Multiscale Optimization of nCB-Cement Composites: Effects of Chemical Surfactants on: Dispersion, Conductivity, Mechanical Performances

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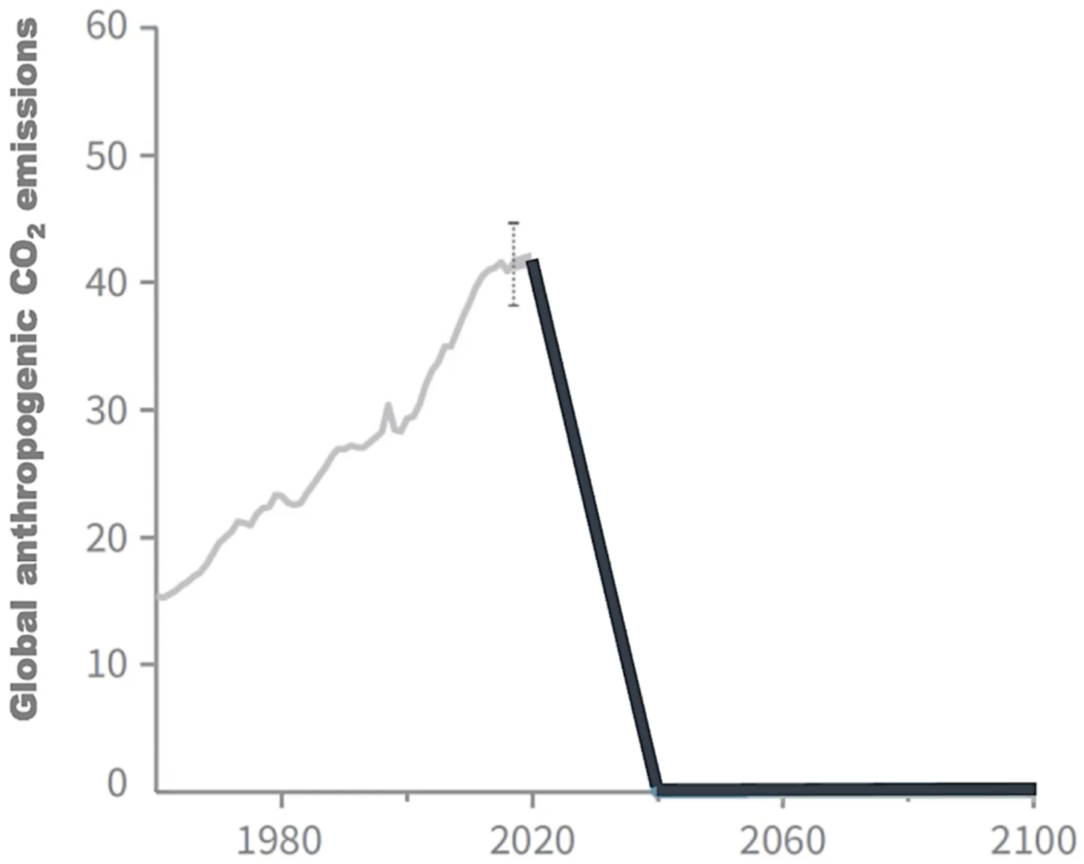
ACI Fall Convention - Boston MA, Oct. 29 – Nov. 2 2023

Motivation

A radical change is needed:
Cut CO_2 emission by 50% in the next 10 years (stay below temperature rise of 1.5 ^oC); reach net zero in 2050

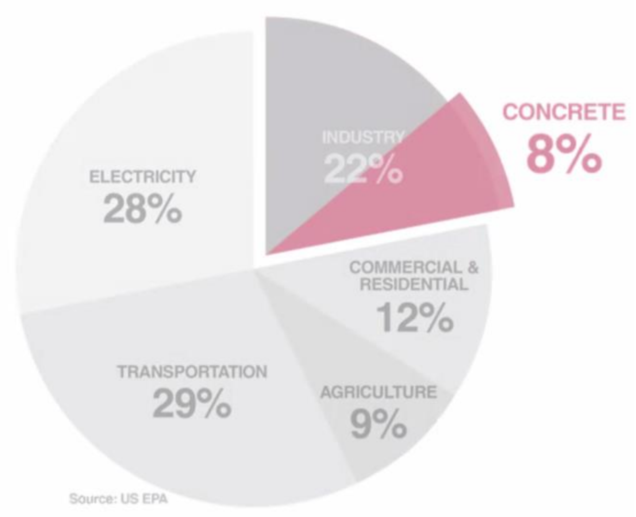


USA has joined over 120 countries in committing to be net-zero emission by 2050

IPCC 2021. 1.5oC report

Does concrete meet social and environmental goals?

<u>Eco-efficient Issues</u>: Cement contributes up to **8%** of global CO_2 emission



CO_2 emissions by business sector

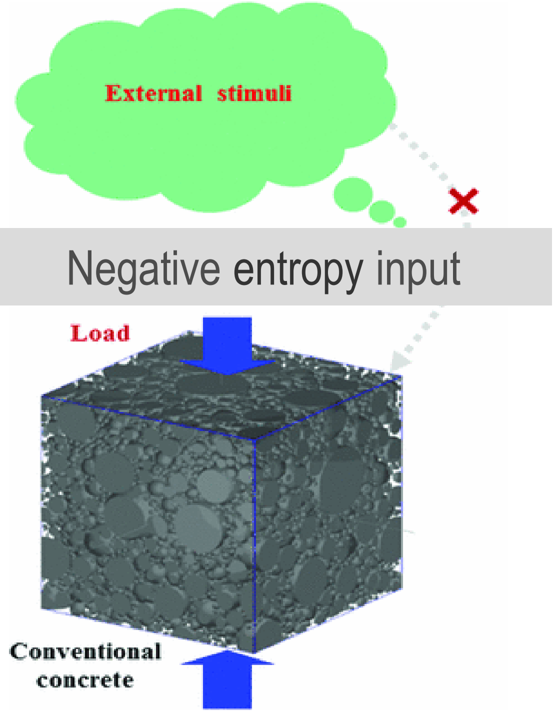
1 ton of cement leads to the emission of 900 kg CO_2 ($CaCO_3$ decomposition and Fuel)

Monteiro, P., Miller, S. & Horvath, A. Nature Mater. 16, 698–699 (2017)

<u>Durability issues:</u> repair of deteriorated infrastructures costs $$$ billions

40% of bridges in US require rehabilitation costing ~ $28 billion annually

<u>Functionality issues:</u> concrete has no negative entropy input through matter or energy with external stimuli



Smart materials are designed with properties that can be changed in a controlled fashion by external stimuli (stress, moisture, electric, chemical compounds

Han et al. 2017

How can concrete be sustainable to meet social and environmental goals?

Reduce CO_2 from clinker production →
- Waste Fuels
- Efficient Plants
- Alternative raw materials

Reduce clinker in cement →
- SCMs
- Local materials
  - Natural materials
  - Waste materials
  - Nano materials

Reduce cement in concrete →
- Aggregate grading
- Appropriate mix design
- Use of admixtures
- Use fillers

Add functionality →
- Self sensing
- Self healing
- Conductivity
- CO_2 capture

Reduce concrete in building →
- Concrete design optimization
- Structure design optimization

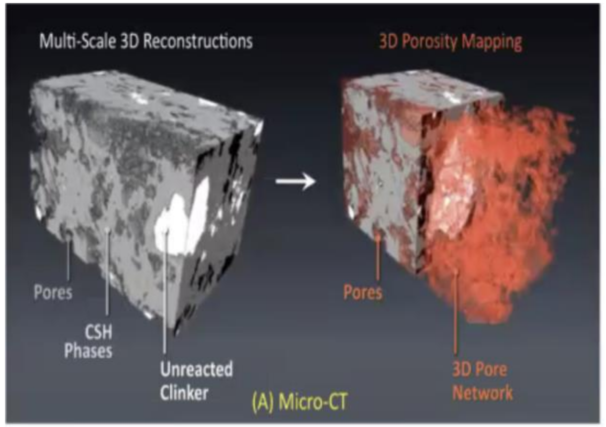
Automate construction →
- Ride of formwork (3D printing)
- Switch to robotic fabrication

Use concrete more efficiently

RECYCLE

Electron conducting carbon-based cement

Capillary pores network of CSH: 95% connected...



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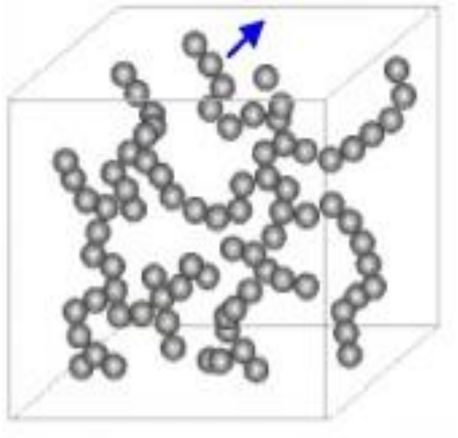
Nano-Carbon Black (nCB)



Low cost & high electrical conductivity

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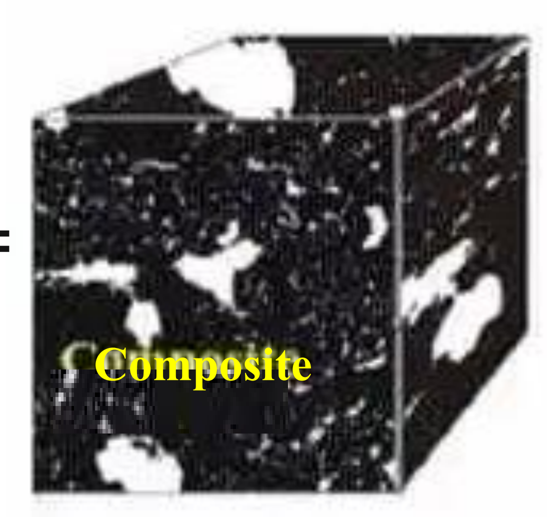
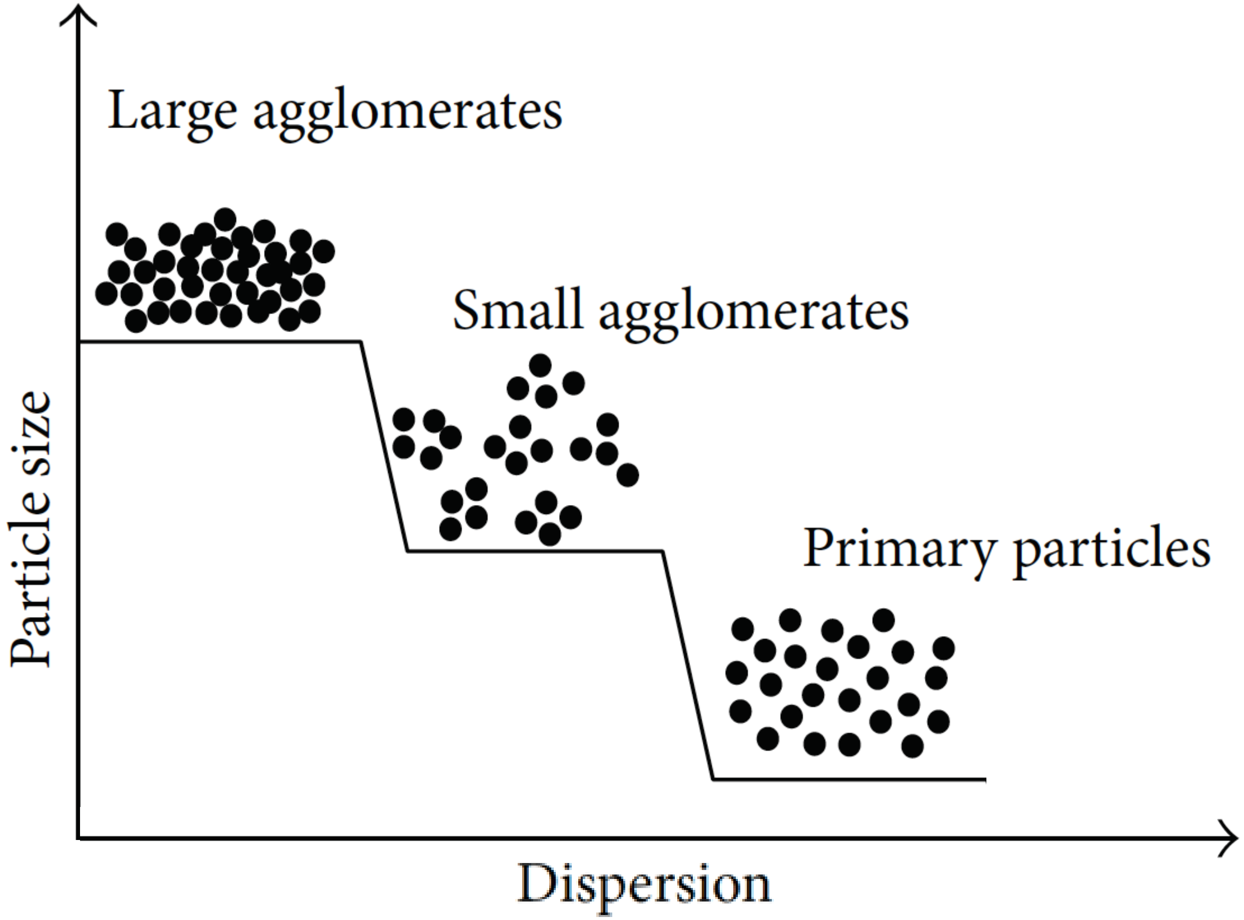


- Electrically conductive
- Self-heating
- Energy storage (capacitors)

Pellenq et al., MIT-CNRS, United States Patent, Dec 2020

What is the effect of nCB dispersion on mechanical and electrical conductivity?



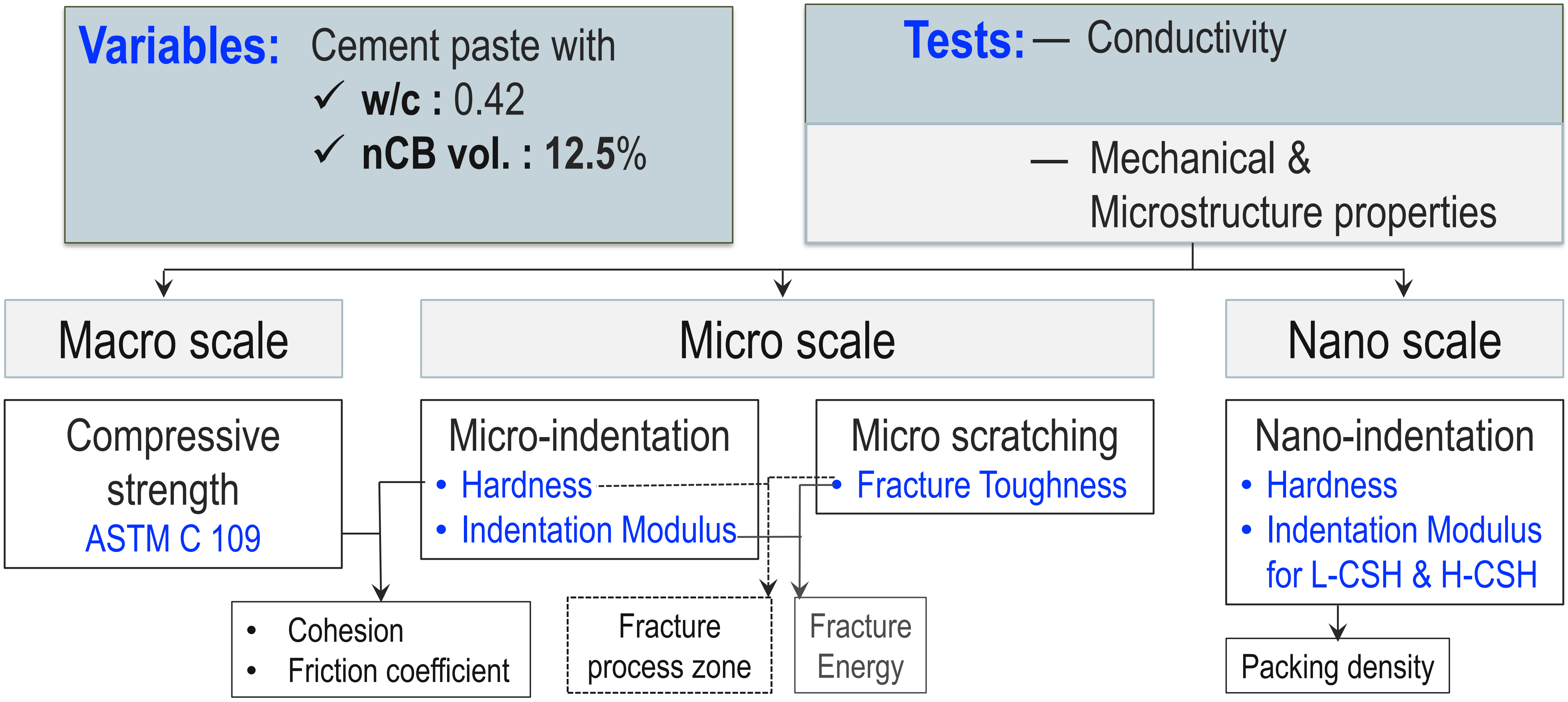
Chemical surfactants

Carboxymethyl cellulose (CMC)
Polycarboxylate (PCE)
CMC+PCE
Polynaphthalene (PNS)

Physical

Sonication

Mechanical and microstructural properties: multiscale engineering chemo–mechanical material characterization



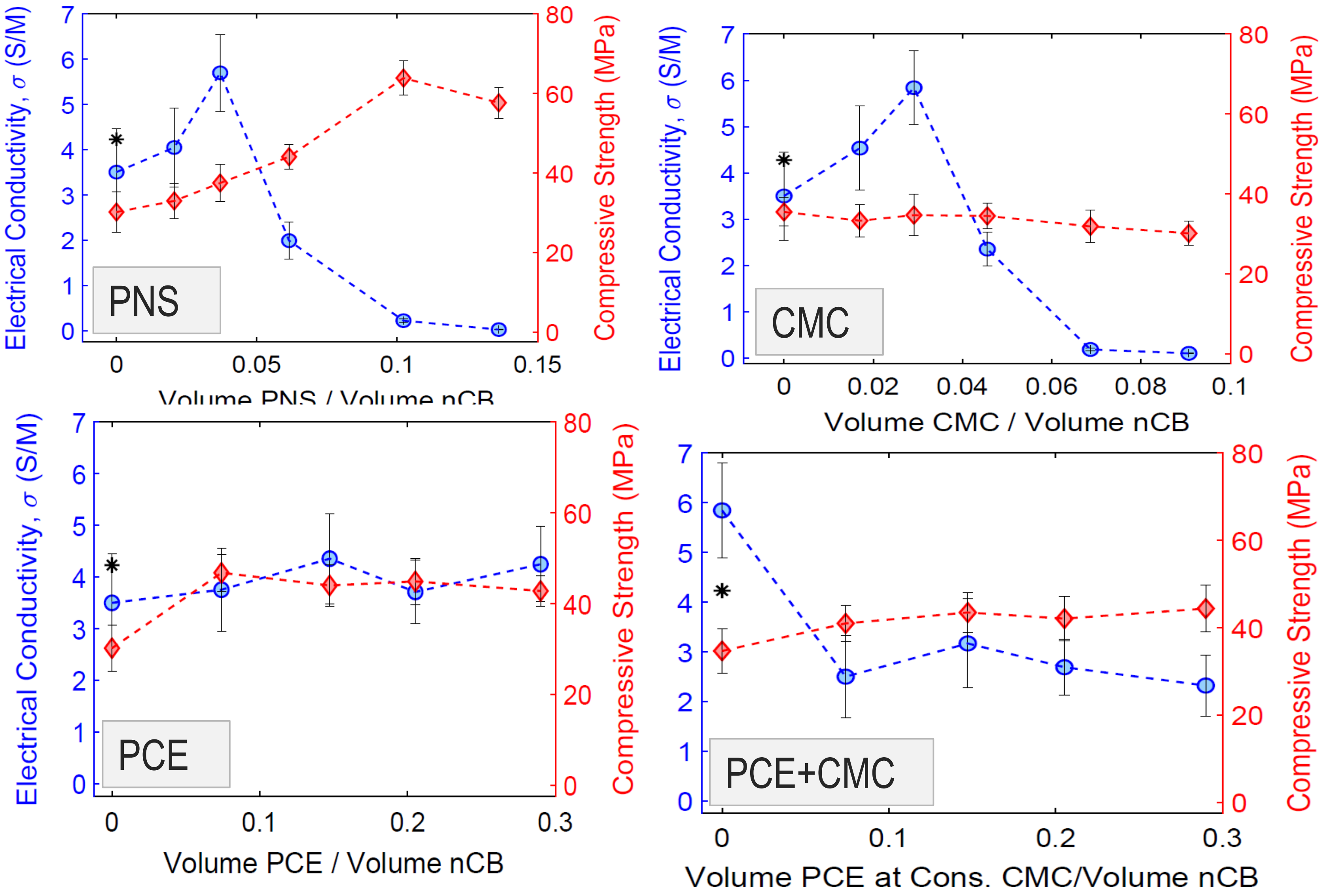
Trade-off between strength and conductivity

Electrical Conductivity:

- Enhanced by moderate PNS and CMC; high concentration prevents the formation of conductive nCB networks.
- PCE's effect is neutral, indicating a lack of interaction with nCB particles.
- CMC+PCE shows a balanced conductivity, suggesting an optimal nCB particle dispersion.

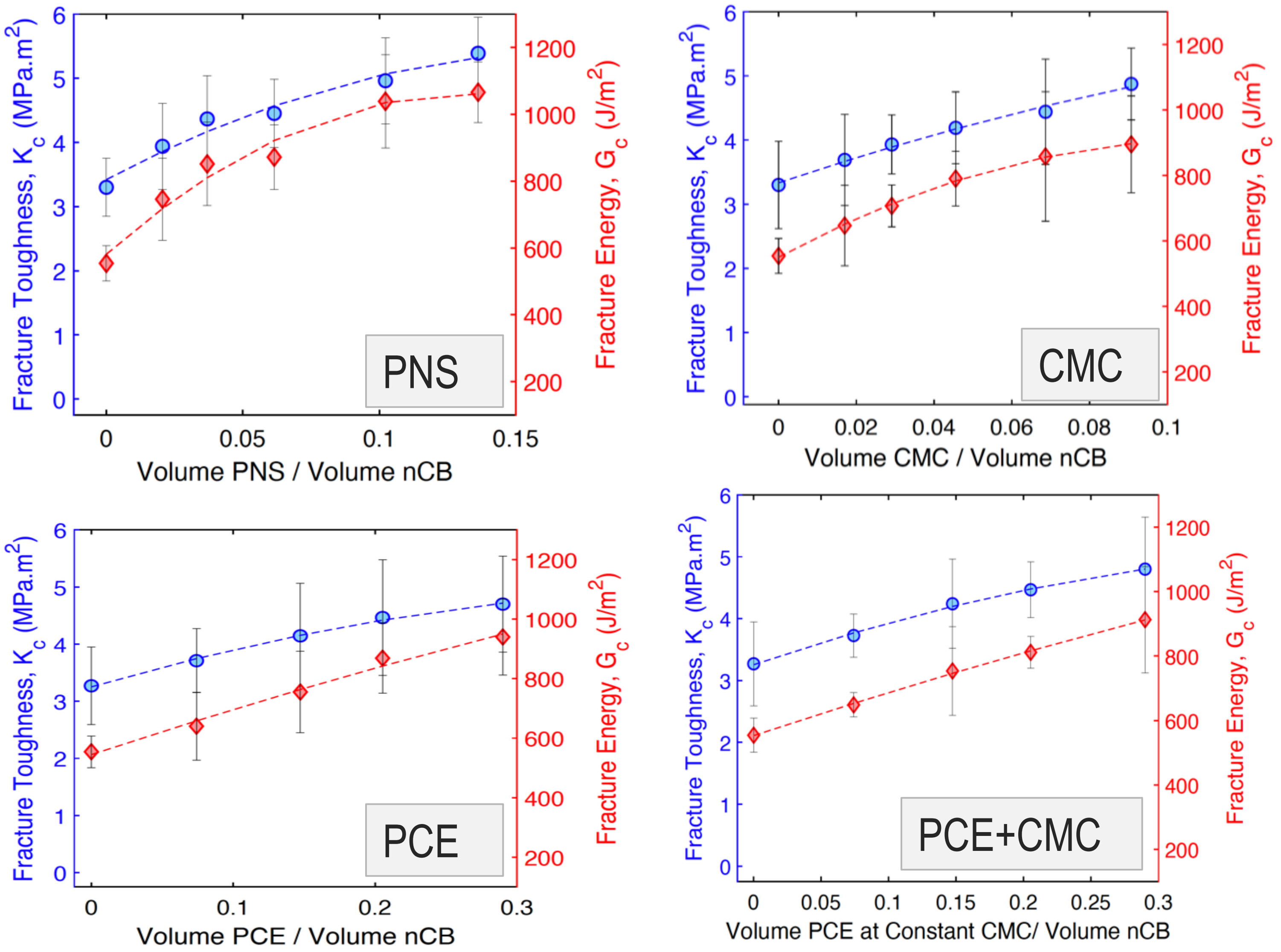
Macro-scale Mechanical Strength:

- Improved with PNS due to uniform nCB distribution, contrary to the weakening effect of CMC.
- PCE maintains/improves strength, indicating effective cement hydration and nCB integration.



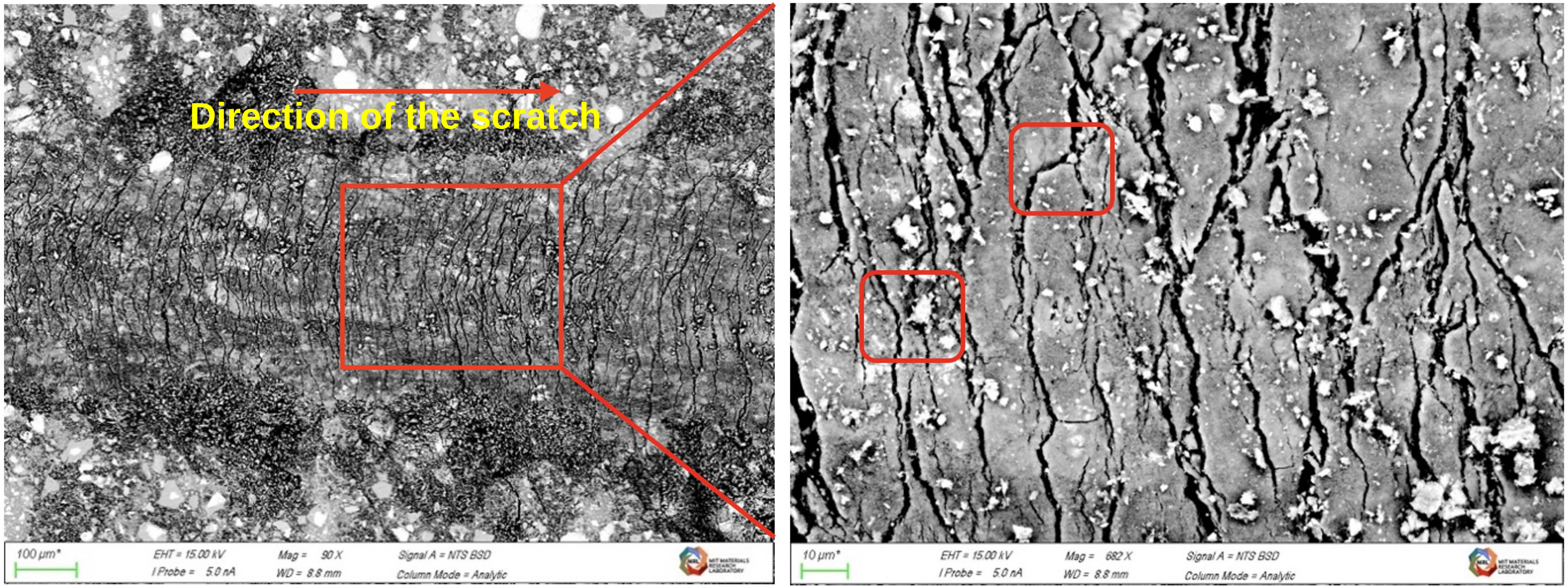
Fracture analysis via scratch test – microscale: Progression of Fracture toughness and energy

- nCB dispersion using any dosage ➔ increases fracture toughness
- Improvement on fracture toughness is originated from **crack deflection** effect, which results from nCB inclusion in cement matrix



Examining fracture mechanisms through SEM of scratch groove

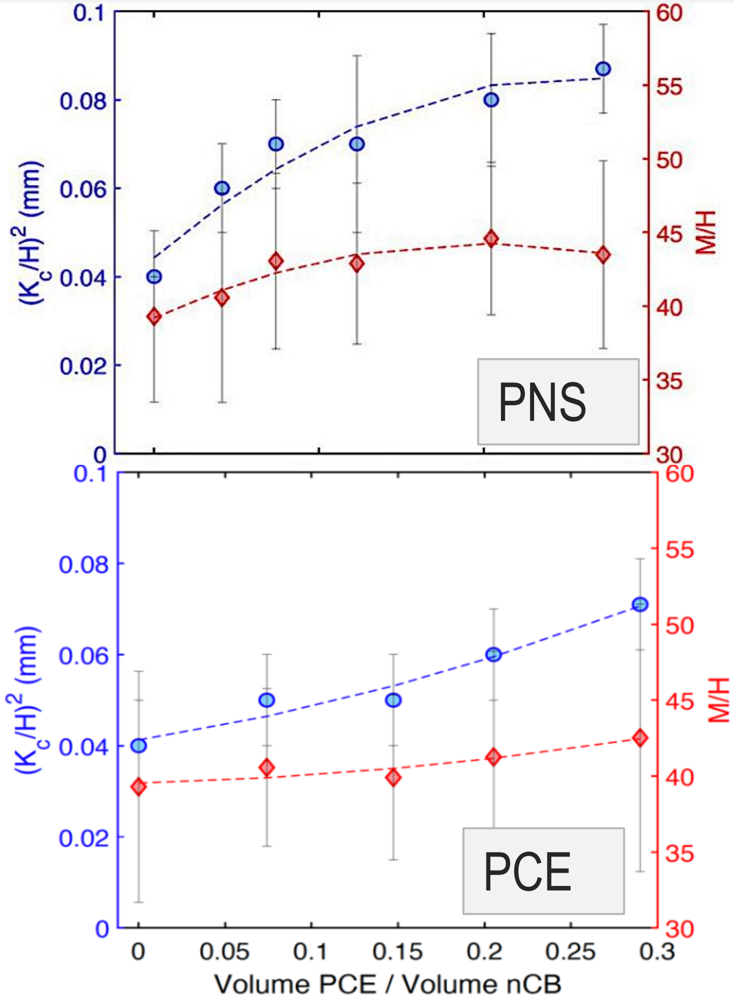
12.5% nCB volume fraction, 0.42 *w/c*, 0.35% PNS



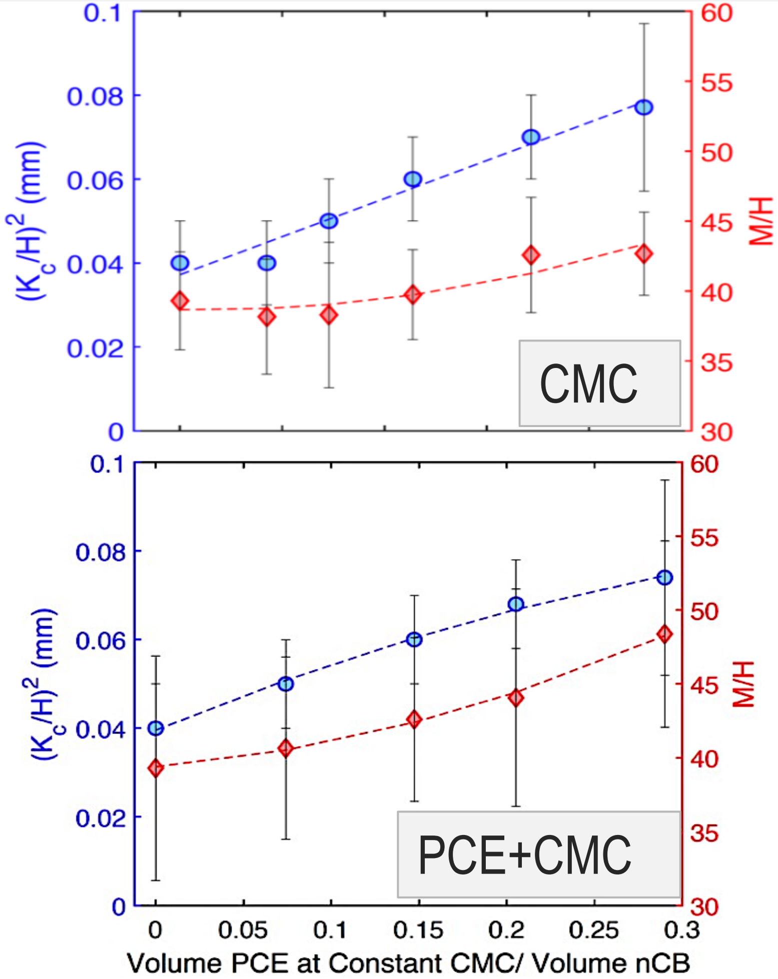
The tortuosity (non-planar geometry) of a crack path is visible along with crack surface.

Ductility: M/H, Fracture Processing Zone $(K_c/H)^2$

Indentation Modulus/Indentation Hardness (M/H): competition of plastic dissipation and elastic energy storage



FPZ of a material at the head of the crack tip where the stress decreases from the maximum value to the far-field stress.



- nCB inclusion ➔ increases ductility (M/H) and fracture process zone
- Plastic dissipation capacity is increased and hence FPZ becomes smaller

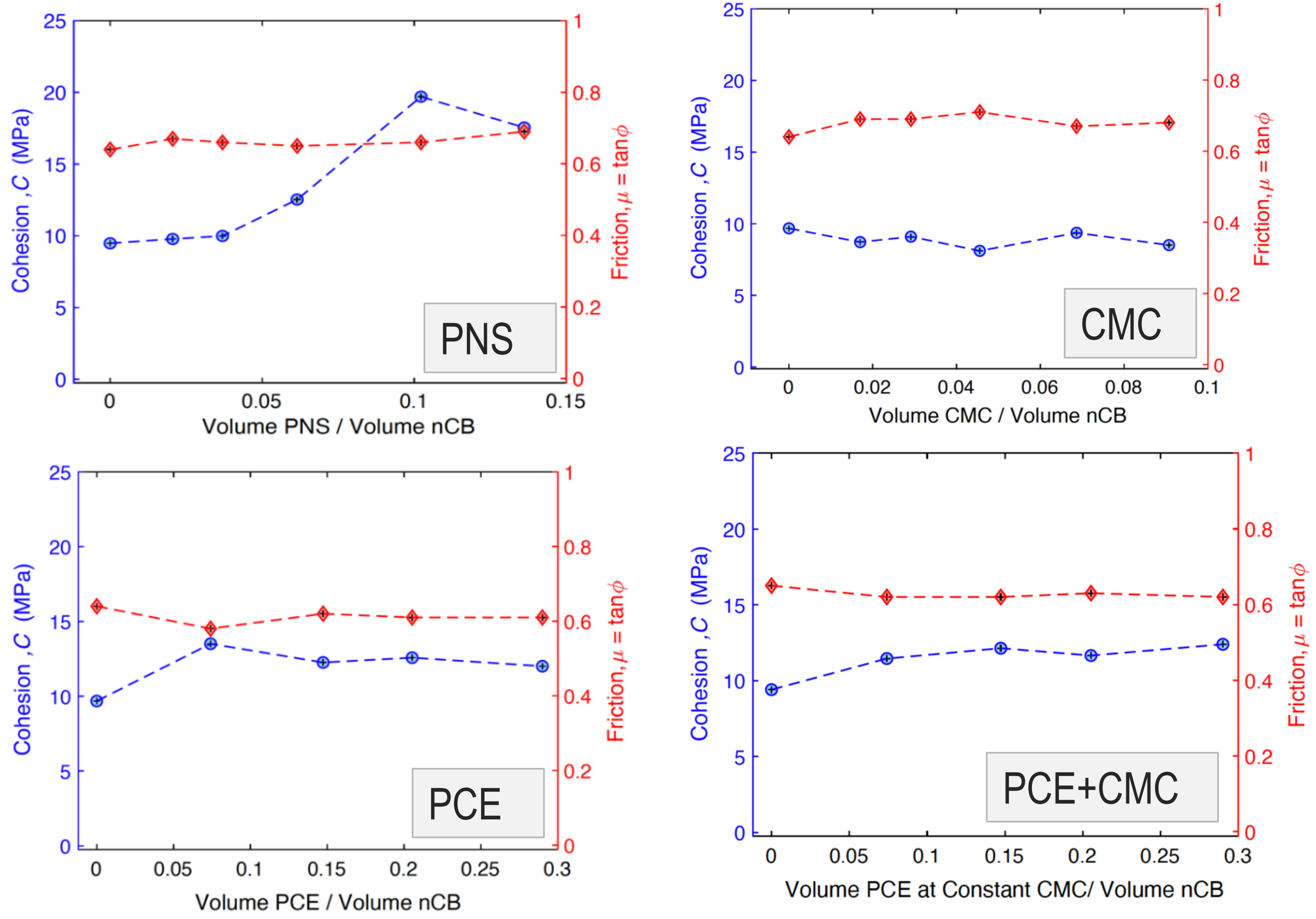
Evolution of friction coefficient and cohesion

- Using nCB with surfactants ➔ slightly boosts friction coefficient (*due to filling capillary pores with nCB*) ➔ enhances fracture toughness

- PNS significantly increases cohesion ➔ greater macro-scale strength, compared to other surfactants

Friction = f (f'_c, Hardness)

Cohesion = f (f'_c, Friction)

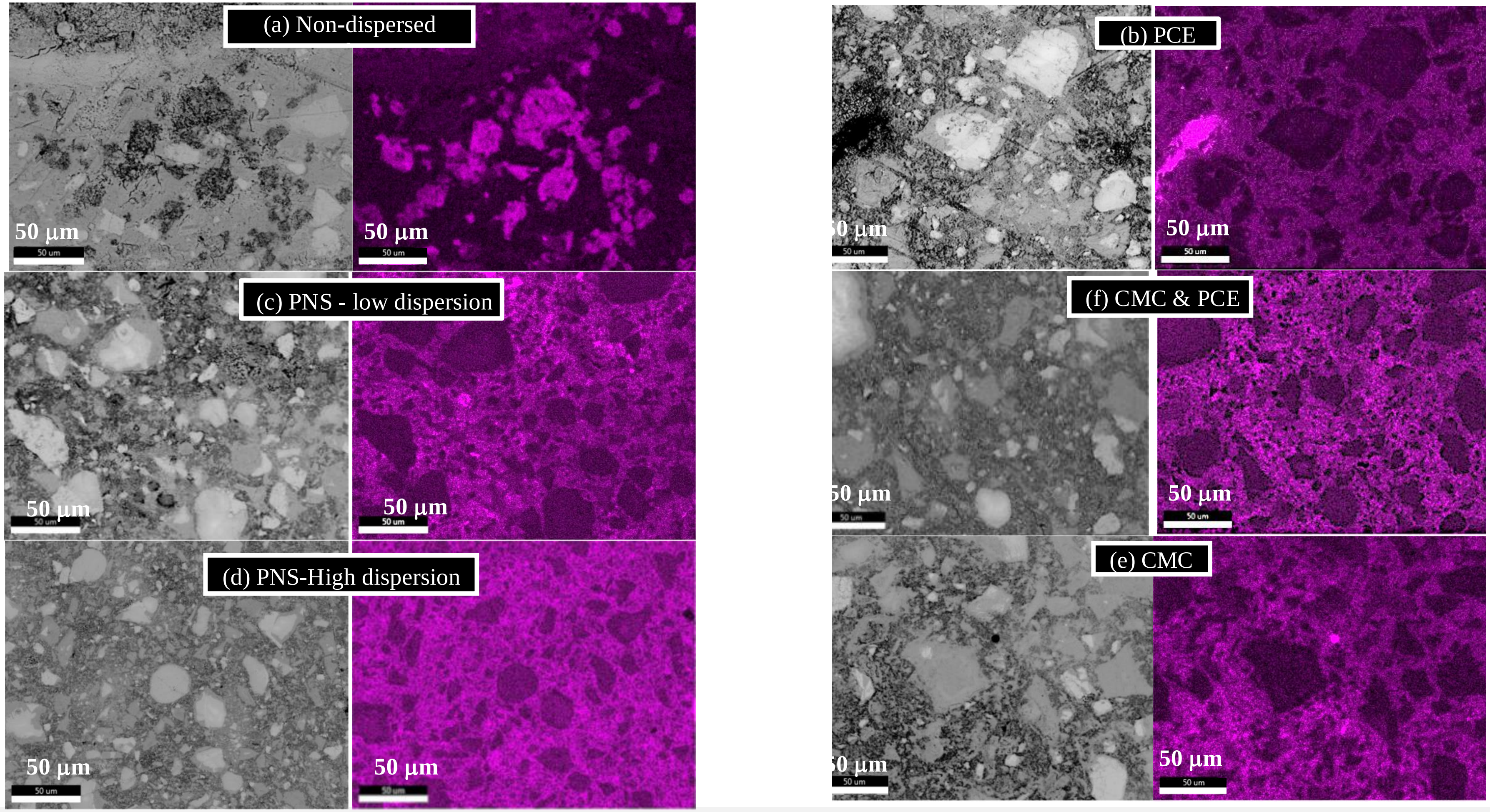


Effect of dispersion of nCB on Nanomechanical properties using Nanoindentation < 1µm

Mixture with:	Indentation H (GPa)				Indentation M (GPa)				Indentation creep (GPa)				Volume friction			
	Phase 1	Phase 2	Phase 3	Phase 4	Phase 1	Phase 2	Phase 3	Phase 4	Phase 1	Phase 2	Phase 3	Phase 4	Phase 1	Phase 2	Phase 3	Phase 4
Blane Cement	1.1±0.3	1.4±0.3	2.0±0.4	--	32±4.3	37±6.8	44±6	--	193±53	387±85	835±333	--	61	24	12	--
No surfactant	0.7±0.3	1.4±0.4	2.3±0.5	5.8±2.8	19±4.5	28±5.4	44±7	77±19	148±48	319±65	698±205	2567±1326	37	23	34	5.8
0.3%PNS	1.0±0.2	1.5±0.23	2.3±0.5	--	25±4.4	37±4.4	52±11	--	132±38	235±63	499±210	--	54.5	30	14	--
1%PNS	1.5±0.4	2.0±0.69	3.1±0.9	--	29±5.2	39±4.4	51±9	--	353±96	537±184	754±283	--	59	31	10	--
1%PCE	1.12±0.4	2.0±0.7	4.7±1.8	--	30±6.4	45±9.6	89±30	--	300±78	592±212	1565±774	--	64	26	11	--
0.25%CMC	0.9±0.4	1.3±0.41	2.0±0.7	--	23±5.3	34±5.2	50±10	--	141±29	285±71	520±271	--	59	30	12	--
1%PCE-CMC	1.2±0.4	1.9±0.7	4.7±1.8	--	29±6.4	45±9.6	89±30	--	300±78	592±212	1565±774	--	63	30	8	--

- No dispersion of nCB decreases M and H of the C-S-H ➔ strength reduction
- Over dispersion of nCB with PNS enhances M and H of the C-S-H ➔ Cohesion & macro-mechanical improvement

Microstructural analysis of nCB-Cement Composite using SEM and EDS



Without dispersing agent: nCB forms large agglomerations, hindering load transfer and affecting mechanical properties.
PCE, CMC inclusions: Fewer agglomerations, more uniform nCB distribution.
High PNS concentration: Best uniformity in nCB distribution, enhancing mechanical strength.`

Conclusions

- ✓ **Conductivity:** Enhanced nCB dispersion via PNS and CMC boosts conductivity; excess dispersion reduces it. PCE has minimal effect.

- ✓ **Strength:** Direct correlation with nCB dispersion. PNS surfactant notably improves strength. No dispersion diminishes strength.

- ✓ **Fracture Properties:** nCB dispersion elevates toughness and ductility due to 'crack deflection' and bridging forces from PCE/CMC.

- ✓ **Friction & Cohesion:** PNS and CMC increase both by enhancing nCB dispersion.

- ✓ **Micromechanical:** PNS dispersion uplifts C-S-H gel properties by 12-25%.

- ✓ **Morphology:** SEM/EDS analysis highlights surfactants' role. PNS optimizes mechanical strength but lowers conductivity.

Next Step

nCB's potential in concrete is transformative. By optimizing balance and delving into nCB surface functionality, we can pioneer a multifunctional concrete that excels in strength and conductivity.

Thank you!

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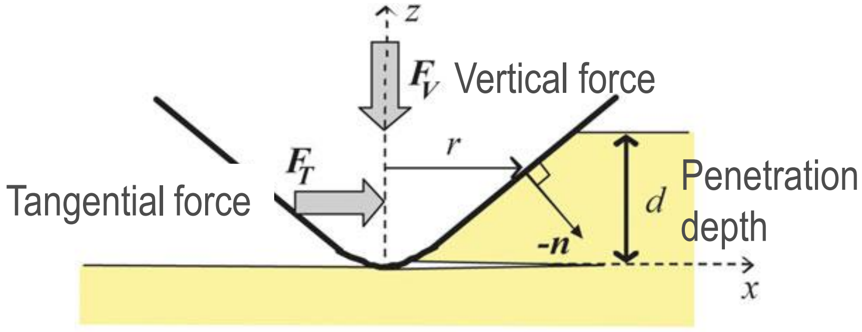
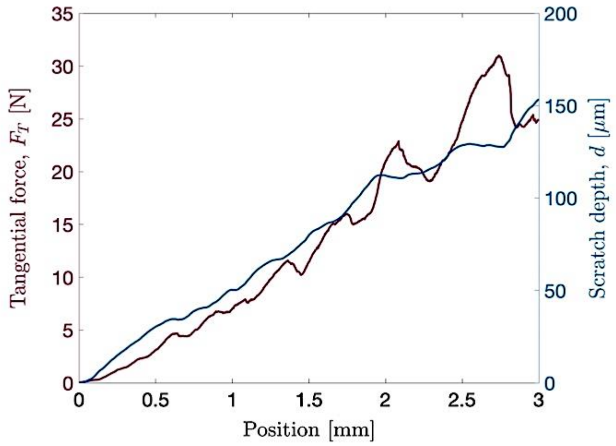
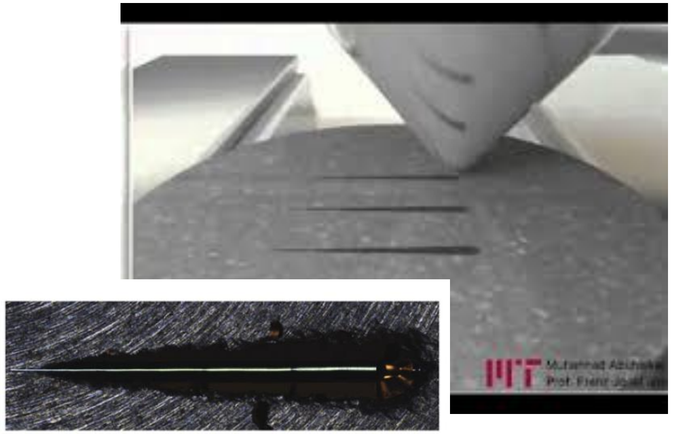
Approach: Micro-scratching protocol

Fracture toughness (K_C): describes the ability of a material to withstand presence of a crack when under stress







Panorama image of 3 mm

CJ Hoover, F-J Ulm (2015)

F_T: Tangential force

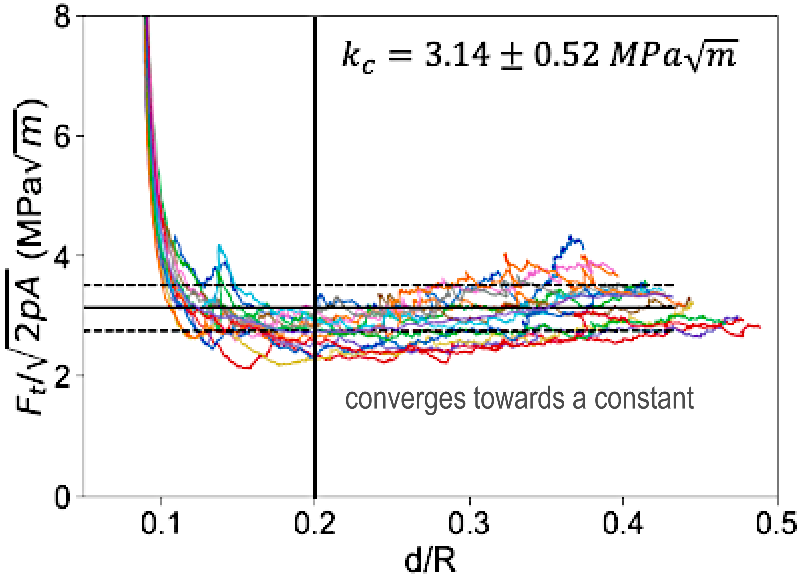
Fracture toughness

$$K_c = \left\langle \frac{F_T}{[2pA]^{\frac{1}{2}}} \right\rangle \Bigg|_{d > \frac{d_{max}}{2}}$$

p: probe perimeter

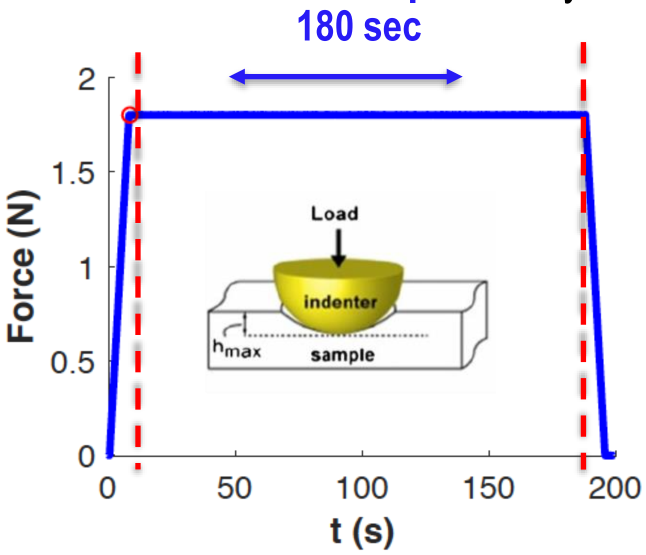
A: projected load bearing area

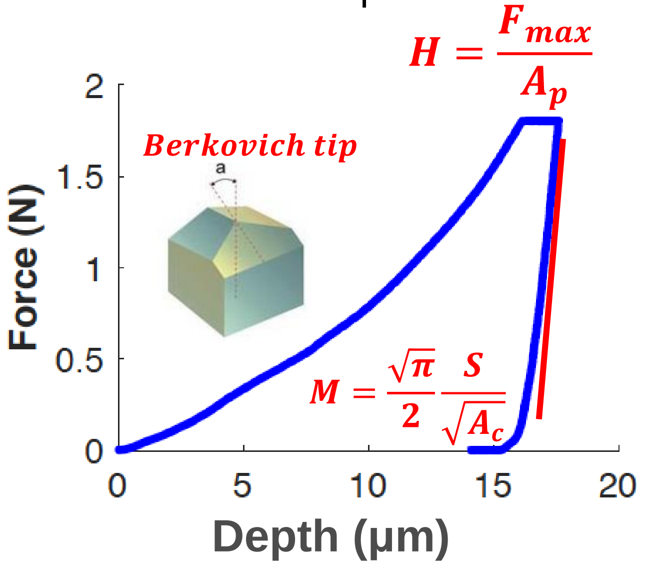
Linear Elastic Fracture Mechanics methods

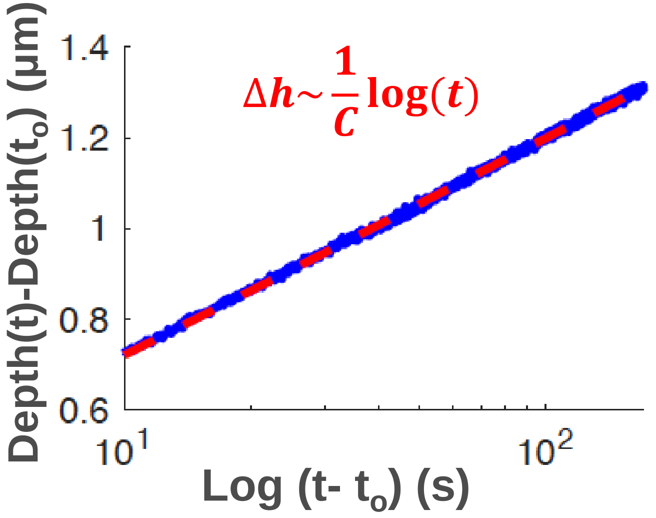


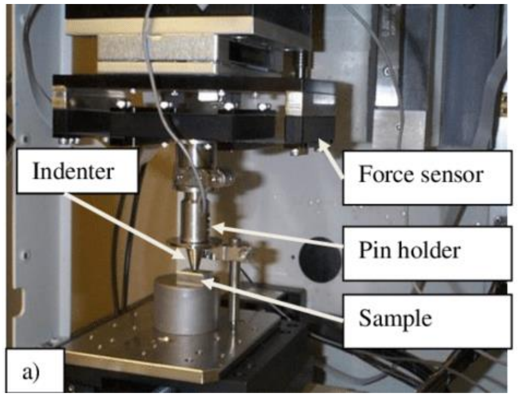
Approach: Indentation protocol

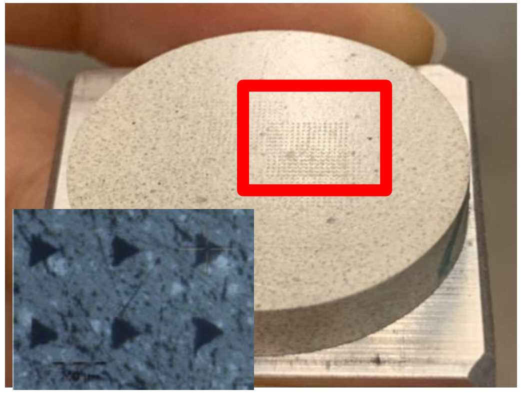
Indentation technique: study small volumes of materials and probe their mechanical properties at the sub-micron scale



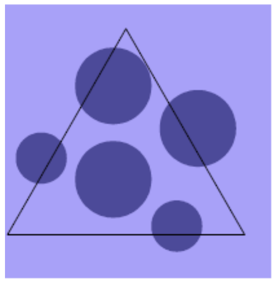




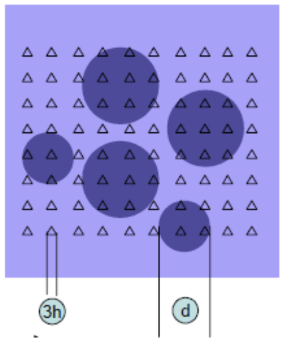




Microscale (~ 100 µm)



Nanoscale (~ 1 µm)



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