Mechanical performance of (bi)metallic nanowires under tension and compression

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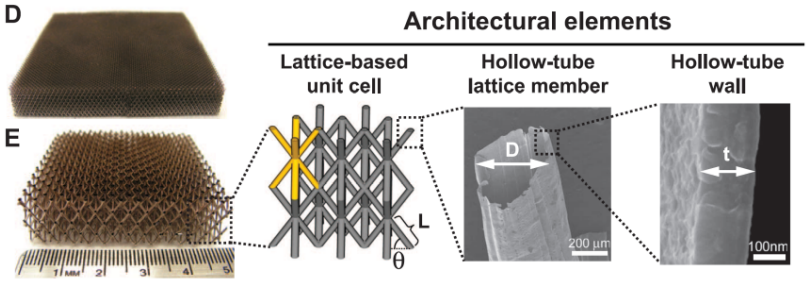
Nanoscale and materials

Building from the ground up

Mechanical properties can be tailored using **architectural elements**, resulting in lightweight materials



Size scale	~ mm - cm	~ μm - mm	~ nm - μm
Controllable architectural features	Unit cell symmetry, spatial location of lattice members	Diameter, wall thickness, node geometry	Microstructure, multilayer, composition

T. A. Schaedler et al., Science 334 (2011) 962-965

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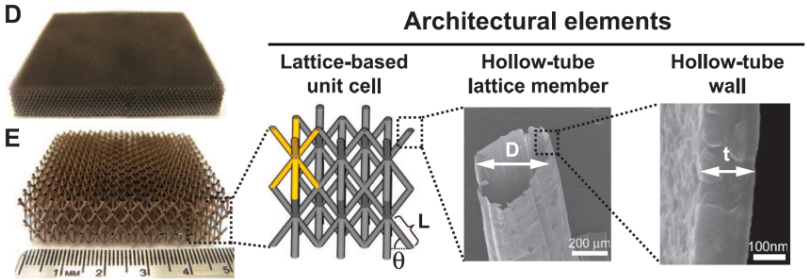
Why not do the same at nano scale?



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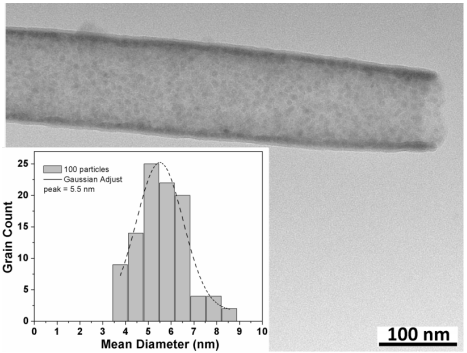
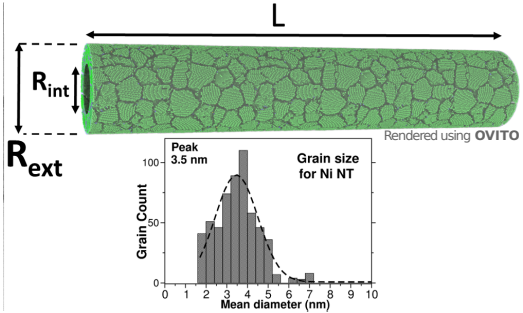
Nanoscale and materials

Nanotailoring

Nano structures can be synthesized by ALD technique over porous alumina membrane.





Our studies are focused on the mechanical response using LAMMPS

J. Rojas-Nunez et al., Computational Materials Science, 168, 81 (2019)

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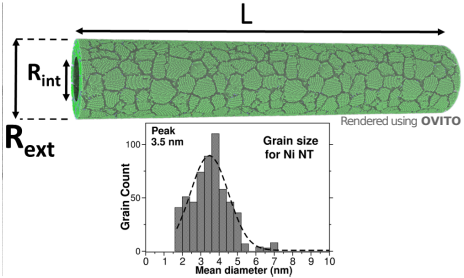
Nanoscale and materials

Nanotailoring

Nanocrystalline structures can be generated using Voronoi tessellation



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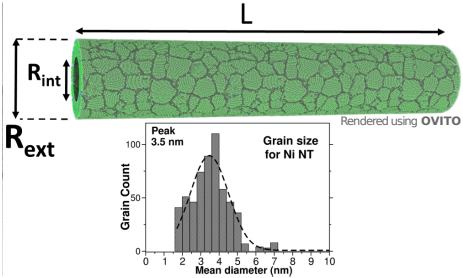

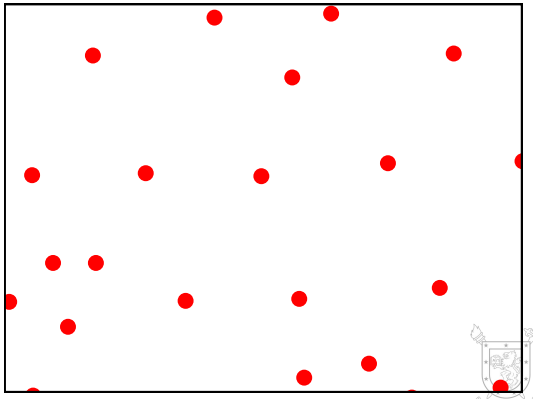

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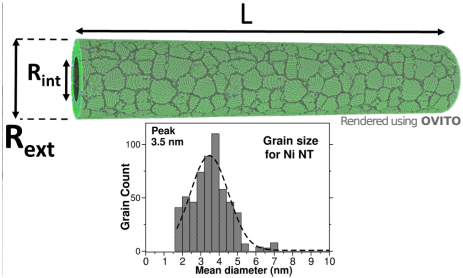

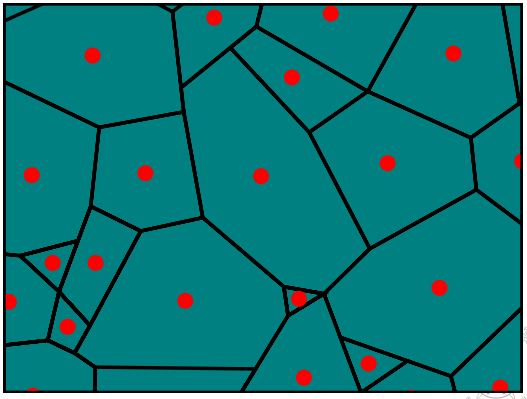

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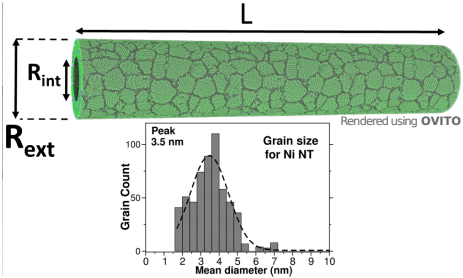

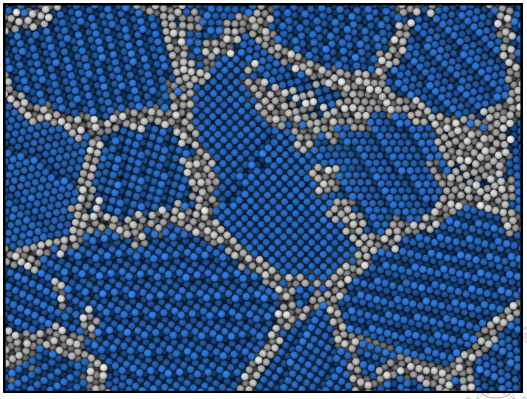

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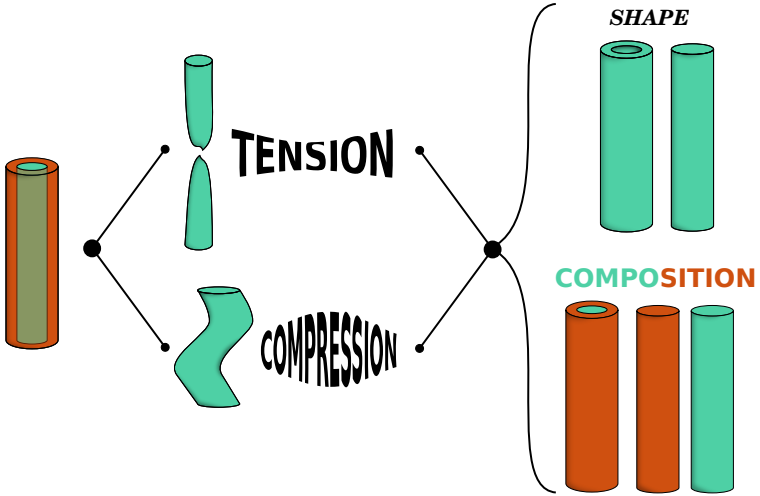
Atomistic simulations

Mechanical behavior using LAMMPS



Stretching and compressing simulations are performed at constant temperature.

LAMMPS parameters

timestep	:	1 fs
erate	:	(-)0.1 % fs^{-1}
temp	:	300 K

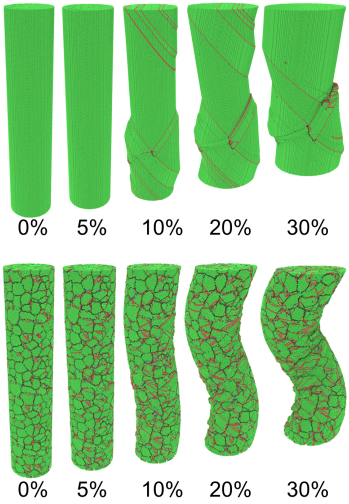
EAM potentials

Ni : Y. Mishin et al., Phys. Rev. B. 59, 3393

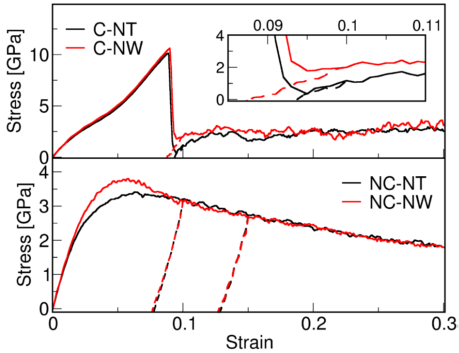
FeNi : G. Bonny et al., Philos. Mag. 89, 3531

Results

Crystalline and Nanocrystalline structures



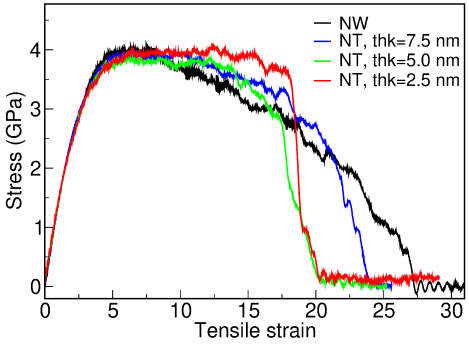
The structures have different mechanical behaviors between crystalline and nanocrystalline arrangements.

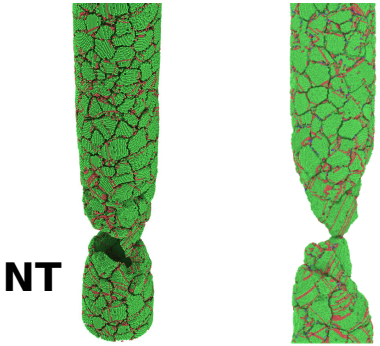


Results

Ni Nanotubes and Nanowires

Changing the shape of the structure between a nanotube (NT) and a nanowire (NW) modifies only the plastic behavior





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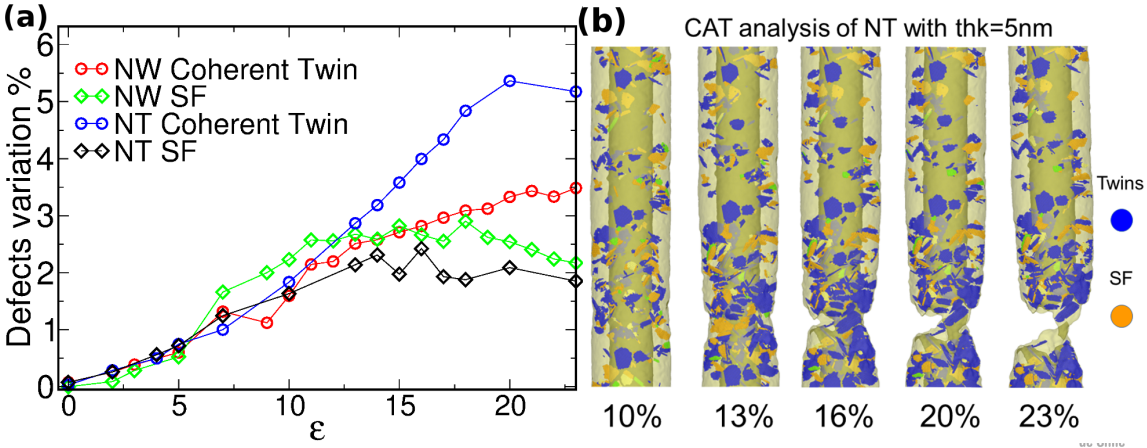
Results

Ni Nanotubes and Nanowires

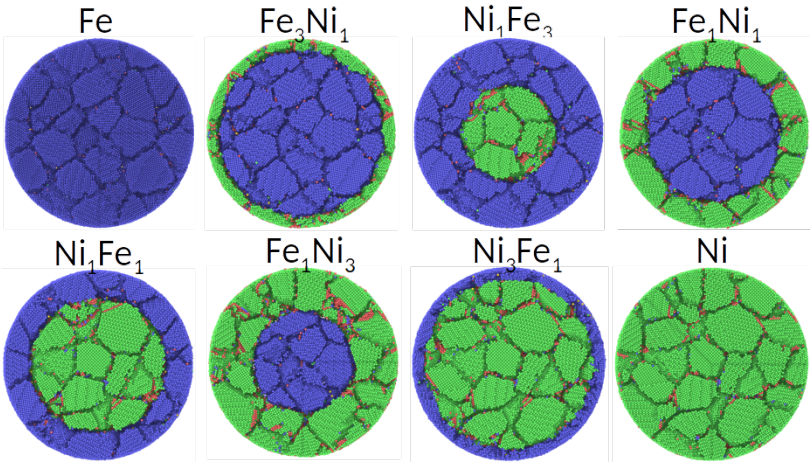
Planar defects are highly concentrated around the fracture point



Results

FeNi Nanowires

Several combinations are being tested for the bimetallic FeNi wire



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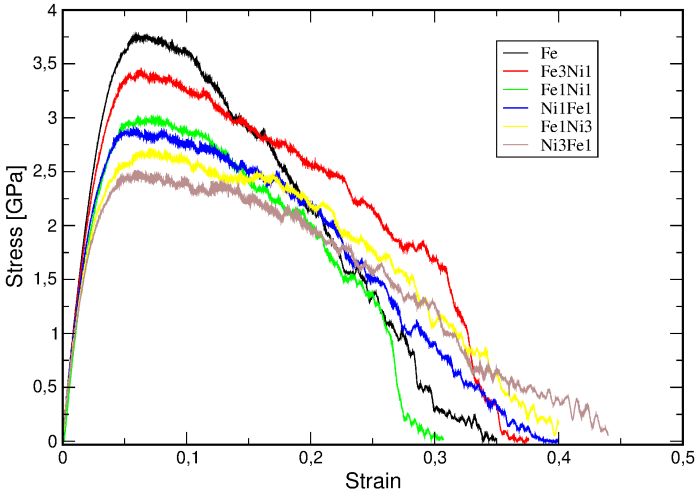
Results

FeNi Nanowires

The results for the tension simulations



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Summary and Conclusions

Nanocrystalline nanostructures were generated and simulated under tensile and compressive strain. Different configurations were tested:

- The nanocrystalline motif changes significantly the mechanical response of the structure
- Changing the shape changes significantly plastic behaviour
- Planar deffects play an important role in the fracture mechanism
- The mechanical response is modified when the structure is made of Fe and Ni

These results are potentially useful to tailor the mechanical properties of new materials.

Acknowledgements

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THANK YOU

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