Stiffness, strength and reusability in architected polycrystals

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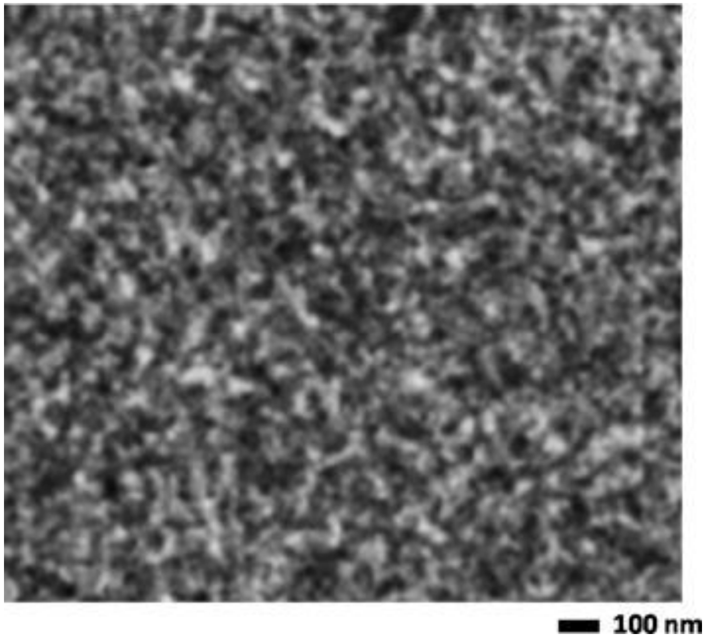
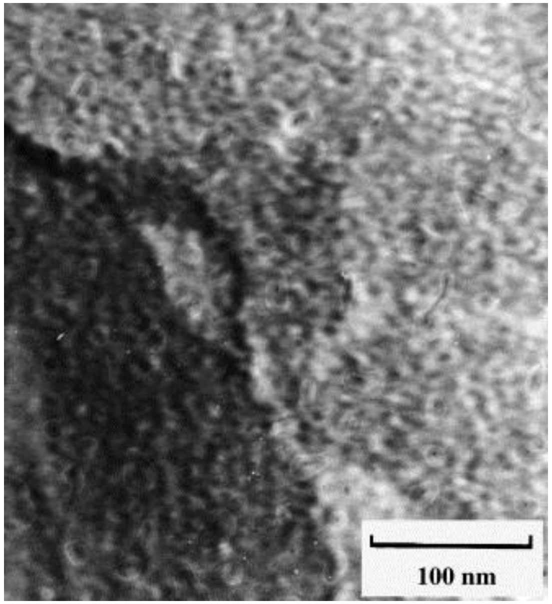
Heterogeneous materials

- Heterogeneous materials (e.g., two-phase elastomers) consist of **hard** and **soft** phases[1-3]
  → **Outstanding properties** including stiffness, strength, energy dissipation and resilience

- **Geometric** and **topological features** in **hard phases** govern the macroscopic mechanical responses in heterogeneous materials



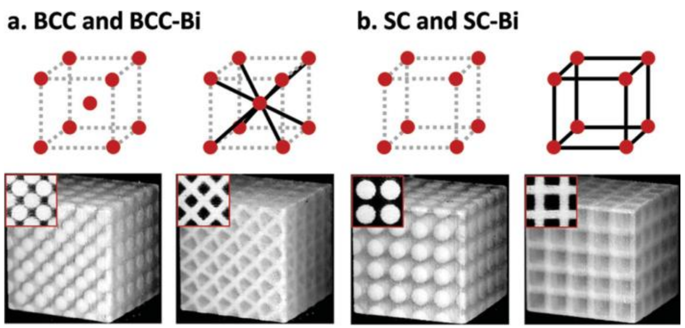


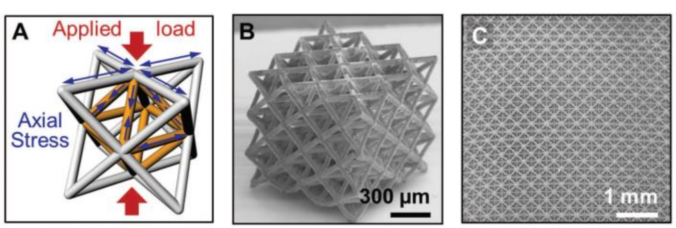
TEM images of thermoplastic polyurethanes[2-3]

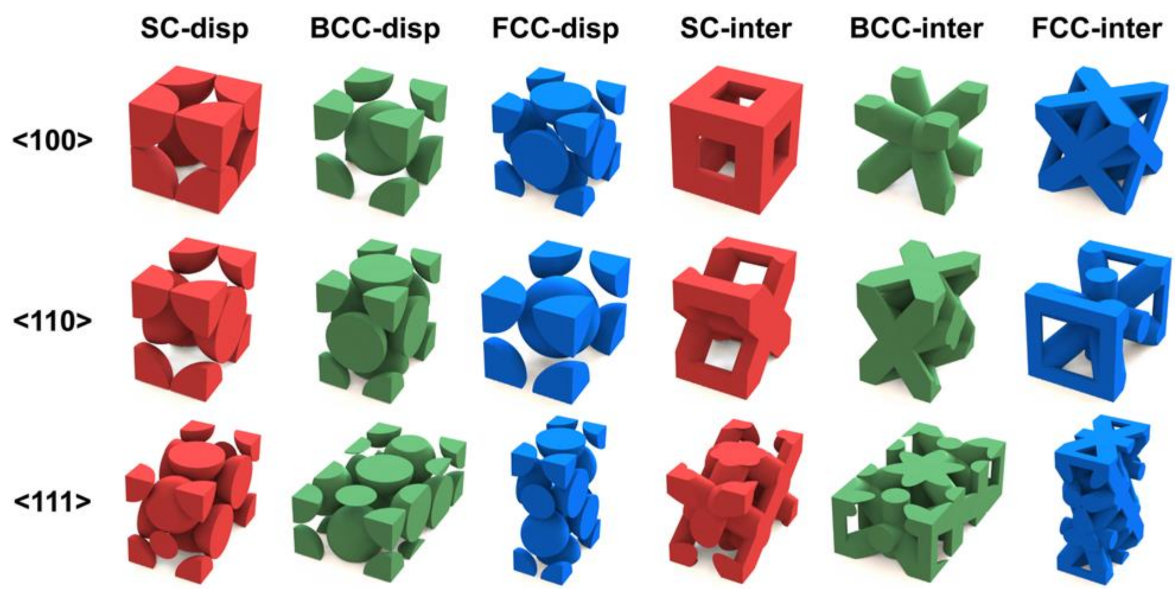
Single-crystalline architected materials

- Architected materials constructed on various **crystal lattices**[4-7]; e.g., simple cubic (SC), body-centered cubic (BCC), face-centered cubic (FCC)

i) **Multi-physical functionalities** for a wide variety of engineering applications
ii) **High** stiffness, strength, mechanical resilience and energy dissipation







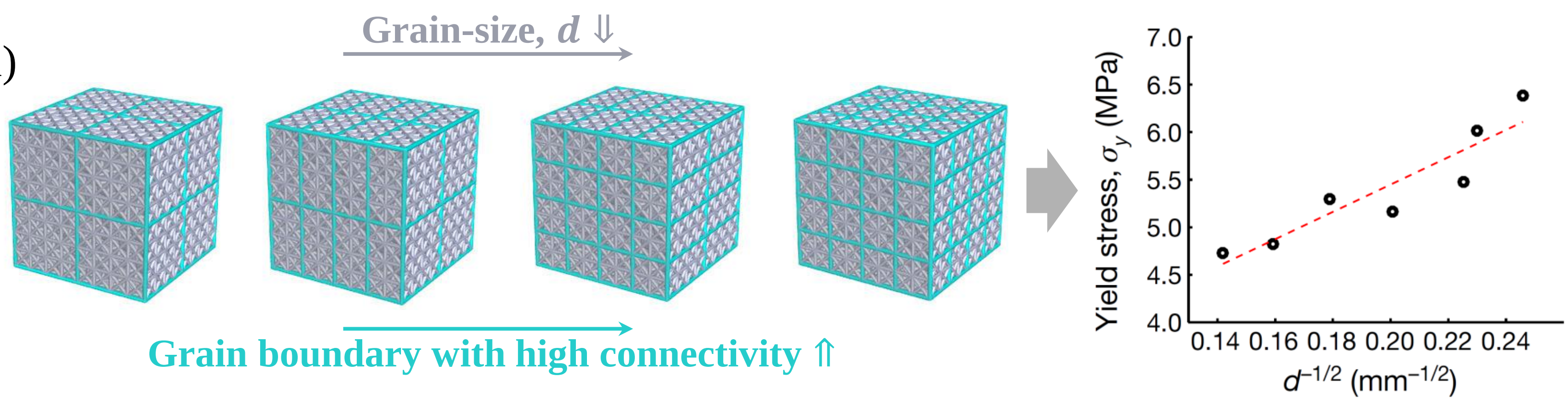
Polycrystalline architected materials

- Mimicry of **polycrystalline microstructures** on a **macroscopic scale**

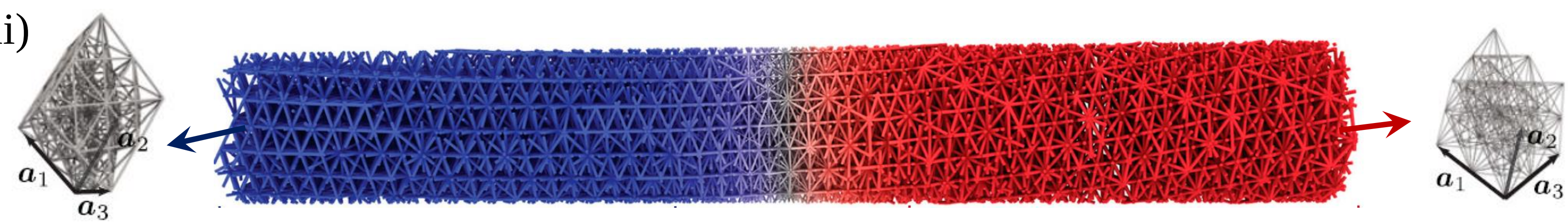
i) Strengthening or hardening mechanisms **(e.g., Hall-Petch relationship)** in physical metallurgy is **applicable**[8-9][10-14]

ii) **Spatially-varying** architected materials[15]

i)

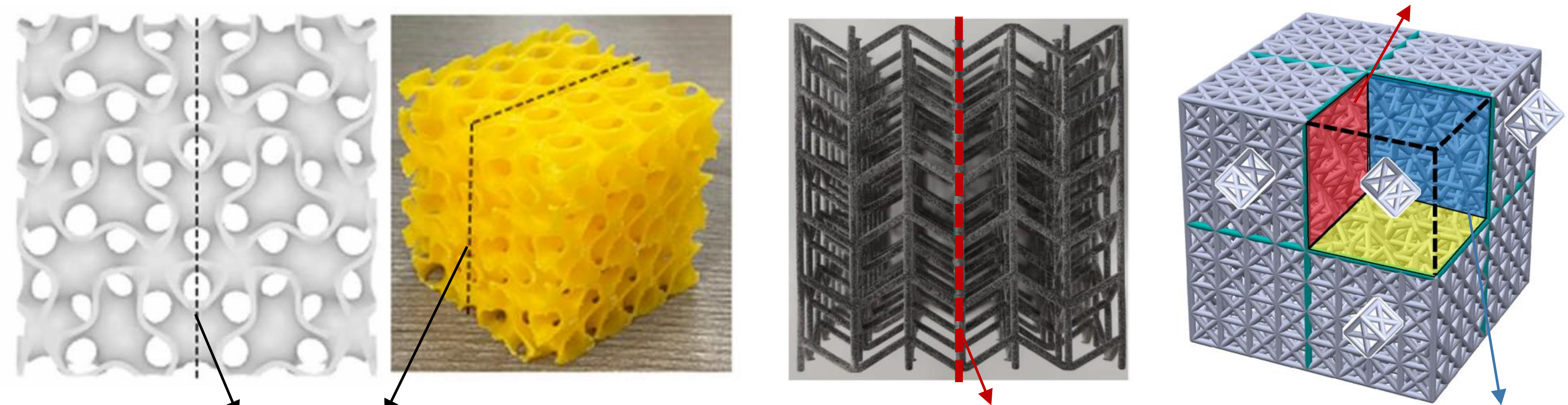


ii)



Polycrystalline architected materials

- **Tremendous potential opportunities** to explore the **structure-property relationships** in polycrystalline architected materials



Role of **a wide variety of grain boundary structures**

Objectives

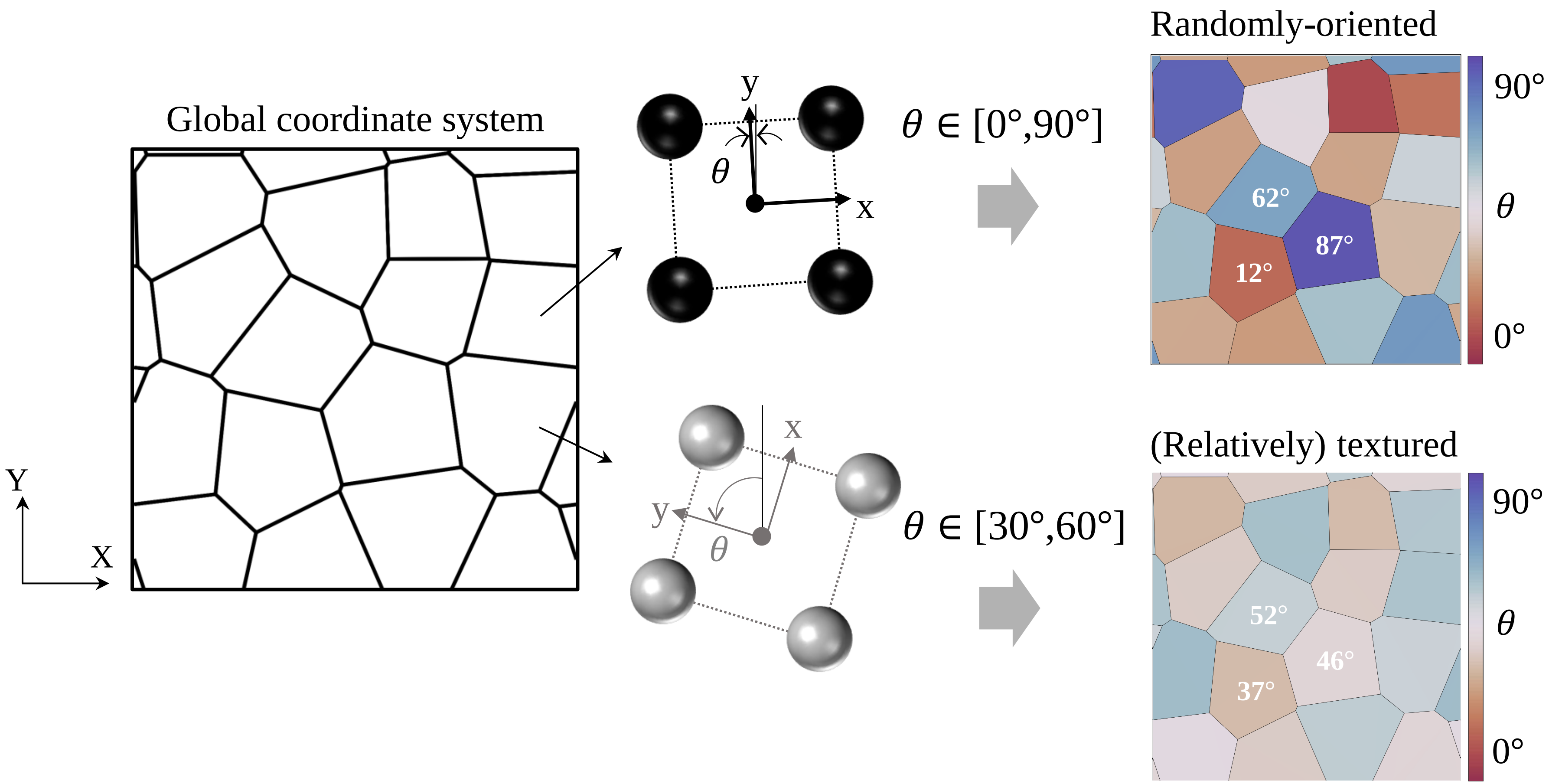
- Emergence of **engineering grain boundary structures** in metallurgy for **polycrystalline architected materials** comprised of **hard** and **soft phases**

- Understanding the role of **grain boundaries** in **grain-size dependent** **mechanical features** and **failures**

Design procedures

i) Microstructural orientation

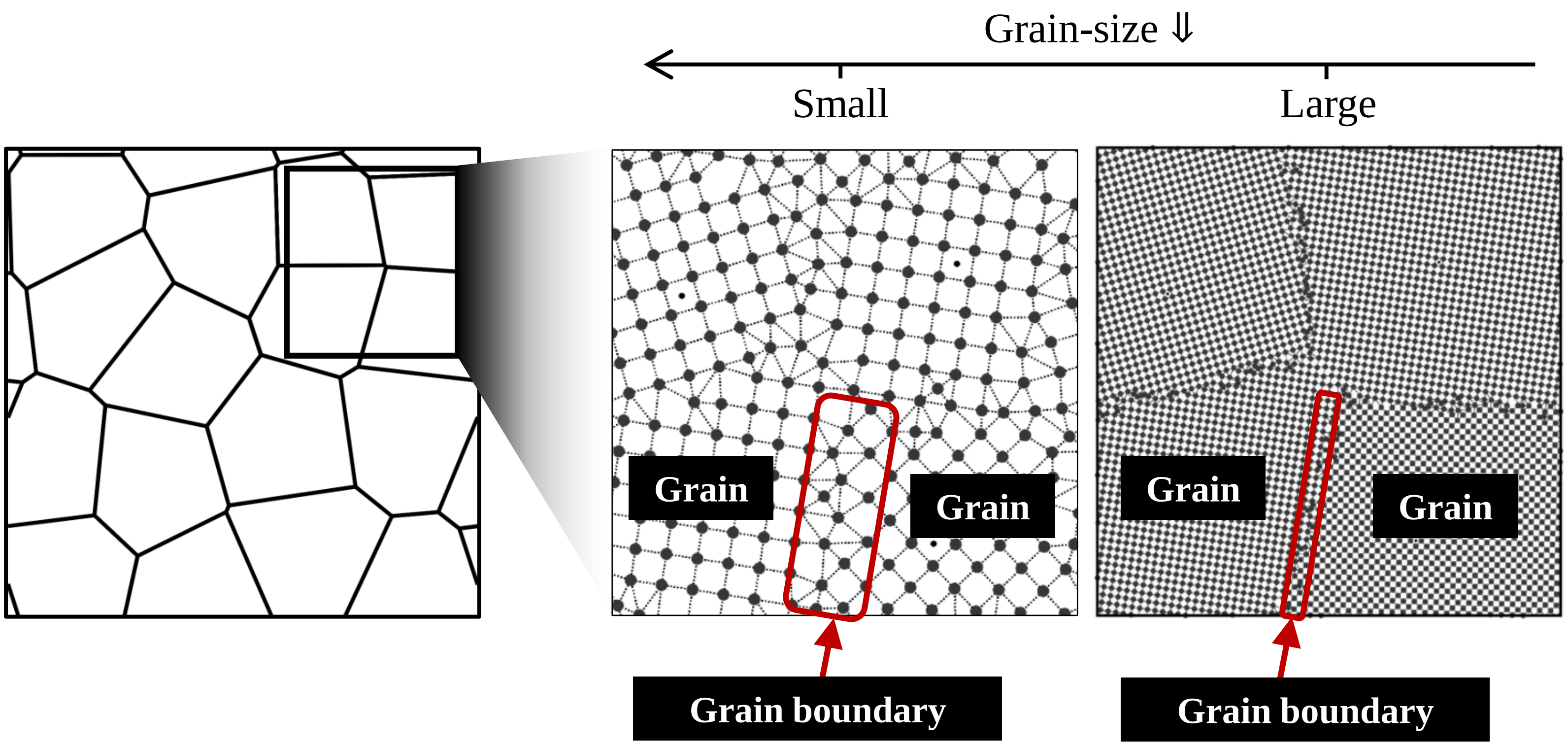
- **Restrict the range** for crystallographic orientations θ[18]



Design procedures

ii) Grain-size

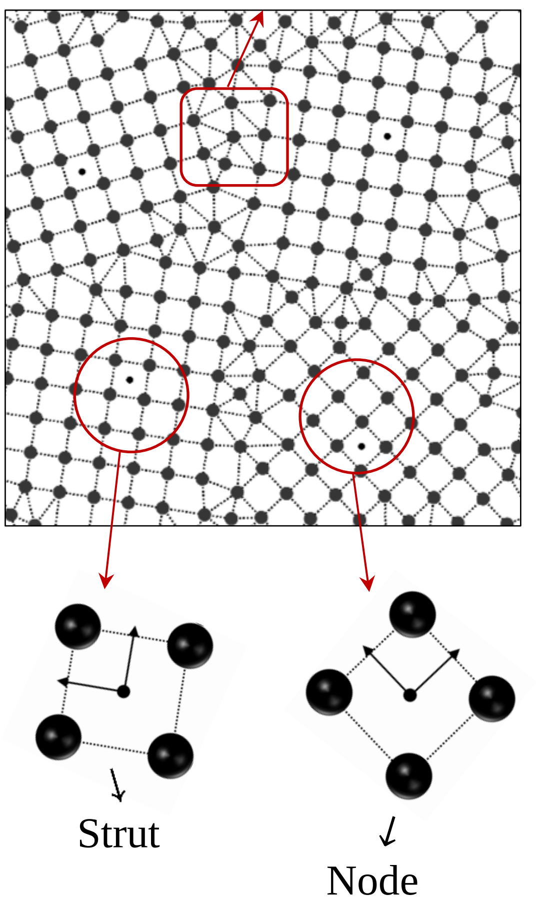
- As **grain-size decreases**, the **volume fraction of grain boundaries** with high strut connectivity **increases**

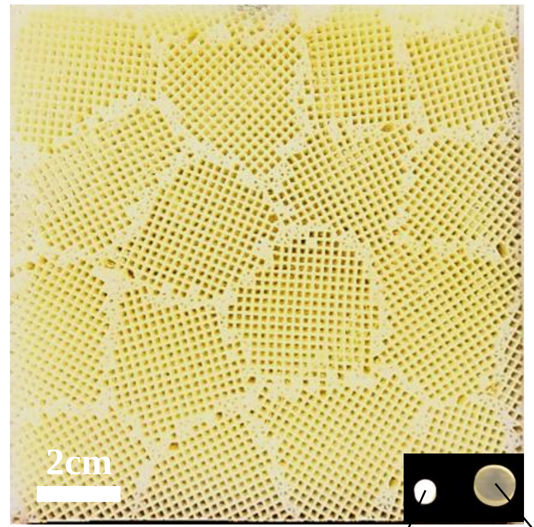


Experimental procedures

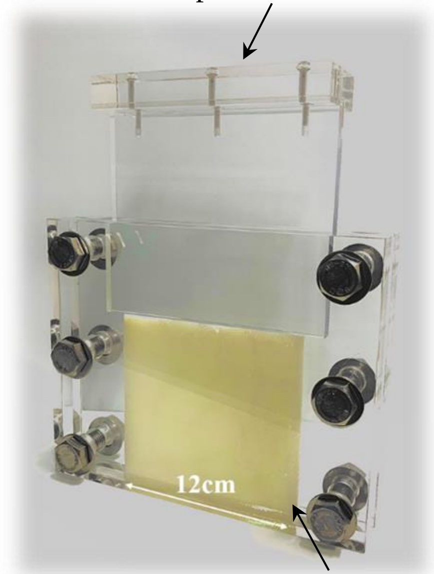
Compression mechanical tests under **plane-strain** conditions

GBs with high connectivity



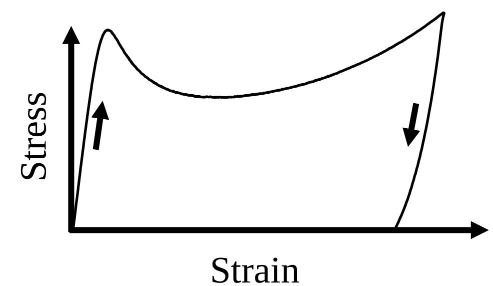


Compression head

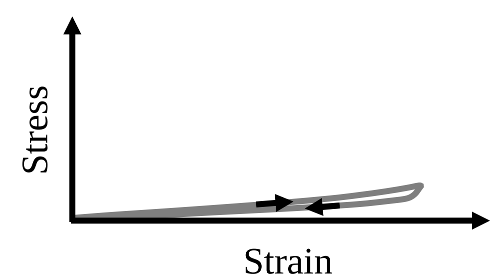


Transparent fixture

Plastomeric hard network



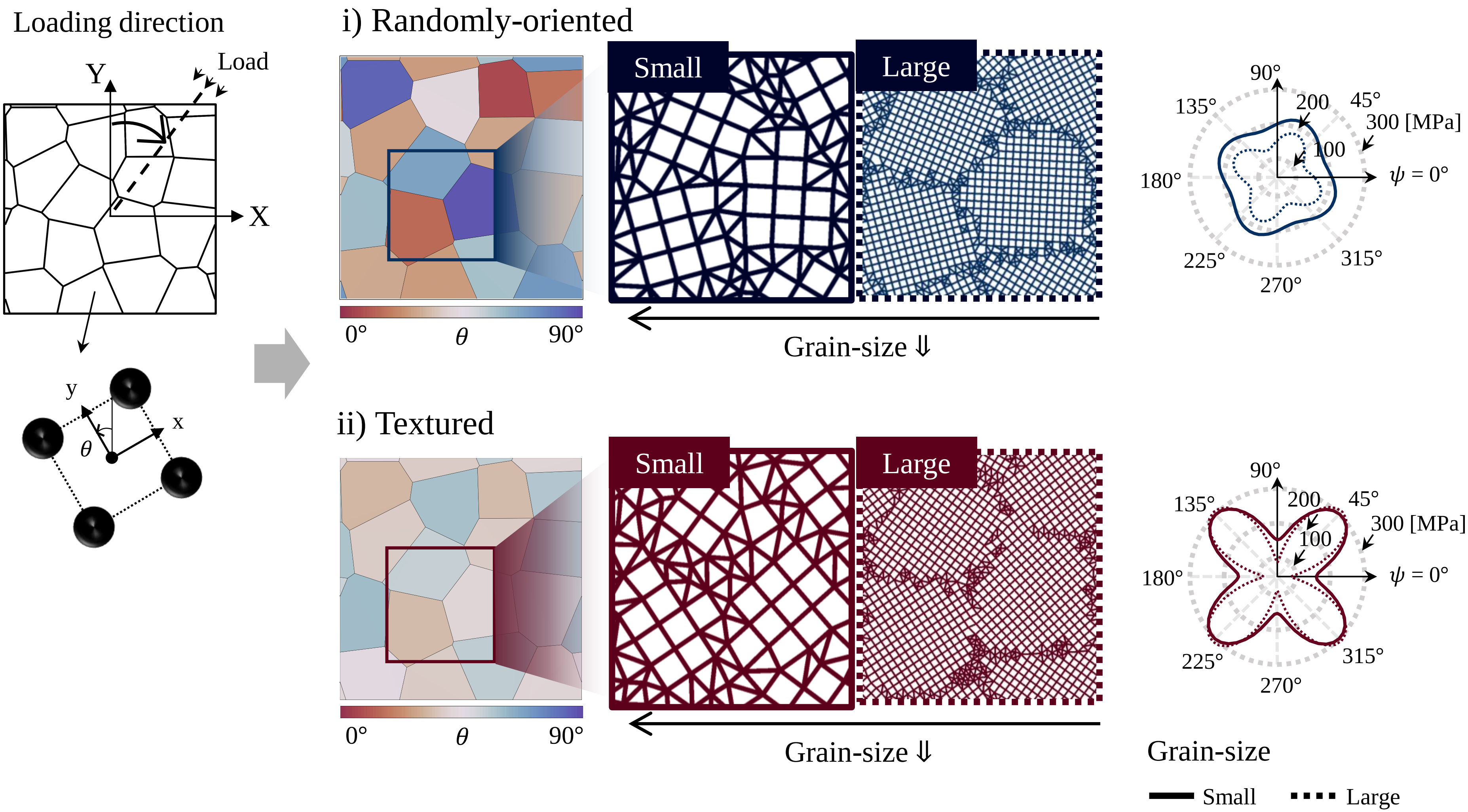
Elastomeric soft matrix



* Volume fraction of the “hard” polycrystalline network = 40%

Directional stiffness - Anisotropy

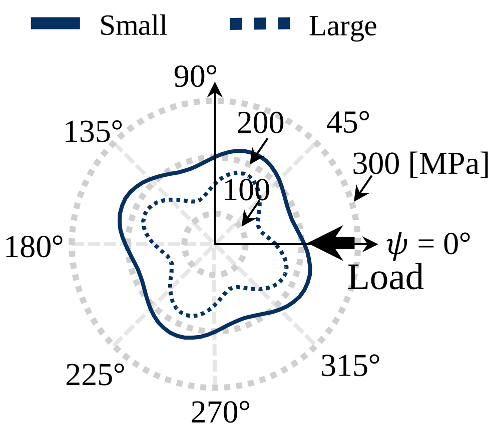
Loading direction-dependent elastic modulus

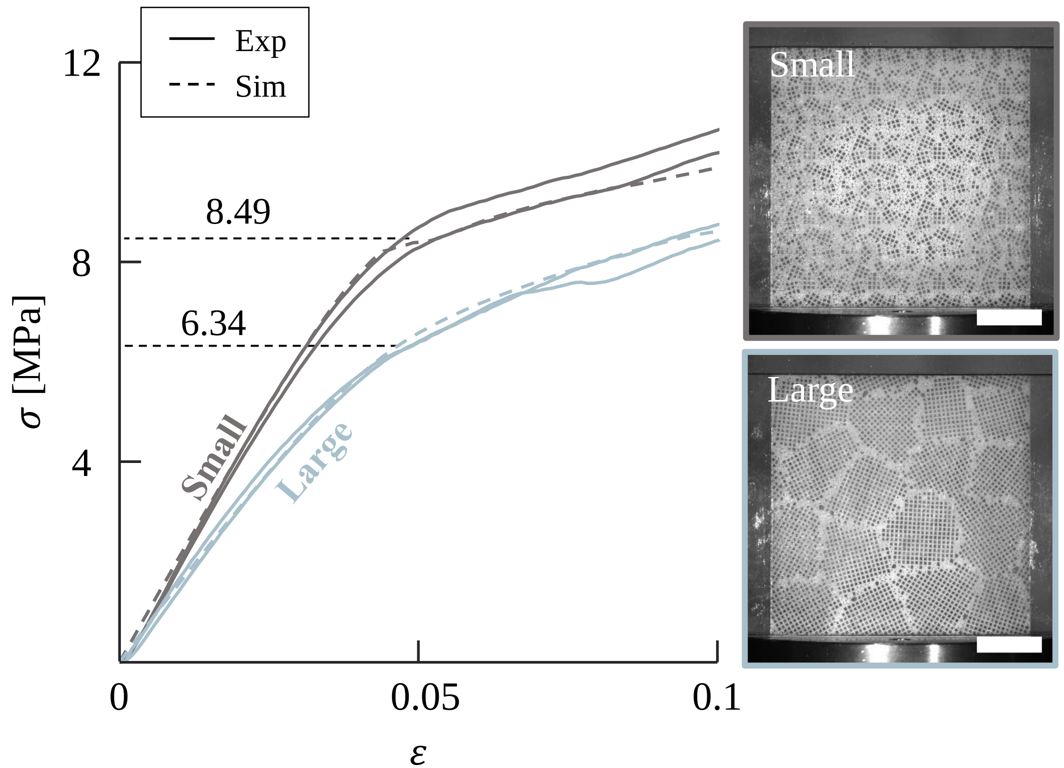


Grain-size effect

i) **Randomly-oriented** polycrystalline architected materials

- **High connectivity throughout grain boundaries** enhances the mechanical responses as grain-size decreases

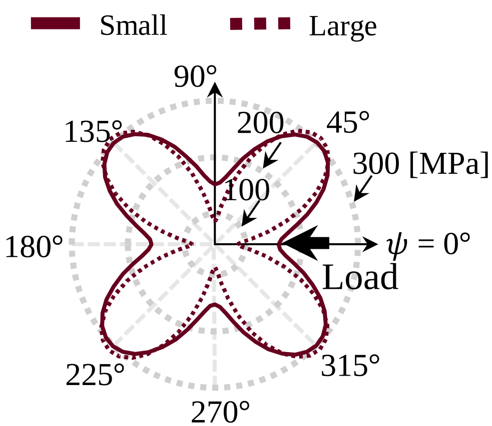


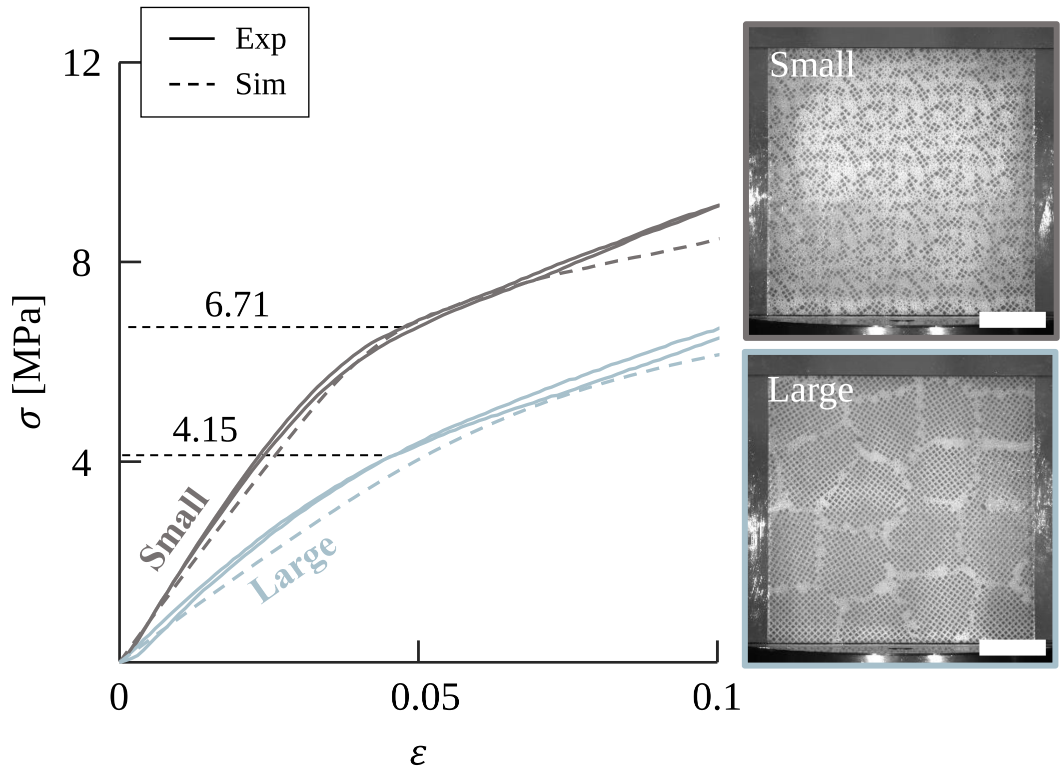


Grain-size effect

ii) **Textured** polycrystalline architected materials

- **High connectivity throughout grain boundaries** enhances the mechanical responses as grain-size decreases

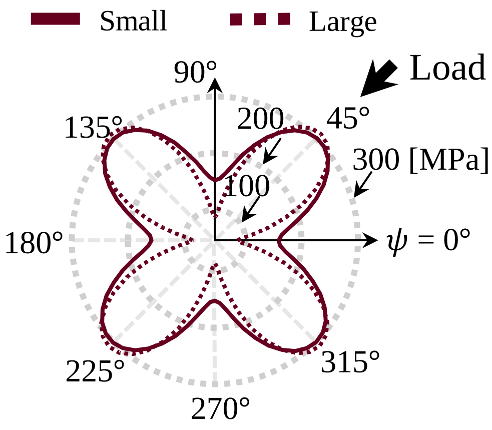


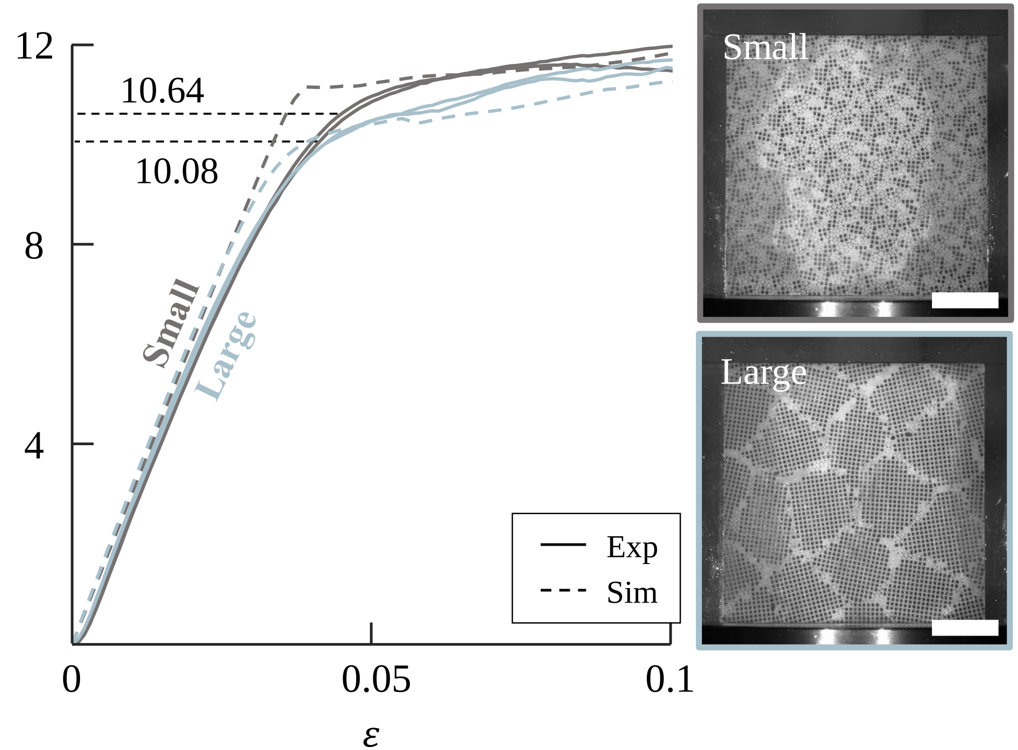


Grain-size effect

ii) **Textured** polycrystalline architected materials

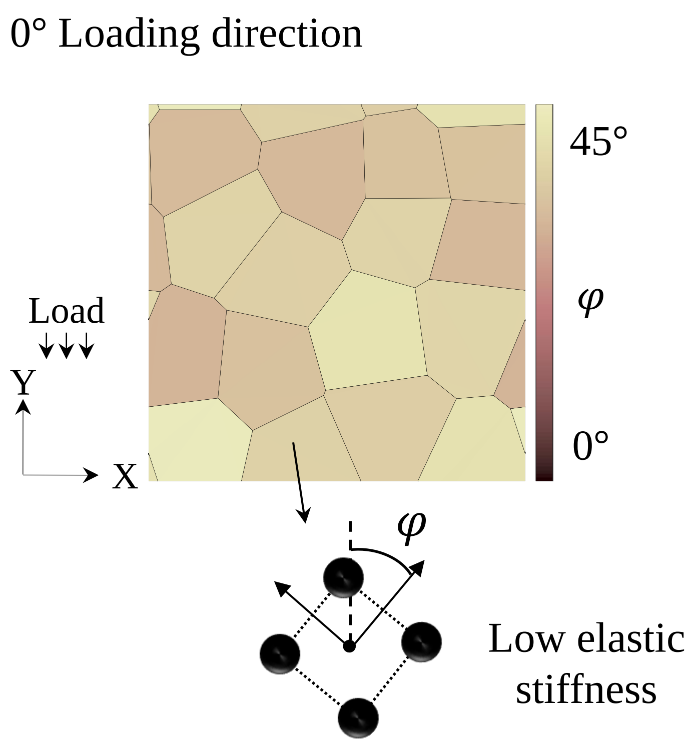
- **Degree of connectivity** throughout grain boundaries **does not sufficiently account for** the grain-size effects

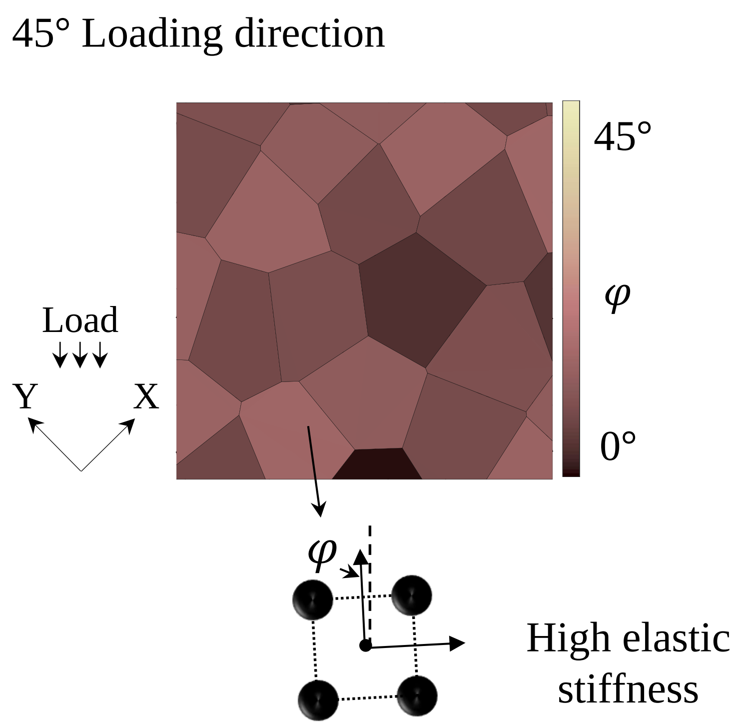




Grain-size effect

- **"Strength" of grain boundaries relative to grains**
  is the key to understanding grain-size dependent mechanical features



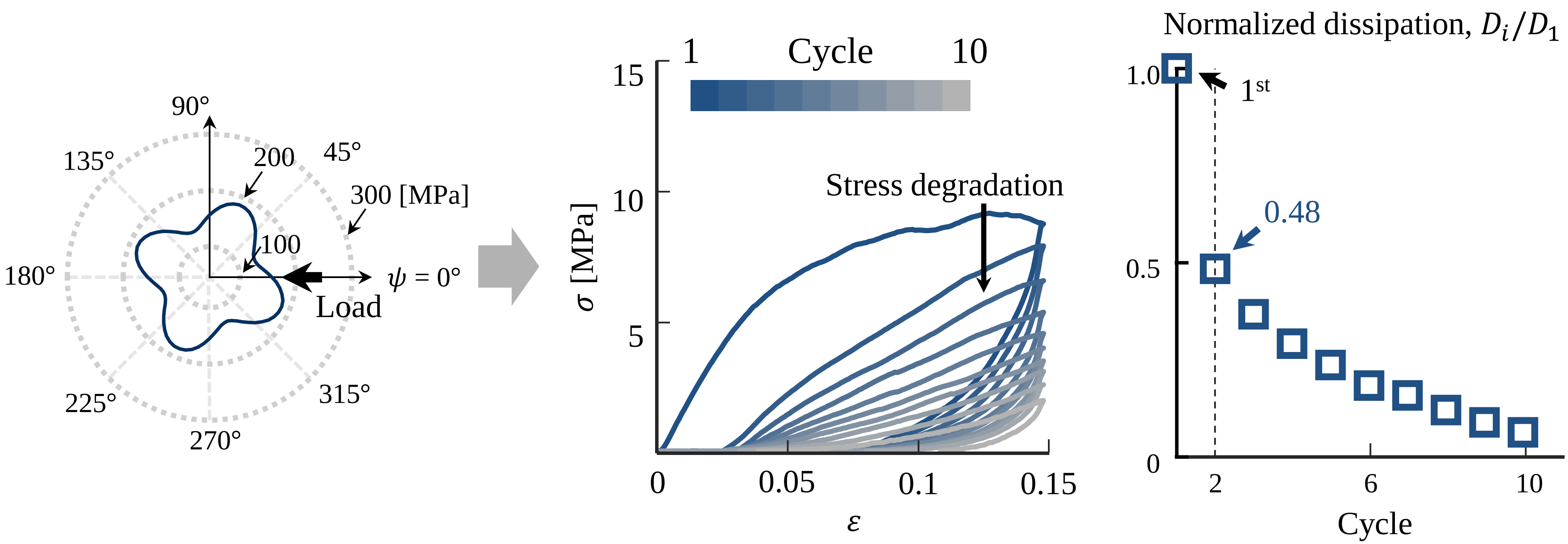


More apparent grain-size effects

Role of GBs in failures

i) **Randomly-oriented** polycrystalline architected materials (Grain-size : Large)

- **Stress degradation** during the multiple cycles ($\dot{\varepsilon}$ = 0.01/s)
- **Local failures** are observed

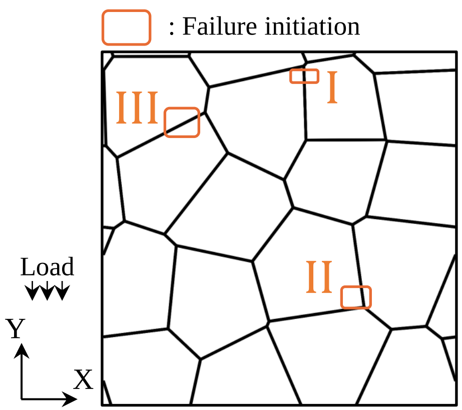


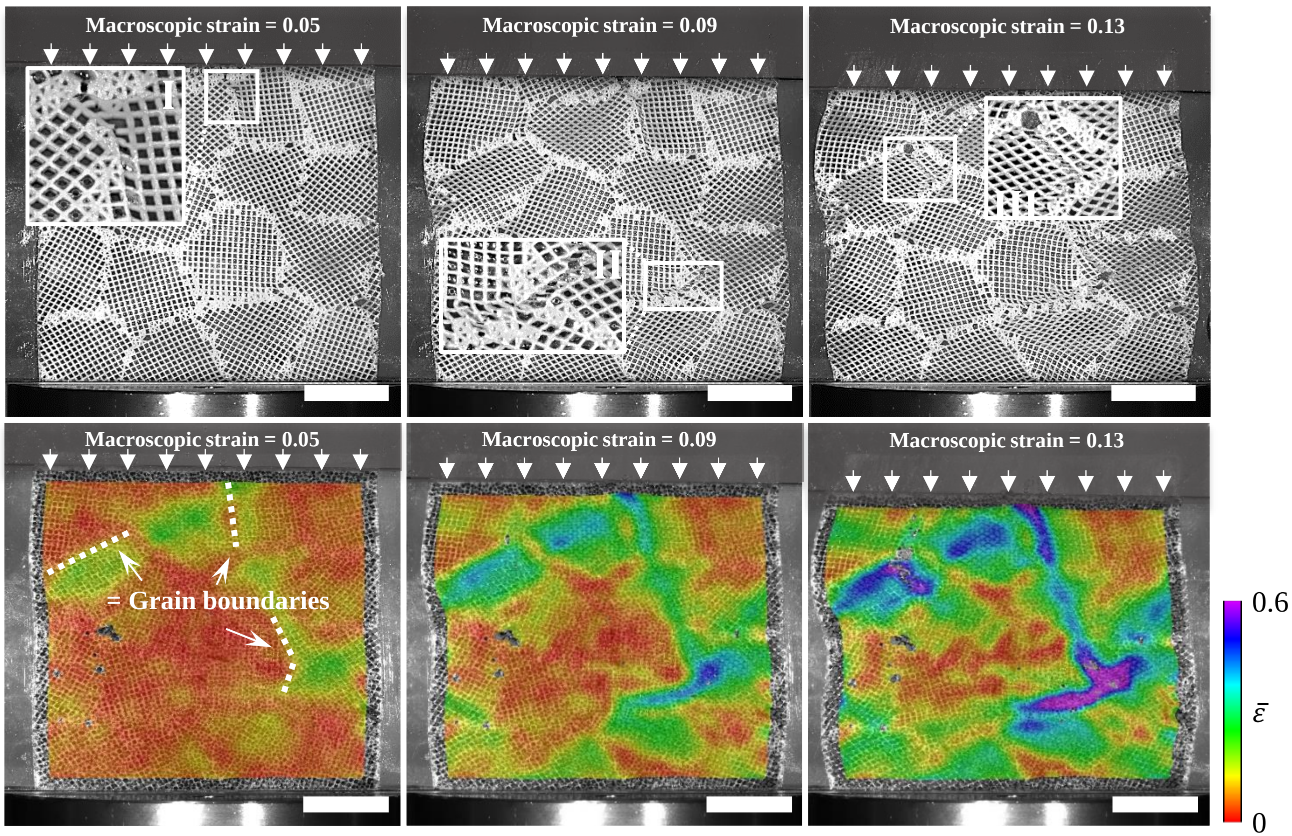
* Idling time for recovery between cycles : 1 hour

Role of GBs in failures

i) **Randomly-oriented** polycrystalline architected materials (Grain-size : Large)

- Local failures are observed to initiate at **grain boundaries** with **significant inhomogeneous deformation**





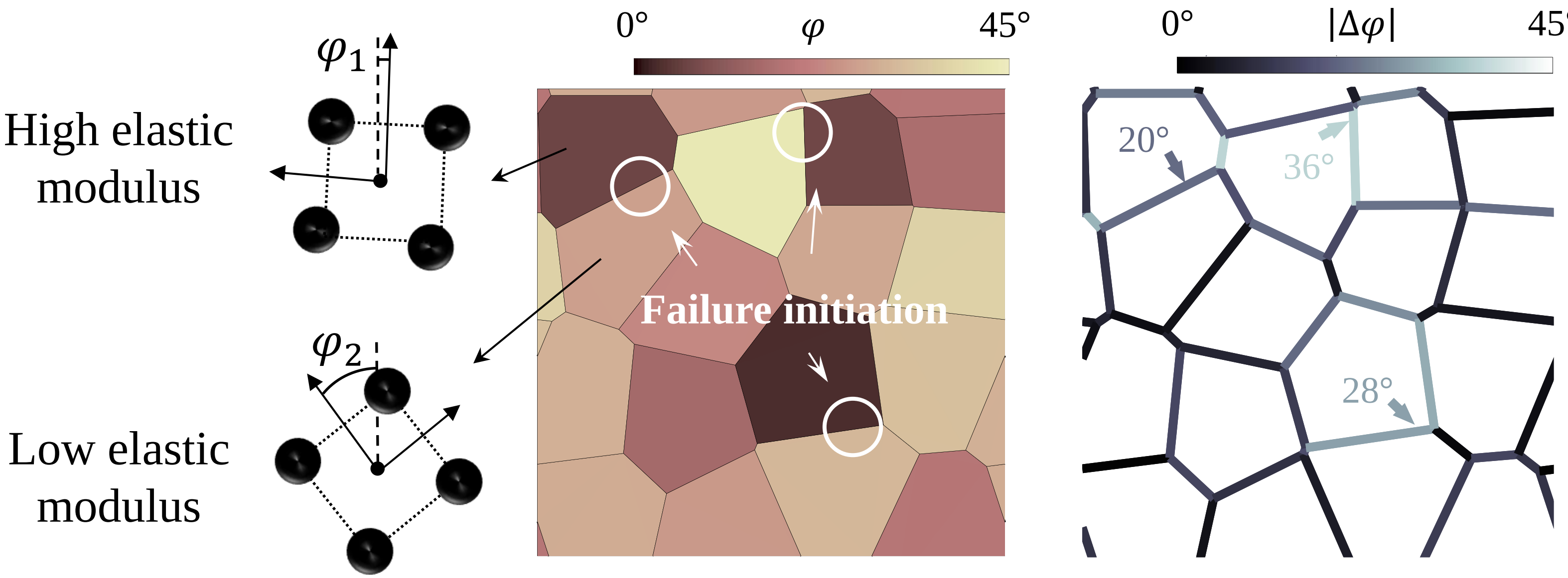
* 1st loading cycle

Role of GBs in failures

i) **Randomly-oriented** polycrystalline architected materials (Grain-size : Large)

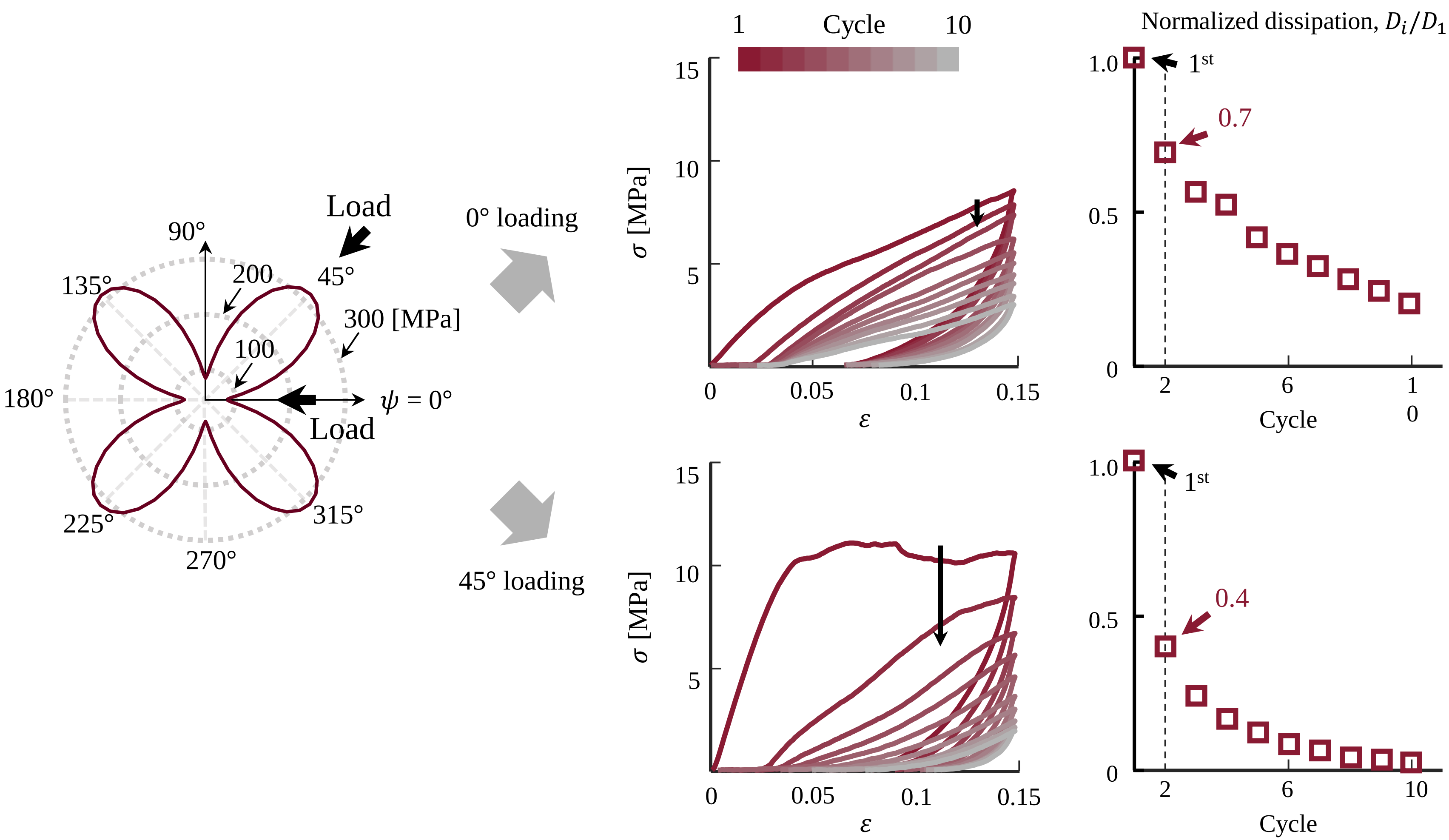
- Inter-grain deformation inhomogeneity due to **elastic anisotropy** of crystal lattice

⇒ **Stress concentration** at grain boundaries



Role of GBs in failures

ii) **Textured** polycrystalline architected materials (Grain-size : Large)



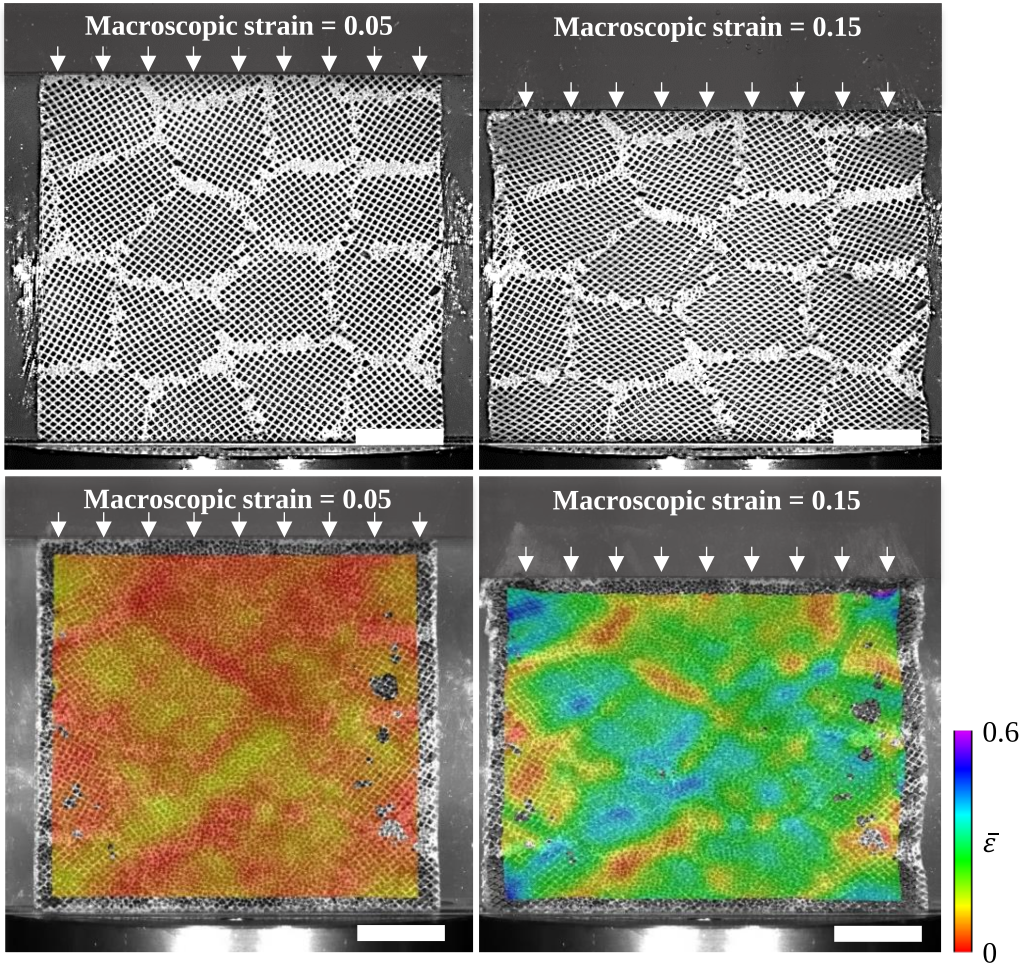
* Idling time for recovery between cycles : 1 hour

Role of GBs in failures

ii) **Textured** polycrystalline architected materials : **0° loading**

- **No significant** local failures

  ⇒ **Low** stress degradation



* 1st loading cycle

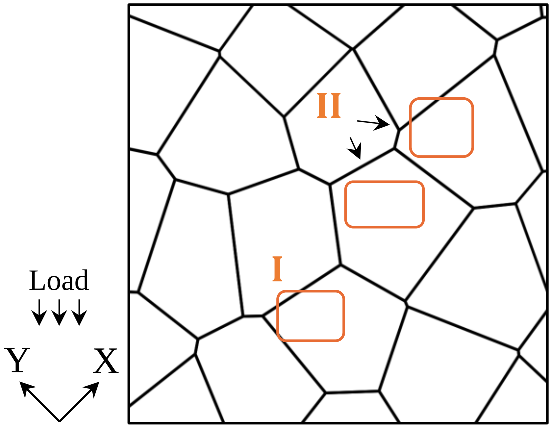
Role of GBs in failures

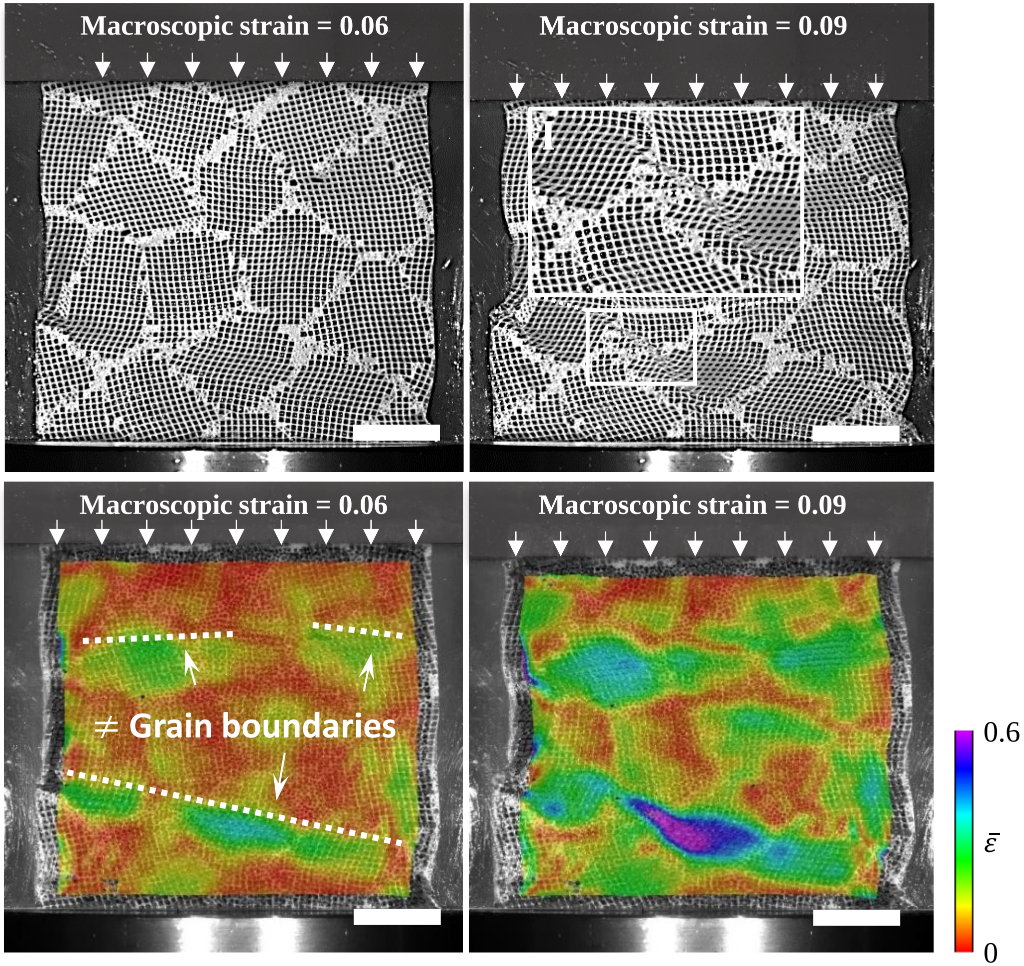
ii) **Textured** polycrystalline architected materials : **45° loading**

- **Significant** local failures

  ⇒ **Large** stress degradation

- Local failures are observed to initiate at **grain interiors**



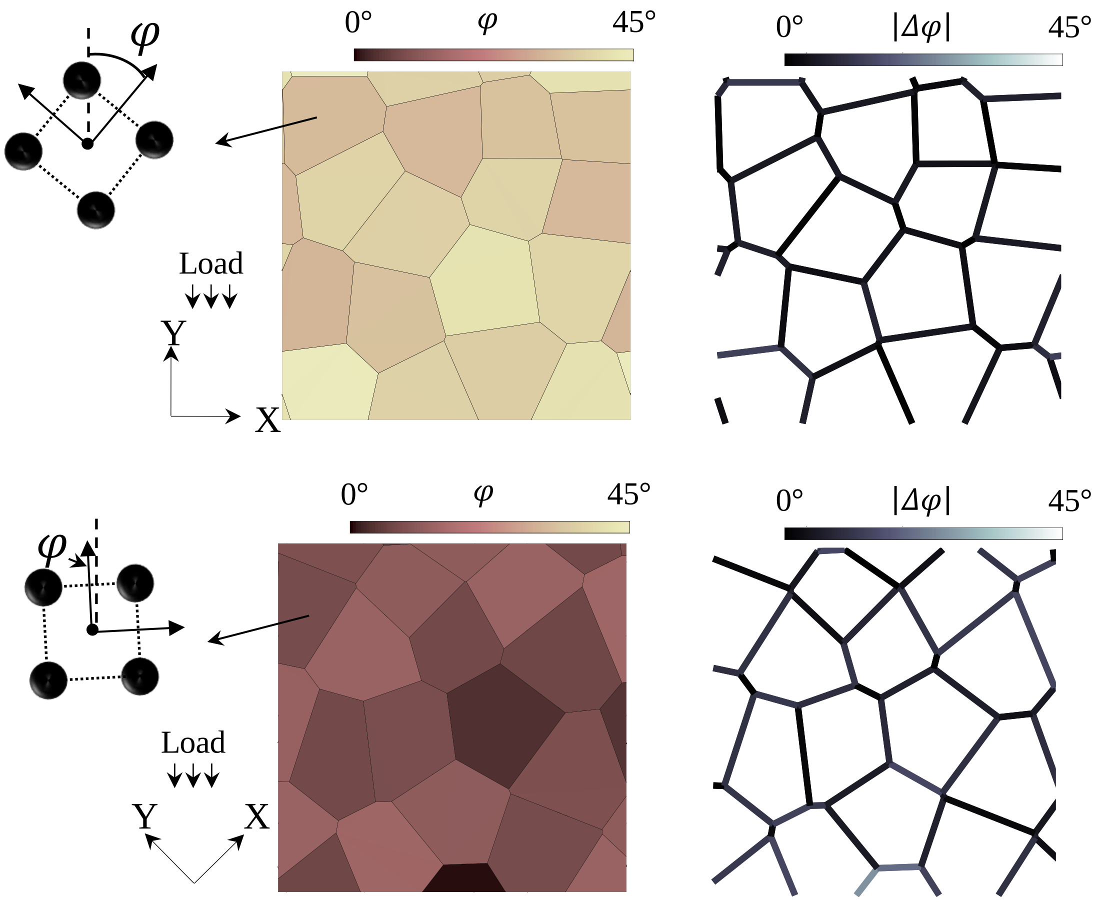


* 1st loading cycle

Role of GBs in failures

ii) **Textured** polycrystalline architected materials

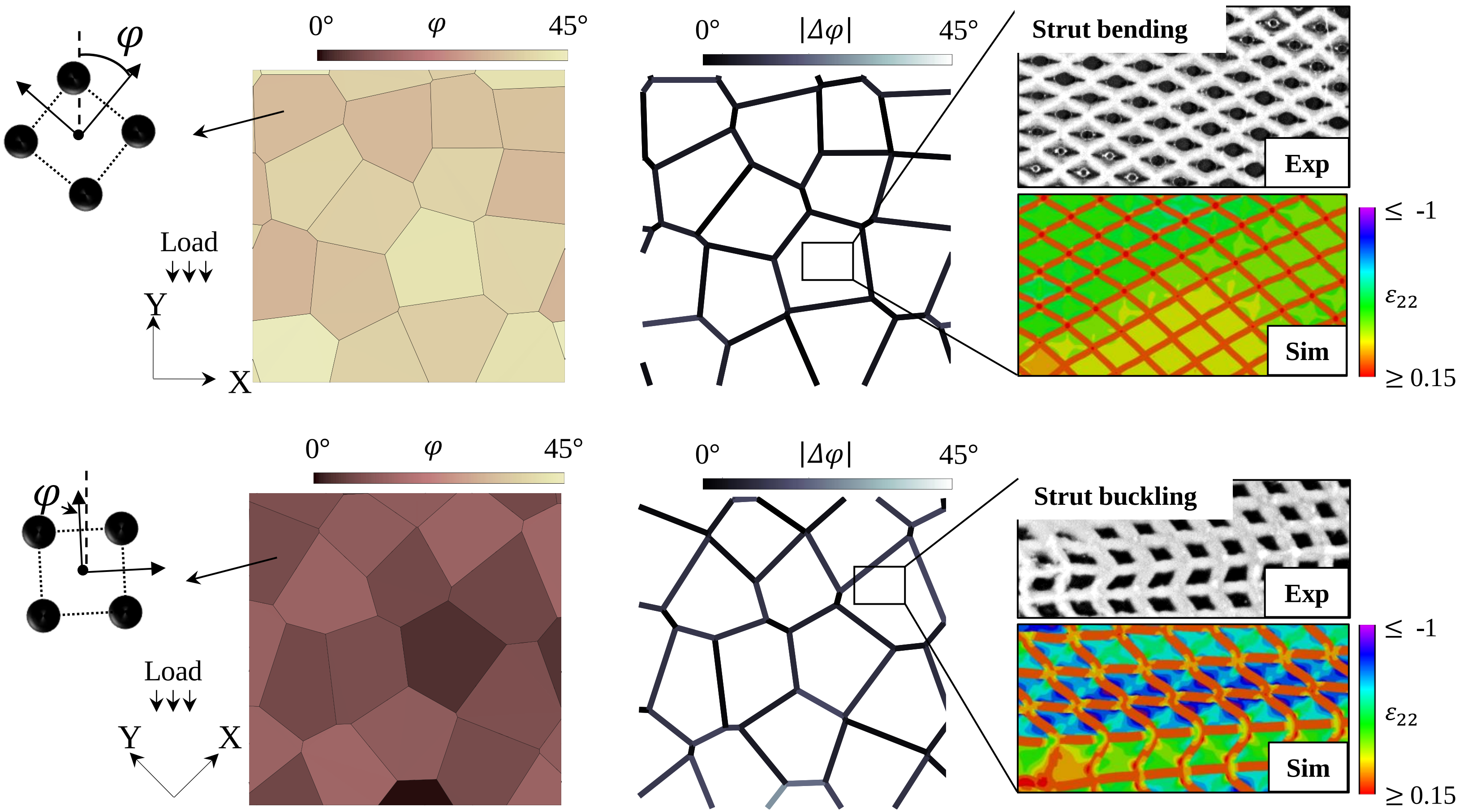
- Grain boundaries **do not strongly influence** the local failures due to **small** $|\Delta\varphi|$



Role of GBs in failures

ii) **Textured** polycrystalline architected materials

- **Microstructures in each of the grains** reveal the underlying failure mechanisms



* Macroscopic engineering strain = 15%

Conclusion and Future works

- **Grain boundaries** play a crucial role in **grain-size dependent mechanical features** and **failures**

  i) The **"strength" of grain boundaries relative to grains** is the key to tailoring grain-size dependent mechanical features

  ii) **Grain boundaries** with **large strain incompatibility** significantly impact **failures** in polycrystalline architected materials

- In future, the **damage**, **fracture** and **toughness** in these polycrystalline architected materials will be explored via **experiments** and **phase-field-based numerical simulations**[19-23]

Acknowledgement

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