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Stiffness, strength and reusability in architected polycrystals

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Mechanics & Extremes
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Heterogeneous materials

- Heterogeneous materials consist of **inelastic** “**hard**” and **elastic** “**soft**” domains[1-3]
  e.g., two-phase elastomers, copolymers, etc.
  → **Outstanding properties** including stiffness, strength, energy dissipation and resilience

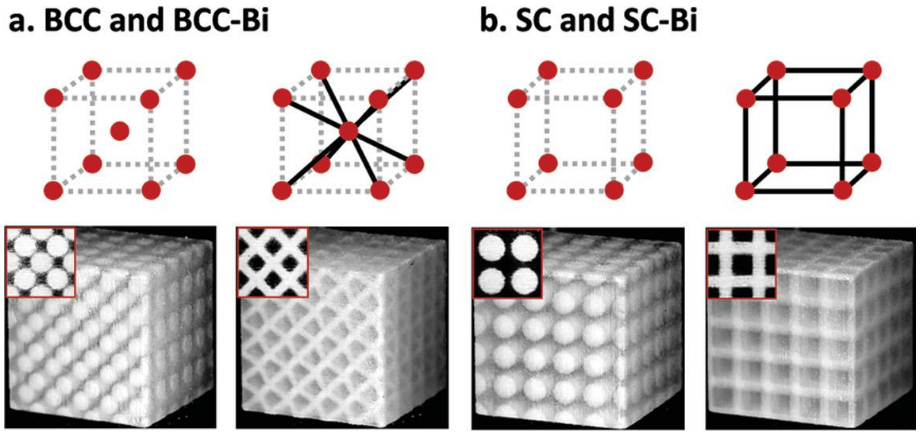
- **Geometric** and **topological features** in **hard phases** govern the macroscopic mechanical responses in heterogeneous materials

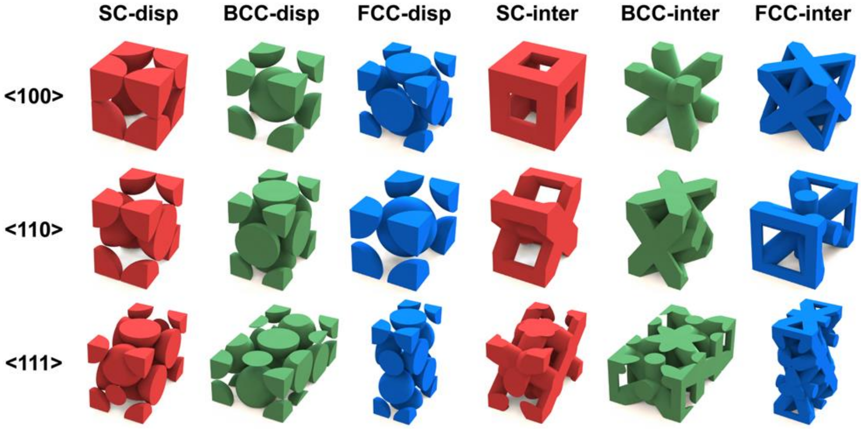
Single-crystalline architected materials

- **Architected** “**heterogenous**” **materials** 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





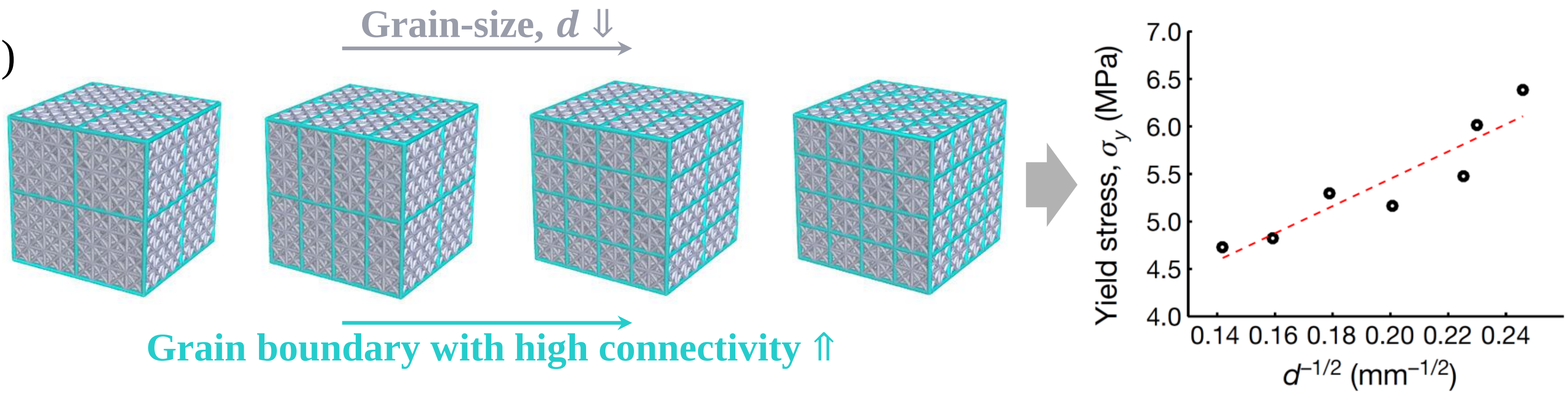
Polycrystalline architected materials

- Mimicking **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]

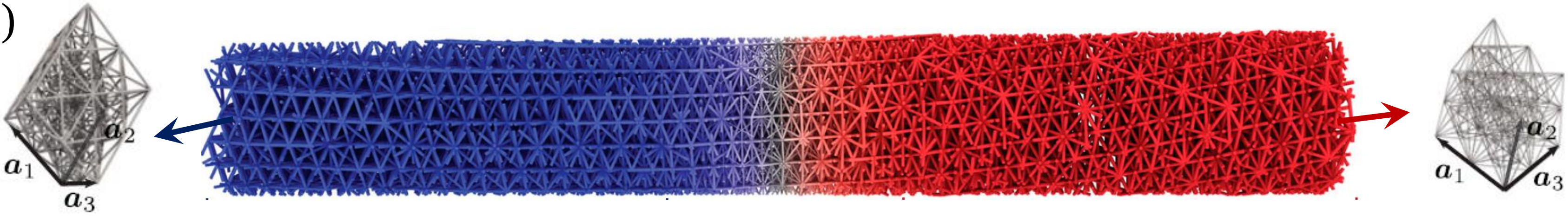
ii) **Spatially-varying** architected materials[15]

i)


Grain-size, *d* ⇓

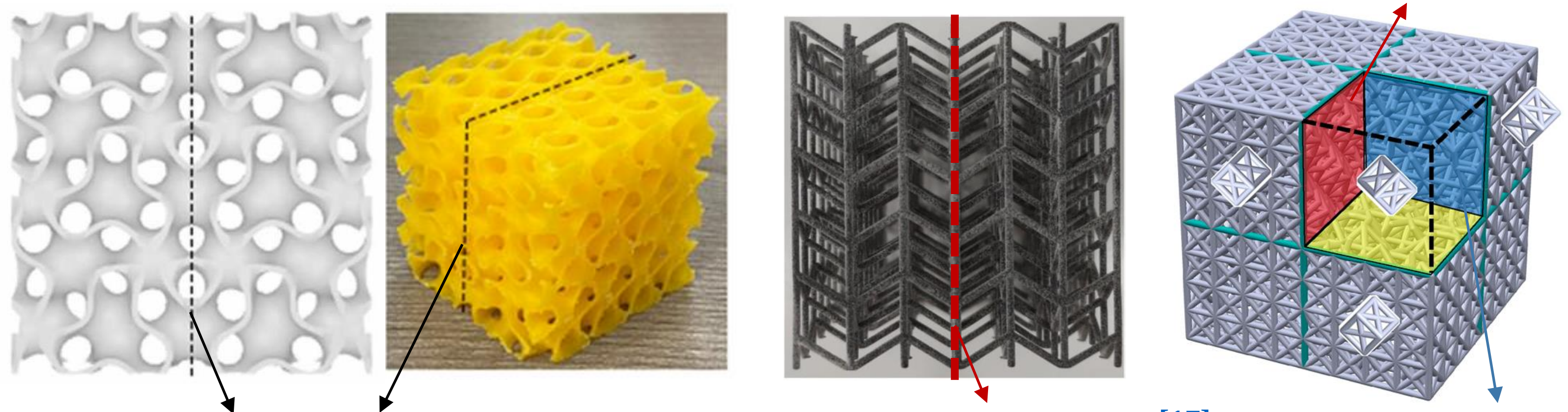
Grain boundary with high connectivity ⇑

ii)



Polycrystalline architected materials

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



Twin boundary[8,9]

Twin boundary[16]

Twin boundary[17]

Twist boundary[8,9]

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

Objectives

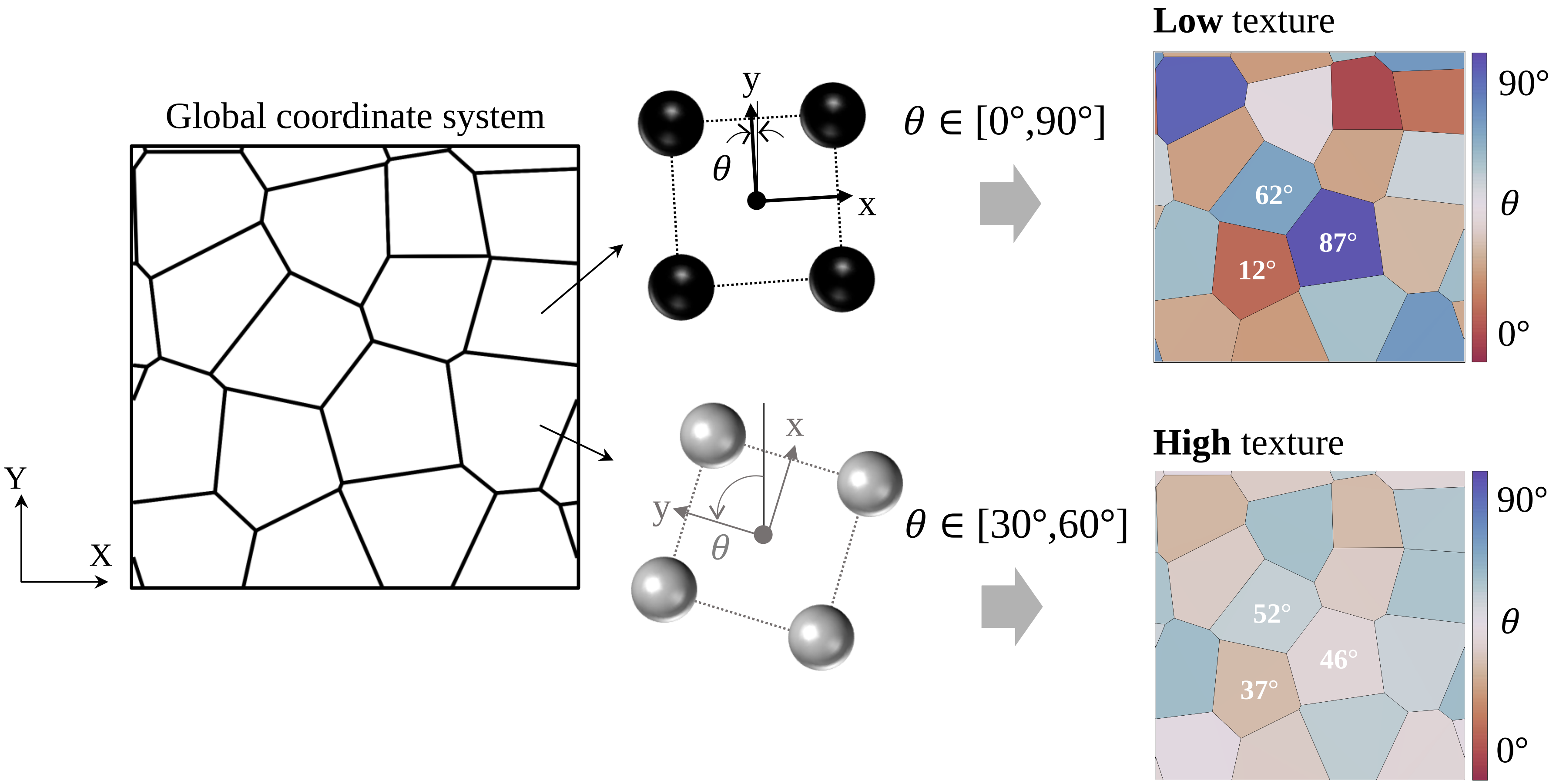
- Emergence of **engineering grain boundary structures** in metallurgy for **architected heterogeneous polycrystals** comprised of **hard** and **soft domains**

- Understanding the role of **grain boundaries** in **grain-size dependent mechanical features** and **reusability** in terms of **energy dissipation** and **load transfer capabilities**

Design procedures

i) Microstructural orientation

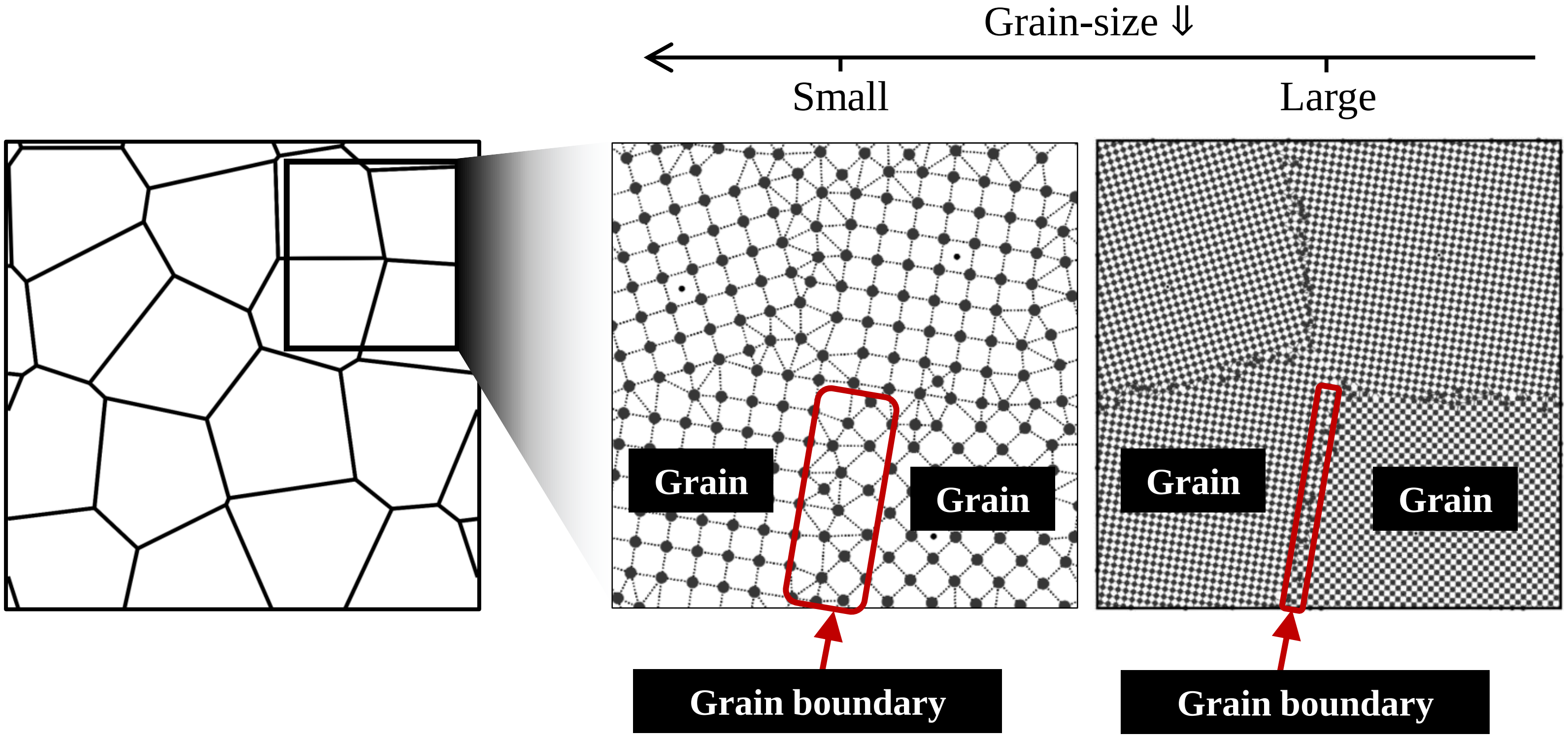
- **Restrict the range** for crystal orientations θ[18]



Design procedures

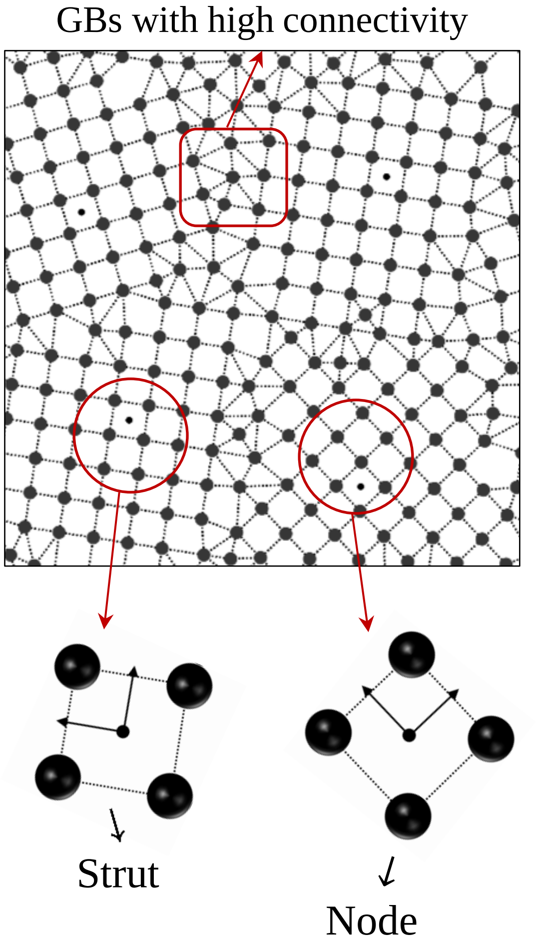
ii) Grain-size

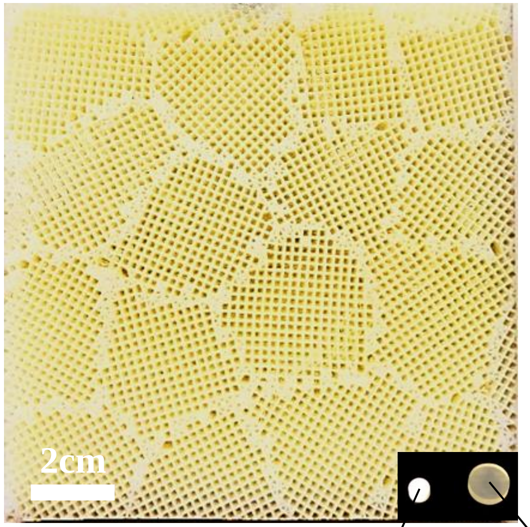
- As **grain-size decreases**, the **volume fraction of grain boundaries** with high strut connectivity **increases**



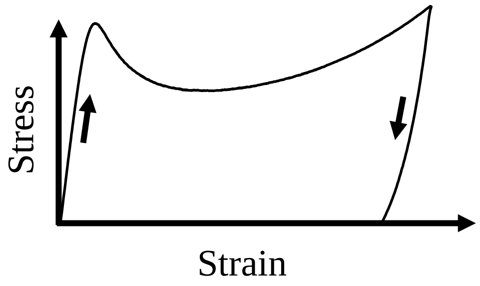
Experimental procedures

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

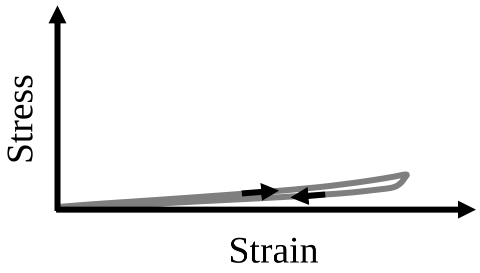




Plastomeric hard network



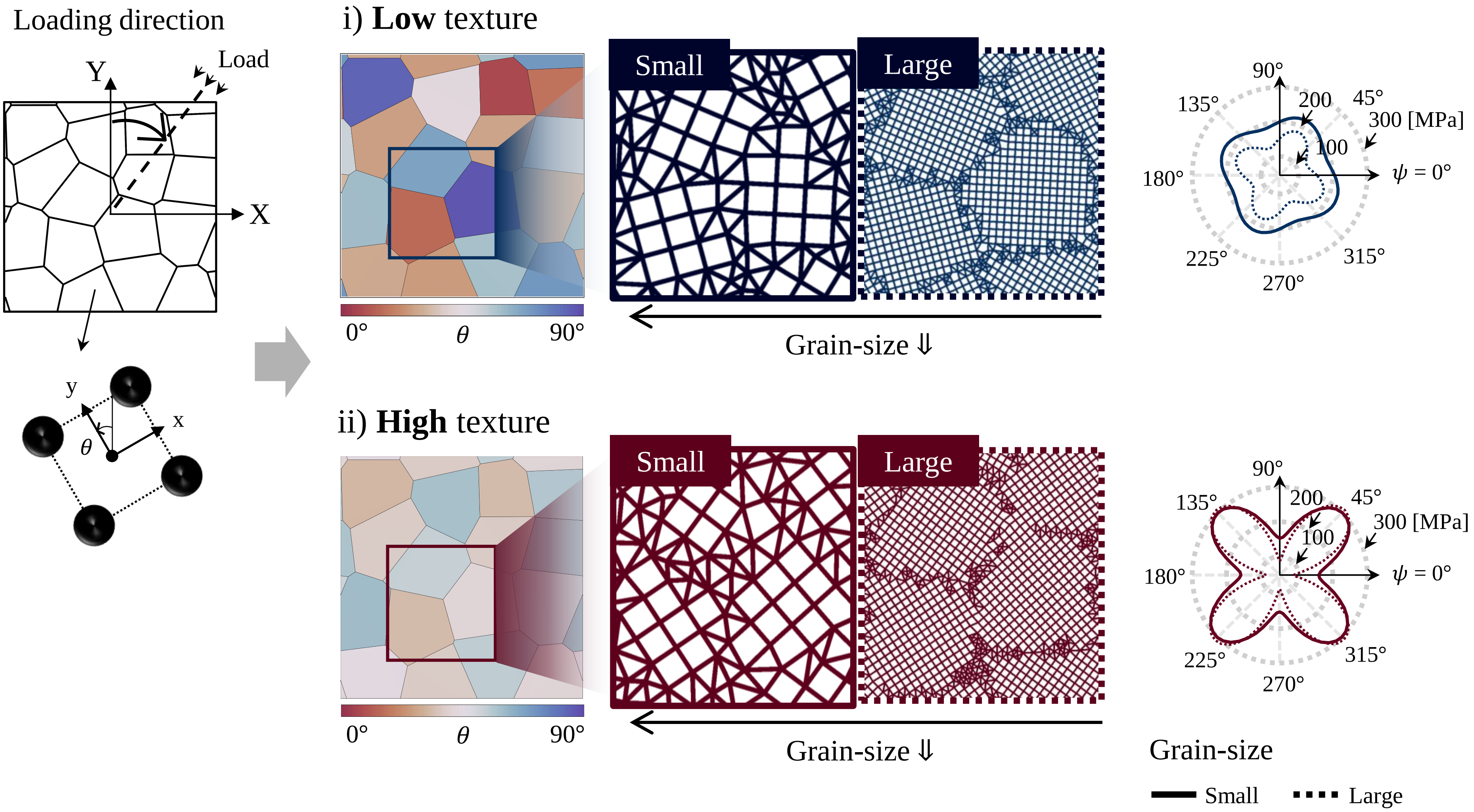
Elastomeric soft matrix



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

Directional stiffness - Anisotropy

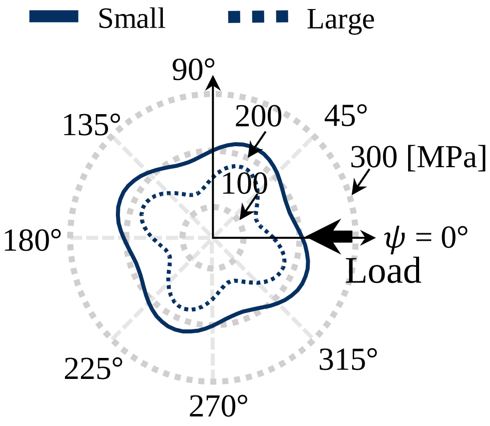
Loading direction-dependent elastic modulus

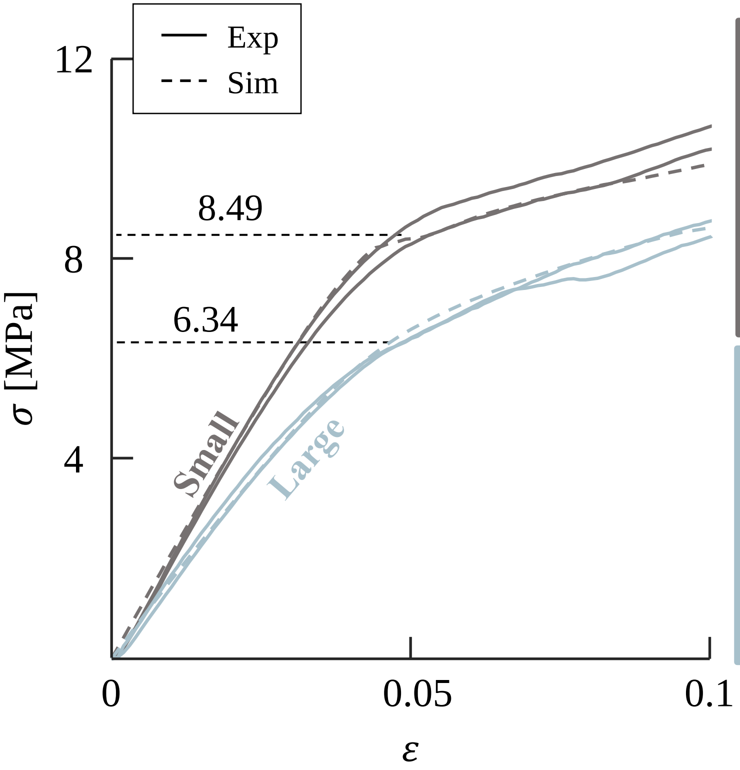


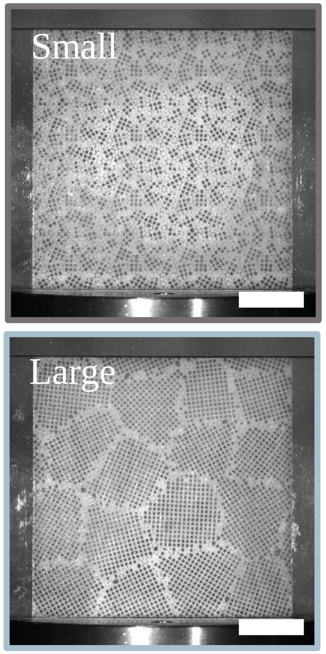
Grain-size effect

i) Architected heterogenous polycrystals with **low texture**

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



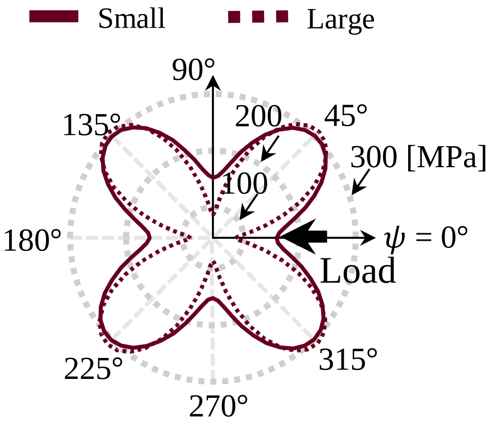


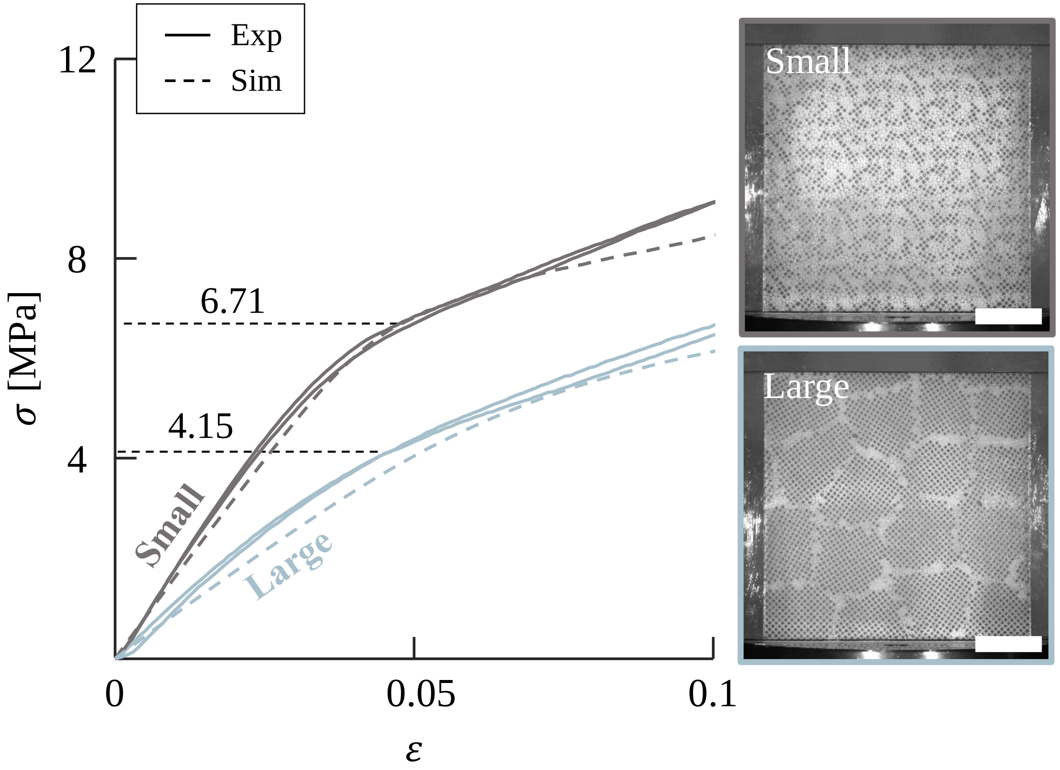


Grain-size effect

ii) Architected heterogenous polycrystals with **high texture**

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

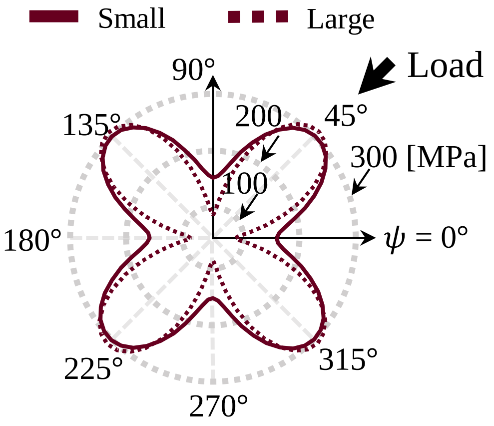


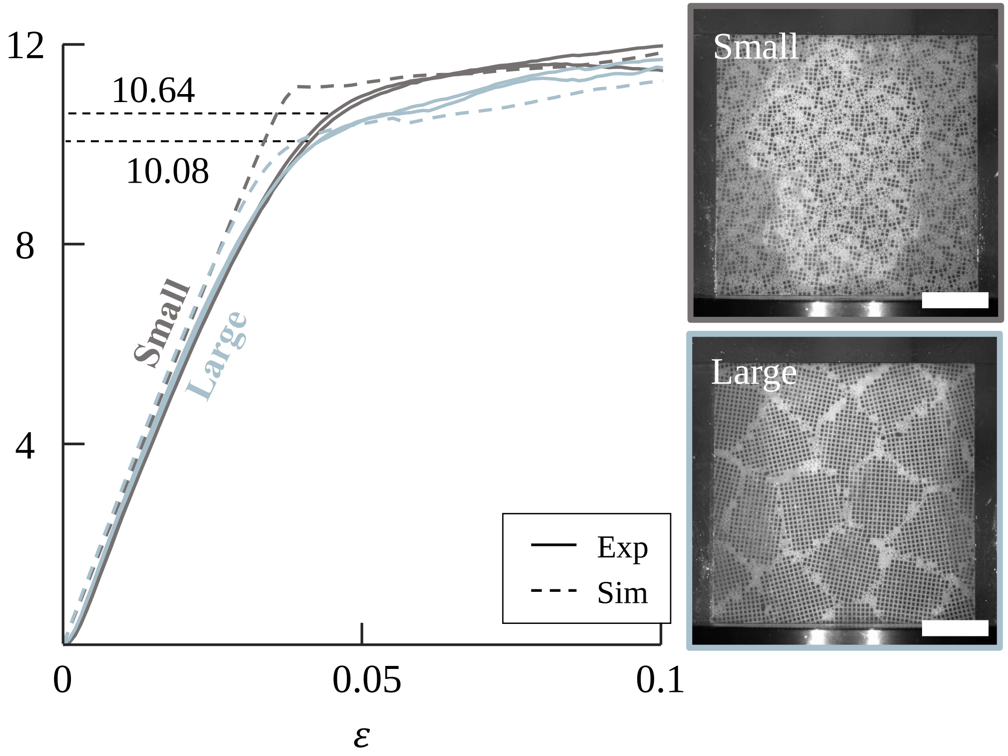


Grain-size effect

ii) Architected heterogenous polycrystals with **high texture**

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

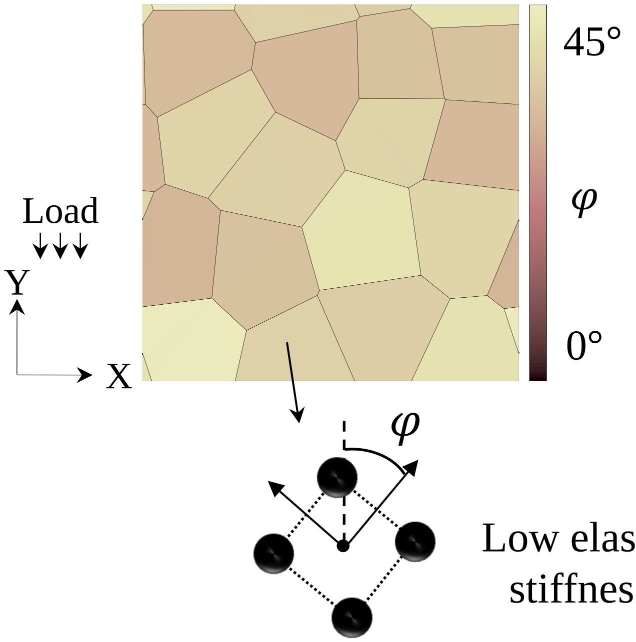




Grain-size effect

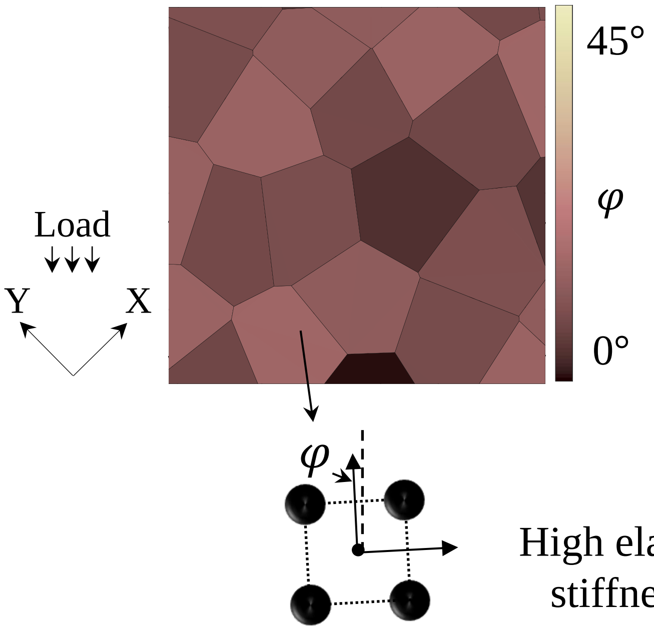
- **“Strength” of grain boundaries relative to grain interiors** is key to understanding grain-size dependent mechanical features

0° Loading direction



Low elastic stiffness

45° Loading direction



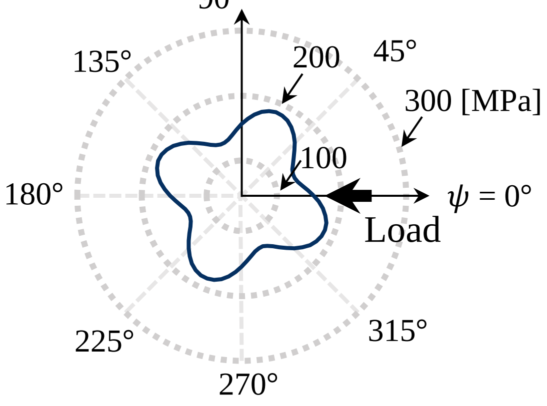
High elastic stiffness

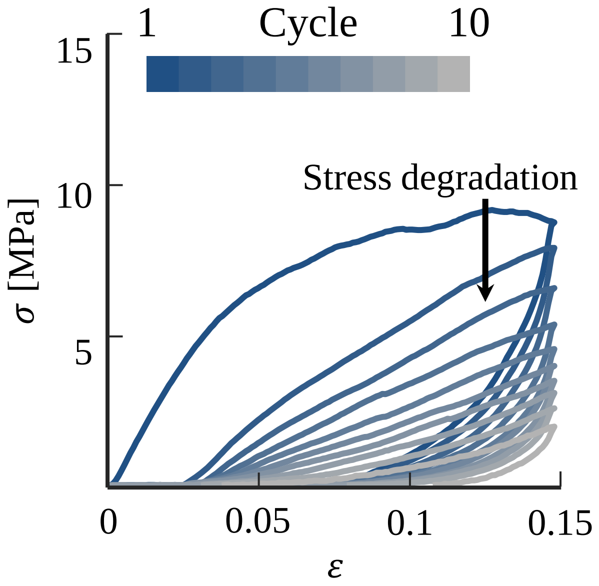
More apparent grain-size effects

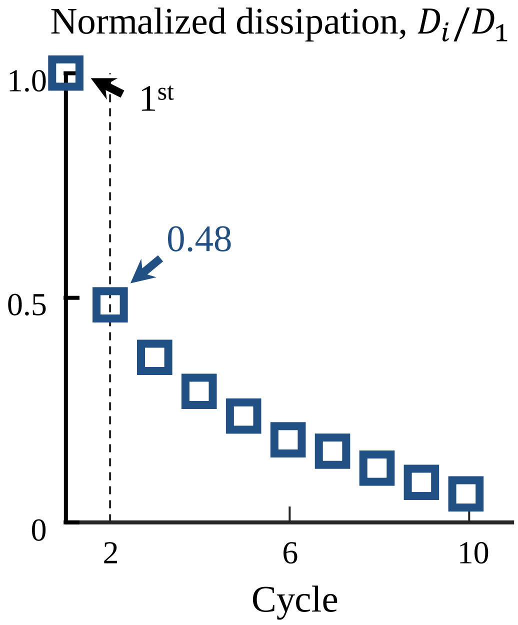
Role of GBs in load transfer and energy dissipation

i) Architected heterogenous polycrystals with **low texture** (Grain-size : Large)

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





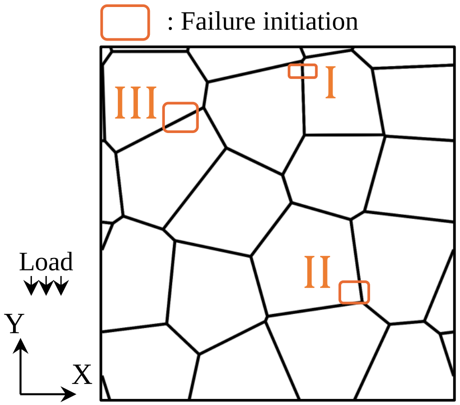


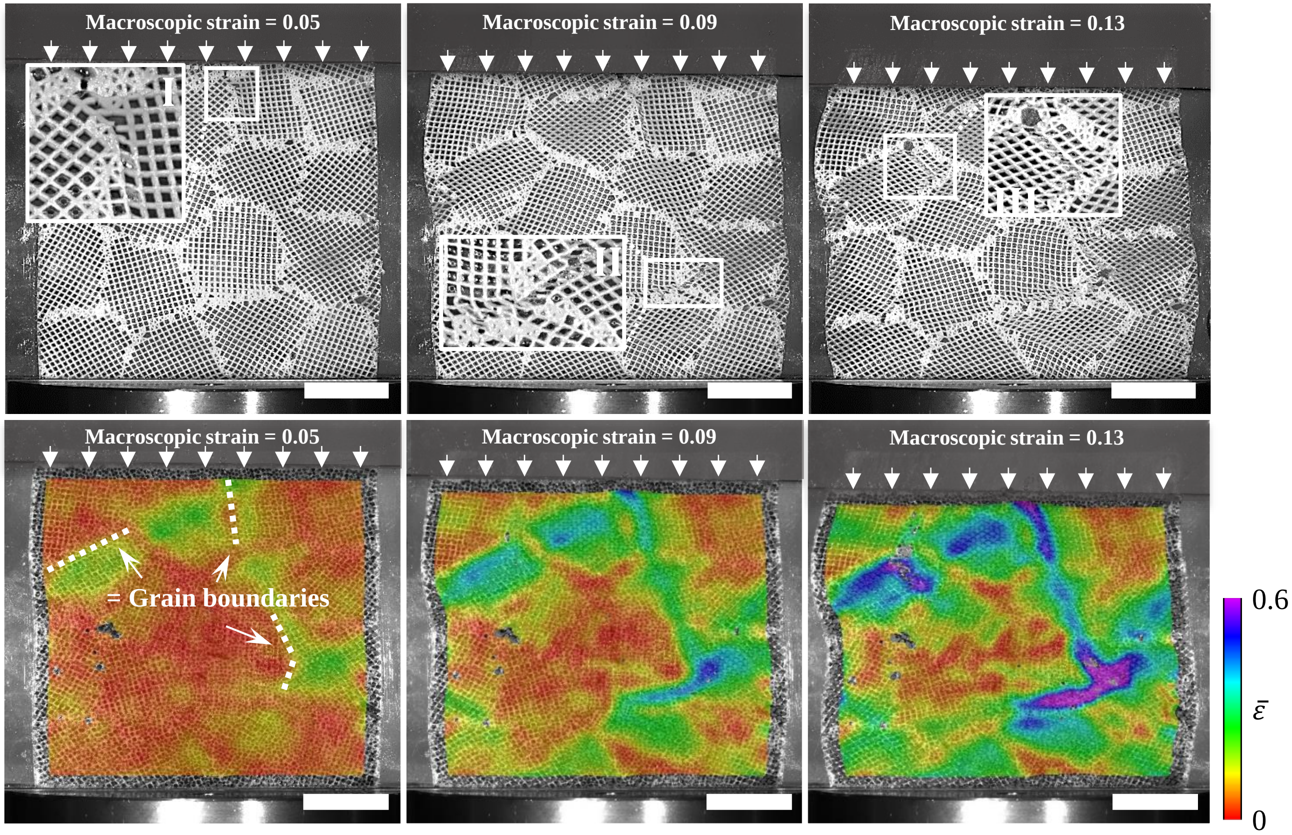
* Idling time for recovery between cycles : 1 hour

Role of GBs in load transfer and energy dissipation

i) Architected heterogenous polycrystals with **low texture** (Grain-size : Large)

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





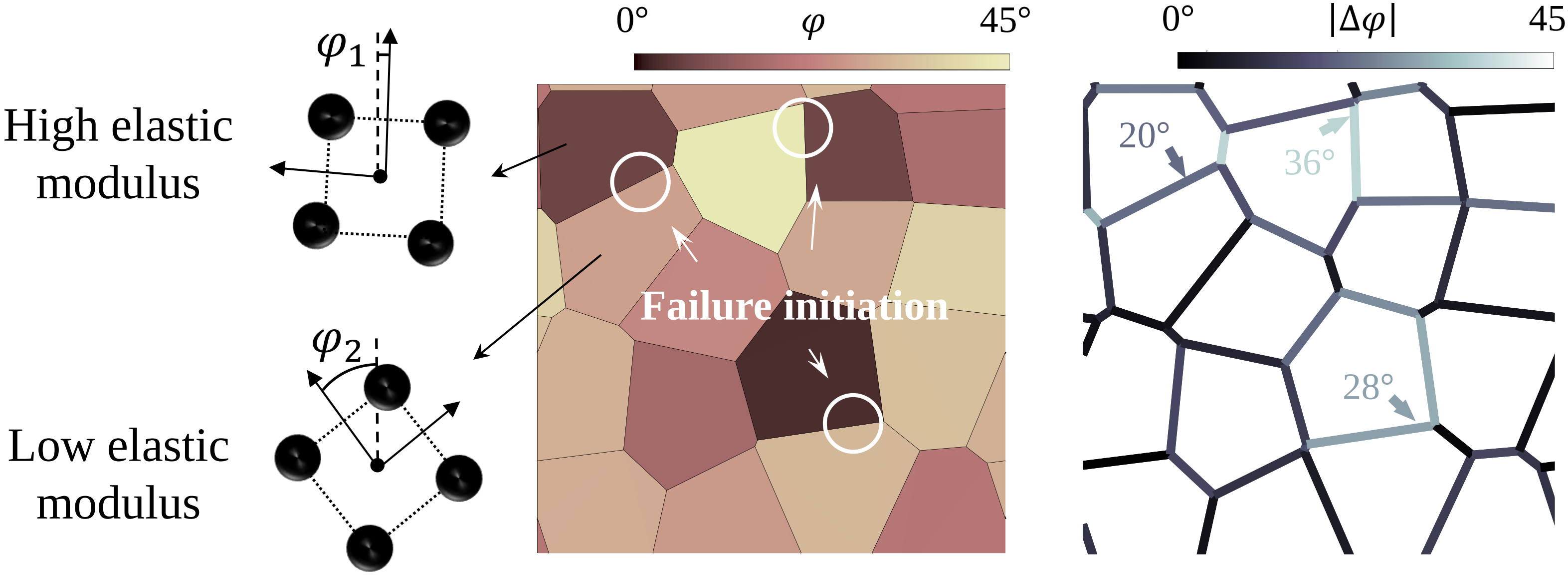
* 1st loading cycle

Role of GBs in load transfer and energy dissipation

i) Architected heterogenous polycrystals with **low texture** (Grain-size : Large)

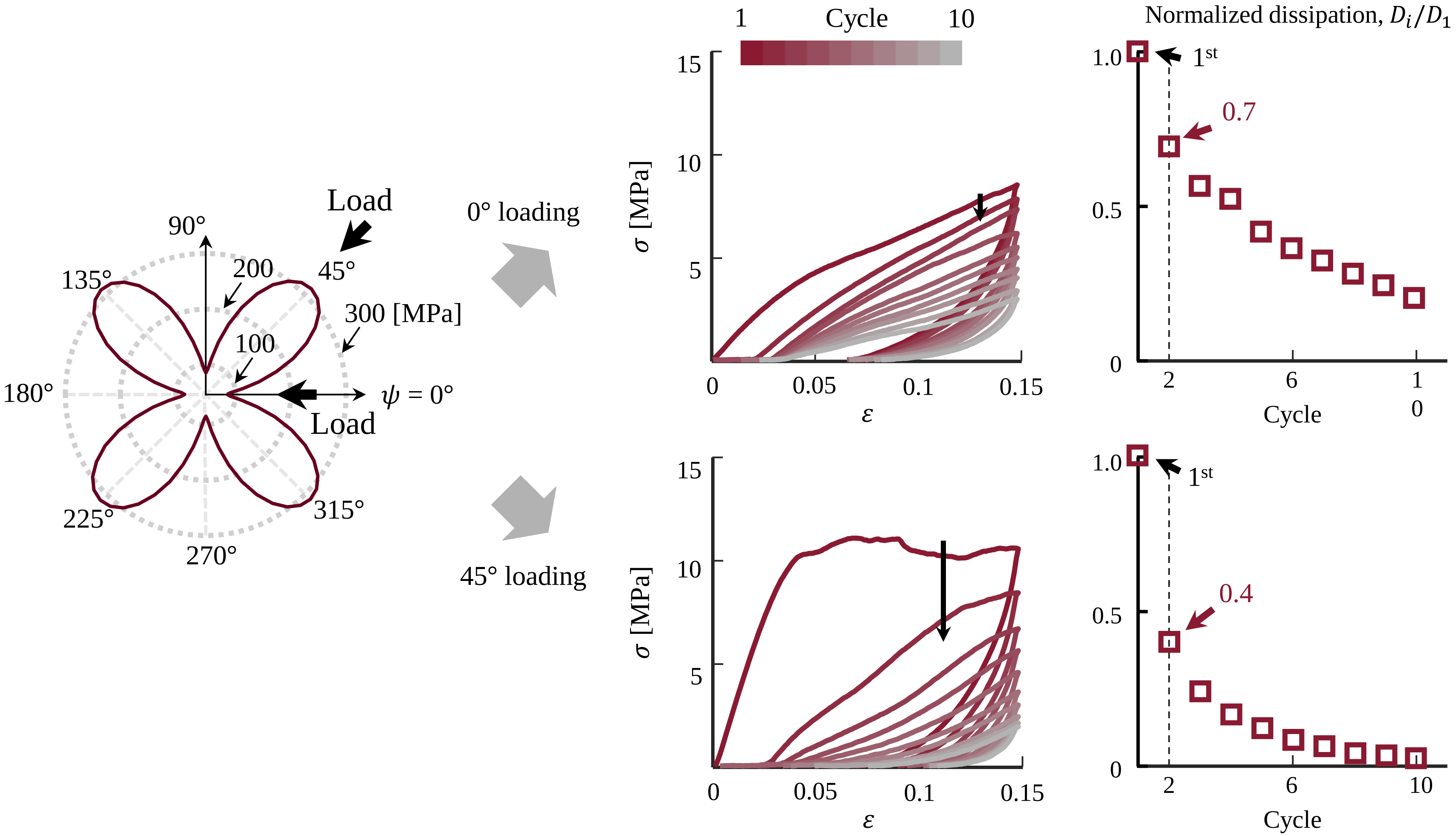
- Inter-grain deformation inhomogeneity due to **elastic anisotropy** of crystal lattice

⇒ **Stress concentration** at grain boundaries



Role of GBs in load transfer and energy dissipation

ii) Architected heterogenous polycrystals with **high texture** (Grain-size : Large)



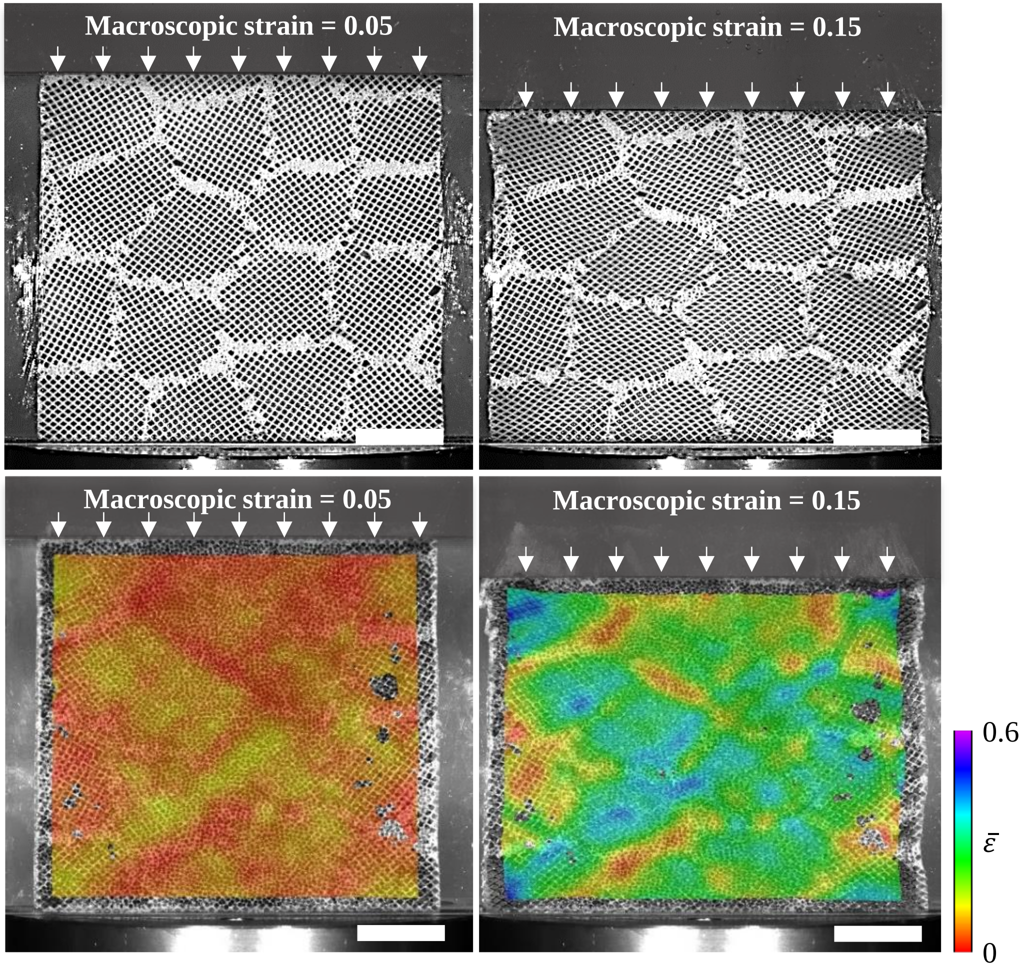
* Idling time for recovery between cycles : 1 hour

Role of GBs in load transfer and energy dissipation

ii) Architected heterogenous polycrystals with **high texture** : **0° loading**

- **No significant** local failures

⇒ **Low** stress degradation



* 1st loading cycle

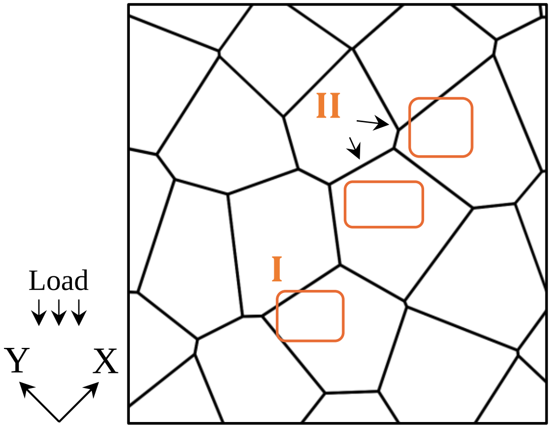
Role of GBs in load transfer and energy dissipation

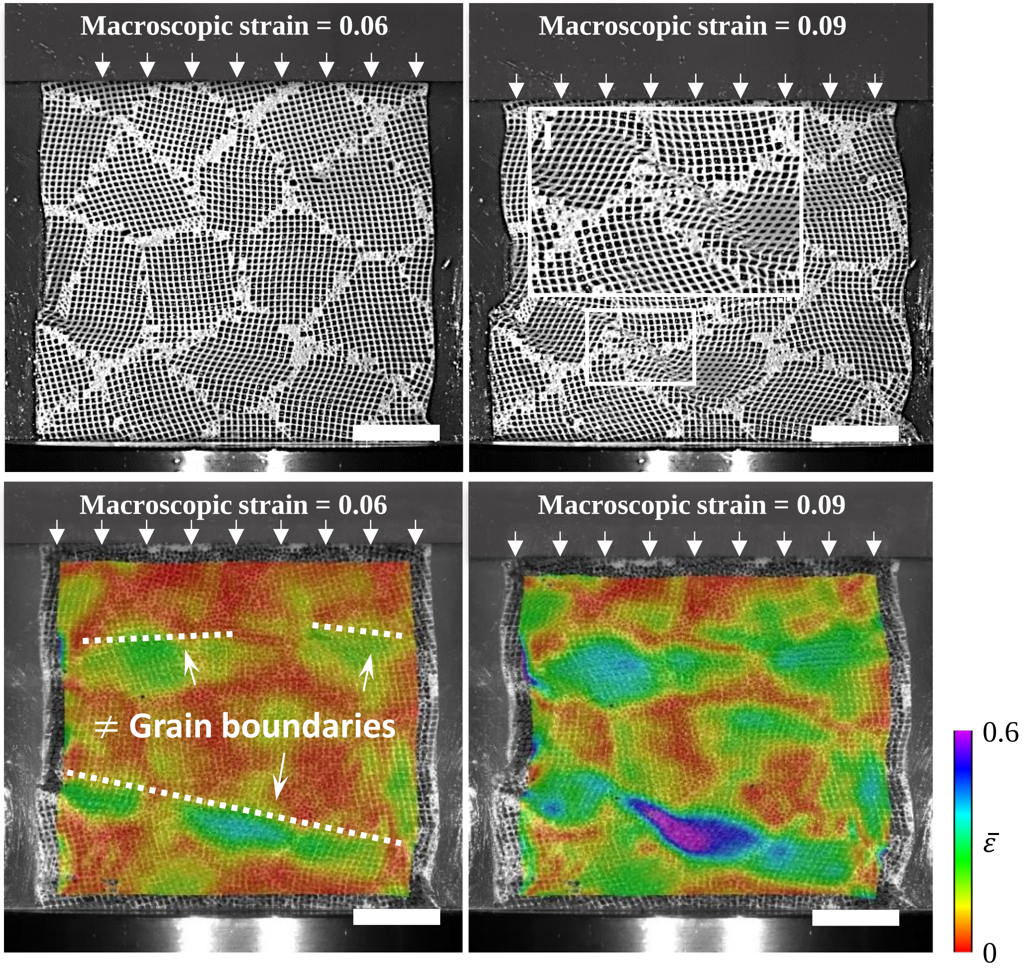
ii) Architected heterogenous polycrystals with **high texture** : **45° loading**

- **Significant** local failures

  ⇒ **Large** stress degradation

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



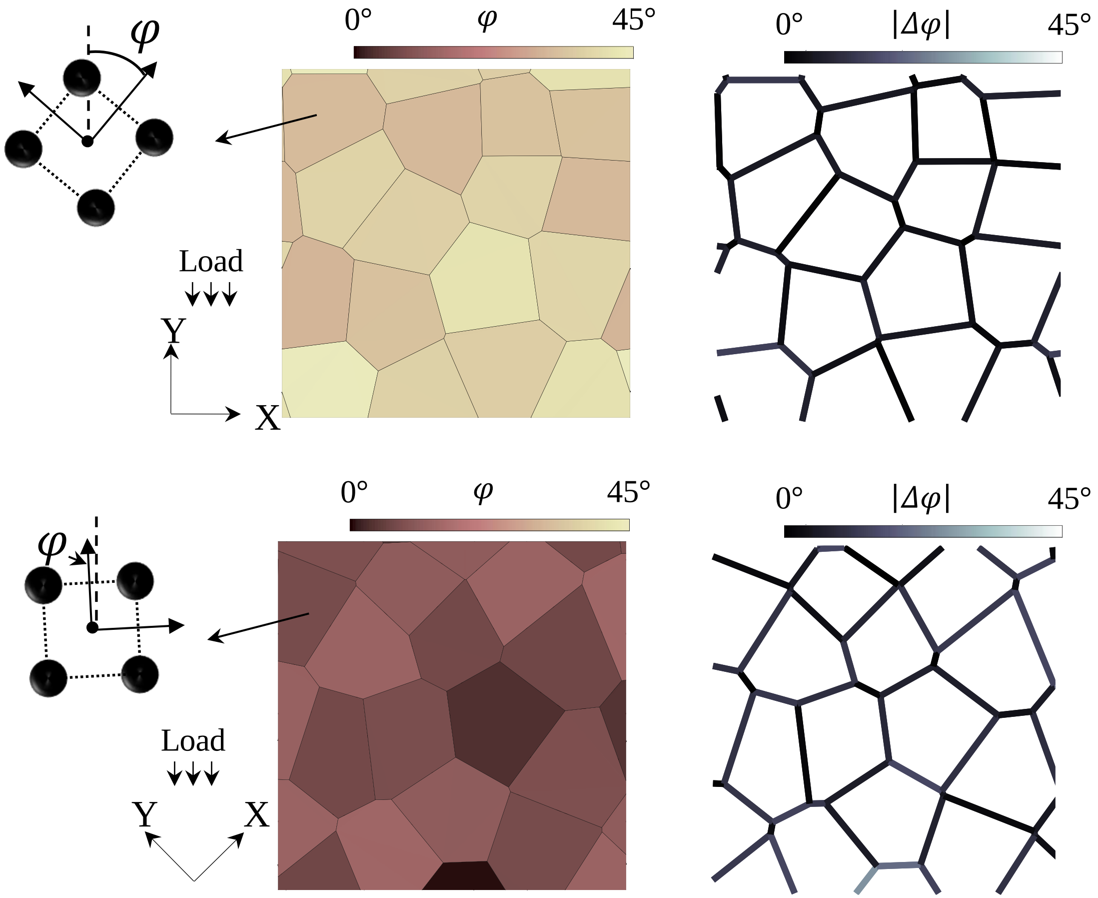


* 1st loading cycle

Role of GBs in load transfer and energy dissipation

ii) Architected heterogenous polycrystals with **high texture**

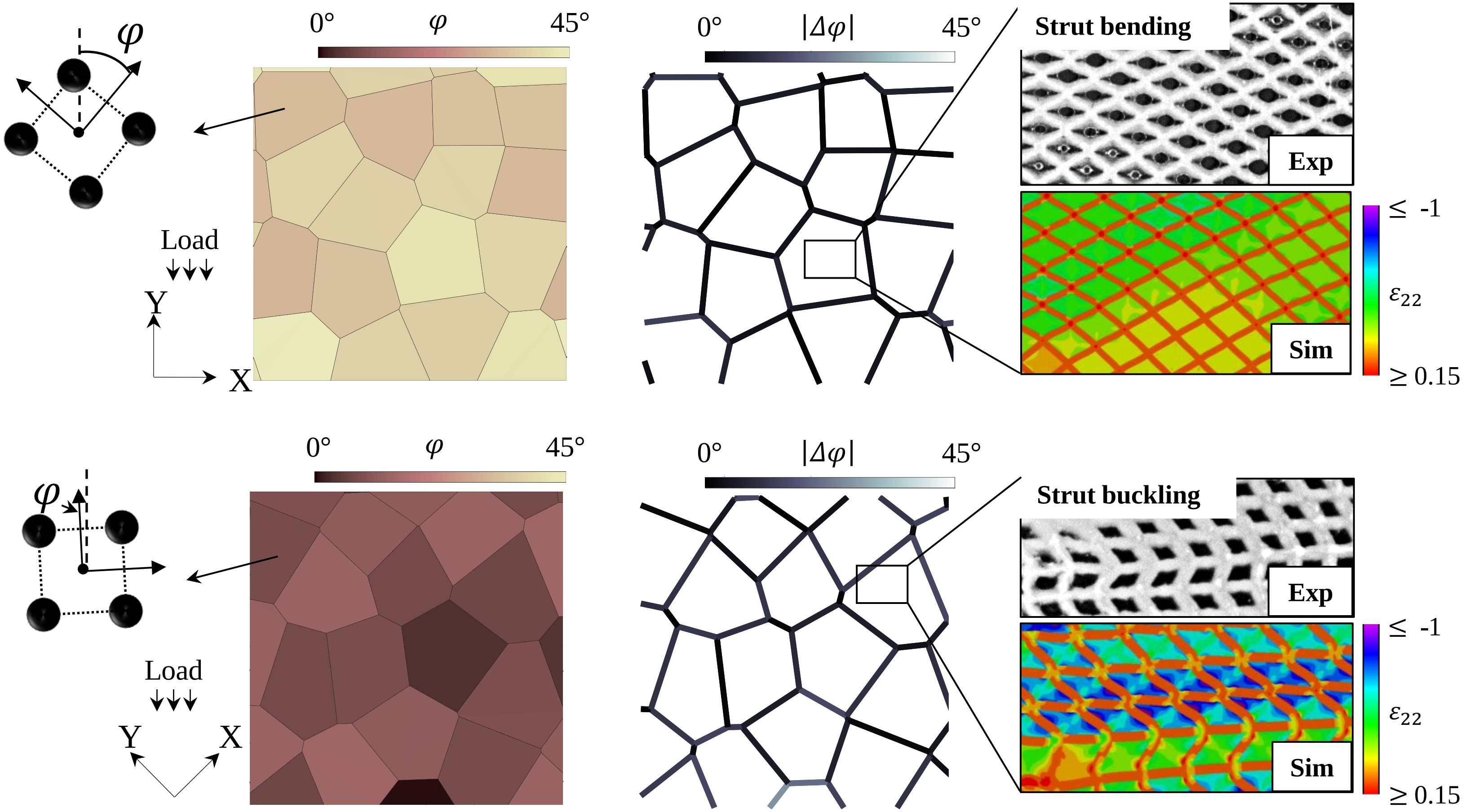
- Grain boundaries **do not strongly influence** the local failures due to **small** |Δφ|



Role of GBs in load transfer and energy dissipation

ii) Architected heterogenous polycrystals with **high texture**

- **The angle between the crystal orientations and the loading direction** (within the **grain interiors**) is key to understand cyclic behaviors in these **highly textured** architected polycrystals



* 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 grain interiors** is key to tailoring grain-size dependent mechanical features

  ii) **Grain boundaries** with significant **deformation inhomogeneity** strongly influence **reusability** of architected heterogenous polycrystals

- 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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References

[1] Lee, J., Veysset, D., Hsieh, A. J., Rutledge, G. C., & Cho, H. (2023). A polyurethane-urea elastomer at low to extreme strain rates. *International Journal of Solids and Structures, 280*, 112360.

[2] Cho, H., Mayer, S., Pöselt, E., Susoff, M., in't Veld, P. J., Rutledge, G. C., & Boyce, M. C. (2017). Deformation mechanisms of thermoplastic elastomers: Stress-strain behavior and constitutive modeling. *Polymer, 128*, 87-99.

[3] Qi, H. J., & Boyce, M. C. (2005). Stress–strain behavior of thermoplastic polyurethanes. *Mechanics of materials, 37*(8), 817-839.

[4] Cho, H., Weaver, J. C., Pöselt, E., in't Veld, P. J., Boyce, M. C., & Rutledge, G. C. (2016). Engineering the mechanics of heterogeneous soft crystals. *Advanced Functional Materials, 26*(38), 6938-6949.

[5] Lee, J. H., Wang, L., Boyce, M. C., & Thomas, E. L. (2012). Periodic bicontinuous composites for high specific energy absorption. *Nano letters, 12*(8), 4392-4396.

[6] Wang, L., Lau, J., Thomas, E. L., & Boyce, M. C. (2011). Co-continuous composite materials for stiffness, strength, and energy dissipation. *Advanced Materials, 23*(13), 1524.

[7] Li, T., Chen, Y., & Wang, L. (2018). Enhanced fracture toughness in architected interpenetrating phase composites by 3D printing. *Composites Science and Technology, 167*, 251-259.

[8] Pham, M. S., Liu, C., Todd, I., & Lertthanasarn, J. (2019). Damage-tolerant architected materials inspired by crystal microstructure. *Nature, 565*(7739), 305-311.

[9] Liu, C., Lertthanasarn, J., & Pham, M. S. (2021). The origin of the boundary strengthening in polycrystal-inspired architected materials. *Nature Communications, 12*(1), 4600.

References

[10] Yu, B., Van Egmond, D. A., Samk, K. A., Erb, U., Wilkinson, D., Embury, D., & Zurob, H. (2023). The design of "Grain Boundary Engineered" architected cellular materials: The role of 5-7 defects in hexagonal honeycombs. *Acta Materialia, 243,* 118513.

[11] Vangelatos, Z., Komvopoulos, K., & Grigoropoulos, C. P. (2020). Regulating the mechanical behavior of metamaterial microlattices by tactical structure modification. *Journal of the Mechanics and Physics of Solids, 144,* 104112.

[12] Yin, S., Guo, W., Wang, H., Huang, Y., Yang, R., Hu, Z., ... & Ritchie, R. O. (2021). Strong and tough bioinspired additive-manufactured dual-phase mechanical metamaterial composites. *Journal of the Mechanics and Physics of Solids, 149,* 104341.

[13] Liu, C., & Pham, M. S. (2024). Spatially programmable architected materials inspired by the metallurgical phase engineering. *Advanced Materials, 36*(8), 2305846.

[14] Zappa, G., Cocchi, L., Candidori, S., Buccino, F., Vergani, L., & Graziosi, S. (2024). Twinning-inspired hexagonal close-packed metamaterials for enhanced energy absorption. *Materials & Design, 244,* 113098.

[15] Bastek, J. H., Kumar, S., Telgen, B., Glaesener, R. N., & Kochmann, D. M. (2022). Inverting the structure–property map of truss metamaterials by deep learning. *Proceedings of the National Academy of Sciences, 119*(1), e2111505119.

[16] Zhang, Y., Zhang, J., Zhao, X., Li, Y., Che, S., Yang, W., & Han, L. (2022). Mechanical behaviors regulation of triply periodic minimal surface structures with crystal twinning. *Additive Manufacturing, 58,* 103036.

[17] Bian, Y., Yang, F., Li, P., Wang, P., Li, W., & Fan, H. (2021). Energy absorption properties of macro triclinic lattice structures with twin boundaries inspired by microstructure of feldspar twinning crystals. *Composite Structures, 271,* 114103.

References

[18] Frary, M., & Schuh, C. A. (2004). Percolation and statistical properties of low-and high-angle interface networks in polycrystalline ensembles. *Physical Review B, 69*(13), 134115.

[19] Karapiperis, K., & Kochmann, D. M. (2023). Prediction and control of fracture paths in disordered architected materials using graph neural networks. *Communications Engineering, 2*(1), 32.

[20] Shaikeea, A. J. D., Cui, H., O'Masta, M., Zheng, X. R., & Deshpande, V. S. (2022). The toughness of mechanical metamaterials. *Nature materials, 21*(3), 297-304.

[21] Lee, J., Lee, S., Chester, S. A., & Cho, H. (2023). Finite element implementation of a gradient-damage theory for fracture in elastomeric materials. *International Journal of Solids and Structures, 279*, 112309.

[22] Narayan, S., & Anand, L. (2021). Fracture of amorphous polymers: A gradient-damage theory. *Journal of the Mechanics and Physics of Solids, 146*, 104164.

[23] Russ, J., Slesarenko, V., Rudykh, S., & Waisman, H. (2020). Rupture of 3D-printed hyperelastic composites: Experiments and phase field fracture modeling. *Journal of the Mechanics and Physics of Solids, 140*, 103941.