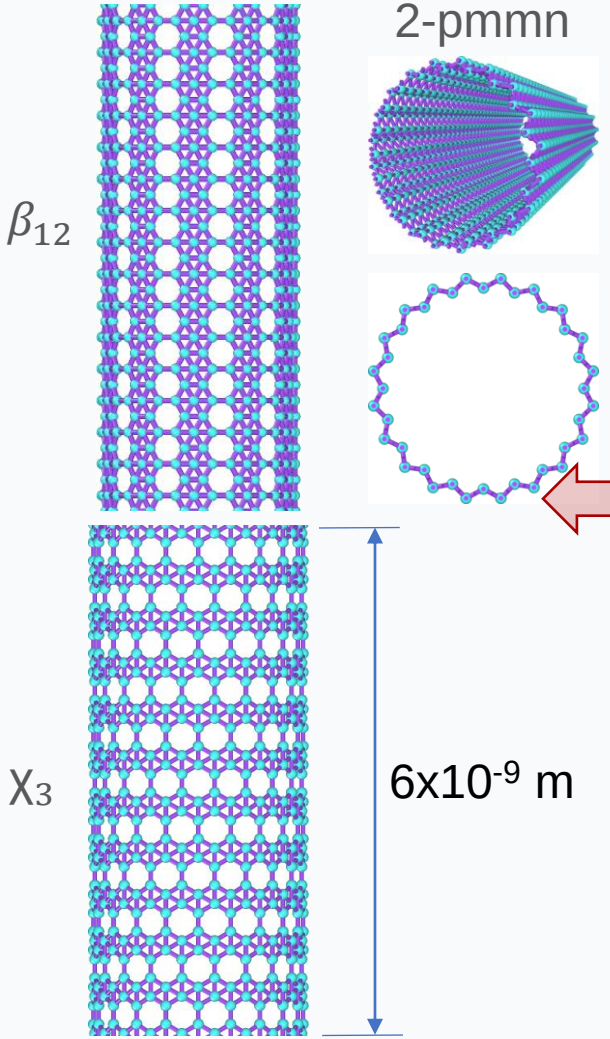
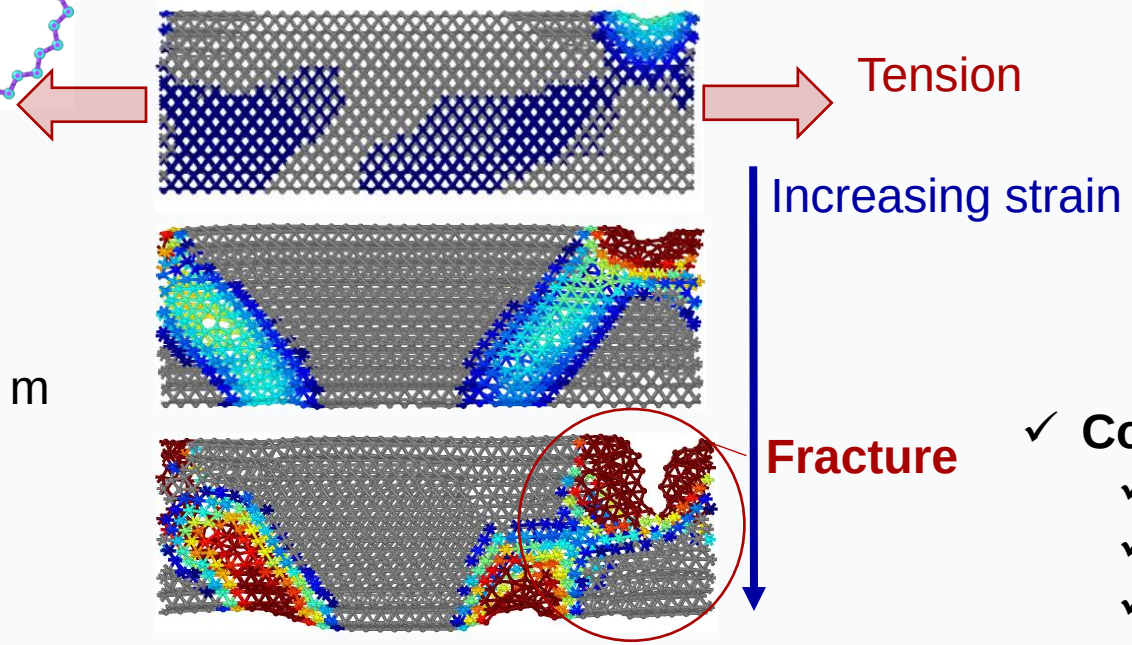
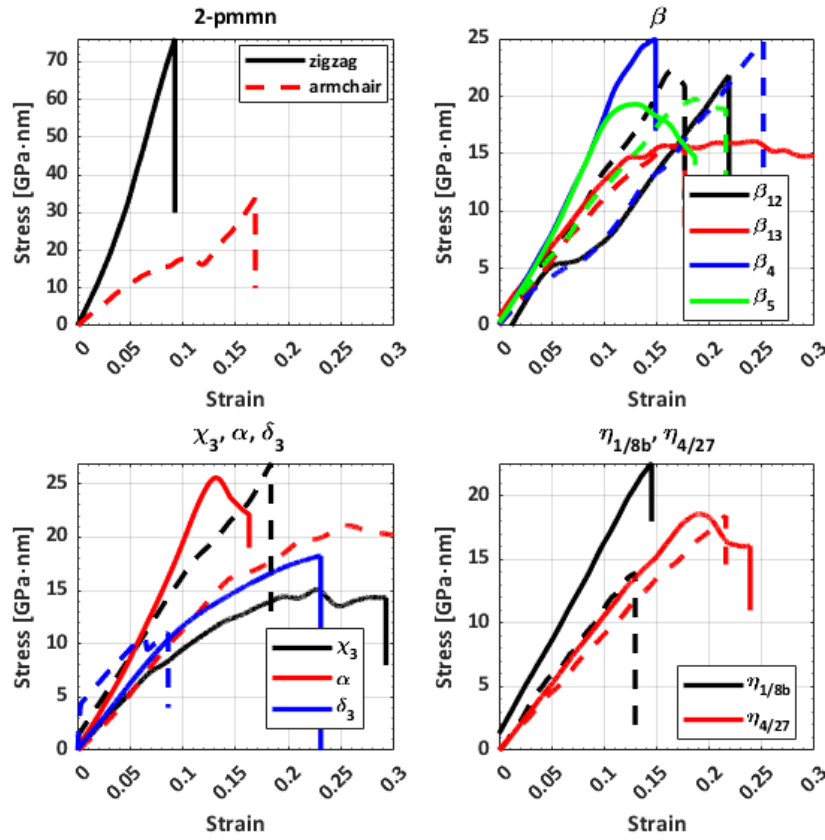
Mechanical Properties of Boron Nanotubes

BNT: Different atomic configurations



- ✓ Excellent electronic and mechanic properties
- ✓ Usage in high-performing nano-devices
- ➢ Uncertainty in the mechanical properties
- ➢ Modeling methods:
  - Quantum mechanics
    - ~1000 atoms
  - ✓ **Molecular Dynamics**
    - **High accuracy**
    - **> 1x10^6 atoms**





- ✓ **Core mechanical properties**
  - ✓ **Young's modulus**
  - ✓ **Fracture strength**
  - ✓ **Fracture strain**

Caliskan, E., & Kirca, M. (2022). Tensile characteristics of boron nanotubes by using reactive molecular dynamics simulations. *Computational Materials Science*, *209*, 111368.

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- **Complex numerical model**
  - Same potential in many different configurations: Long computation time
  - Bond generation/breakage: Reactive Molecular Dynamics
    - ReaxFF (Aktulga vd., 2012)
- **Computational load**
  - Number of atoms ~700-20.000
  - Development of a stable and highly accurate simulation workflow
  - 20 different types of structures
  - Diameter, length, aspect ratio, strain rate, temperature

- ✓ **High-Performance Computing**
  - ✓ **TRUBA**
  - ✓ **UHeM**

- ✓ **Optimization of the calculation time**
  - ✓ Different compilers
  - ✓ MPI / OpenMP
  - ✓ Different architectures
  - Single node, (Lammps: USER-REAXC, USER-OMP)

# MPI tasks x # OpenMP threads	Workflow 1: Thermalization	Workflow 2: Tension
56x1	3.091	1.966
28x2	2.733	1.719
TRUBA - Cascade Lake - Xeon 6258R 2.70GHz Intel oneAPI - icx	ns/day	

# MPI tasks x # OpenMP threads	Workflow 1: Thermalization	Workflow 2: Tension
40x1	2.056	1.397
20x2	2.257	1.808
UHeM - Skylake - Xeon 6148 2.40GHz Intel Parallel Studio - icc	ns/day	

Acknowledgements:The numerical calculations reported in this paper were performed at **TRUBA** and **UHeM** resources

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