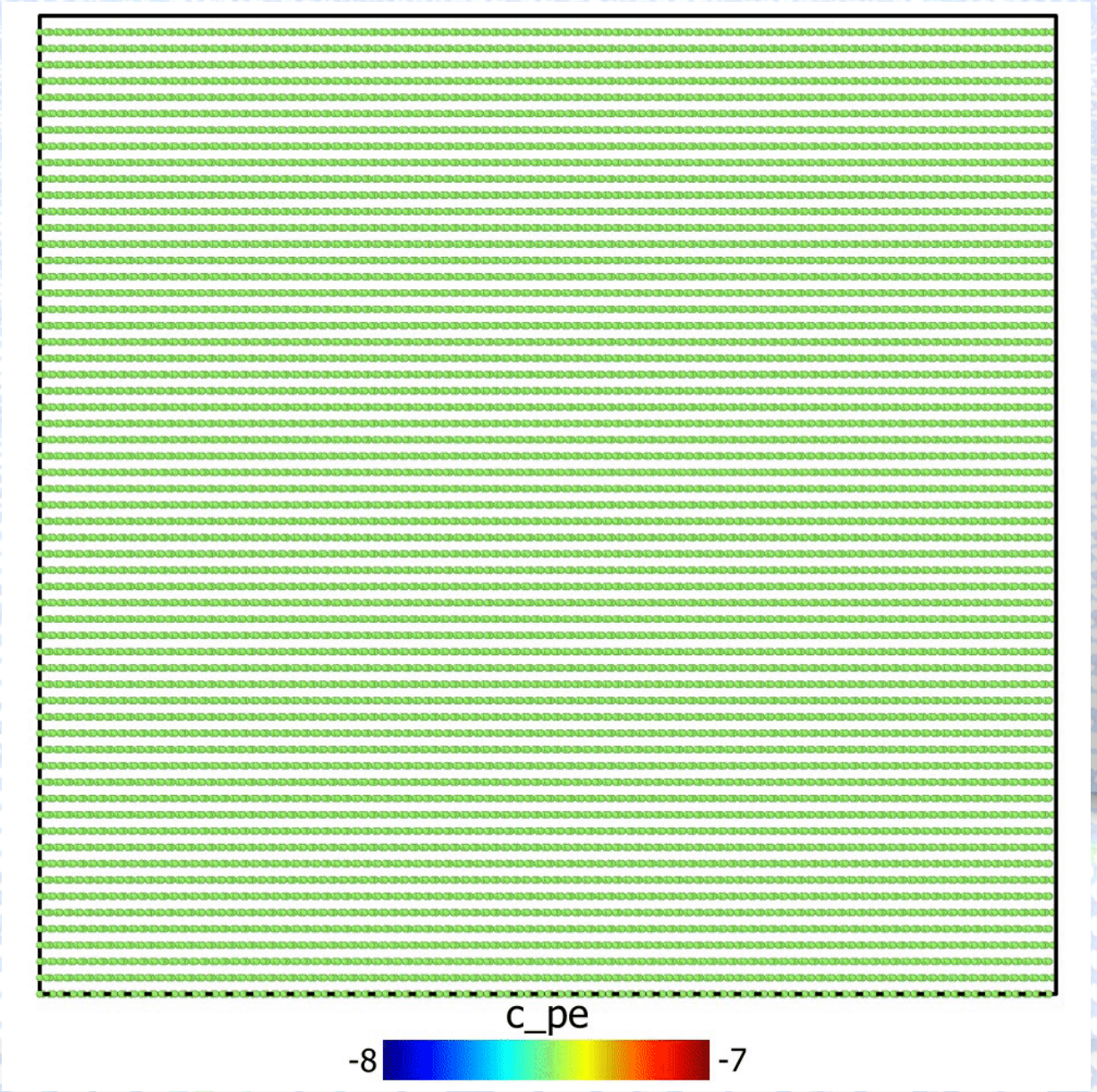
Molecular Dynamics



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