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Mechanics of Metallic Nanolattices: Designing a Future Generation of Cellular Materials on Supercomputers

• Motivation and goals

The ultimate goal of this project is the design of a future generation of metallic nanolattices 'at the very bottom' which requires atomistic simulation methods like molecular statics (MS) and molecular dynamics (MD). While at the macroscale the mechanics of lattices is well understood, on the nanoscale new questions arise; the material behavior is influenced by atomistic (nonlocal interactions, surface effects, competing inelastic deformation mechanicsm, size dependence etc.) which come into the picture for both single-crystalline as well as polycrystalline aggregates. The simulations require supercomputing facilities and a favorable scaling of the simulation performance with the massively parallel hardware.

• Nanolattices with solid struts

The regular, periodic structure of lattices as a cellular material allows for a model prediction to one unit cell (two nodes) along with periodic boundary conditions in the molecular deformation analyses.

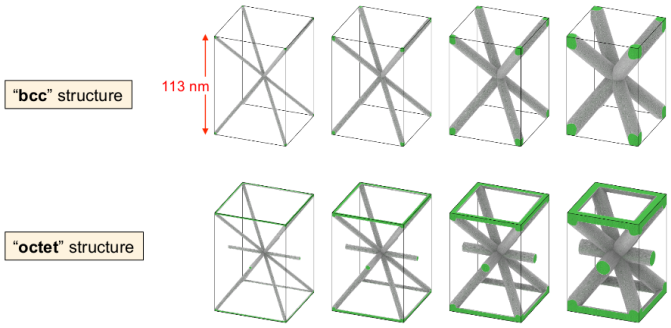

Fig. 1. Solid microlattice structure models with varying density (strut diameter to length ratio) and architecture.

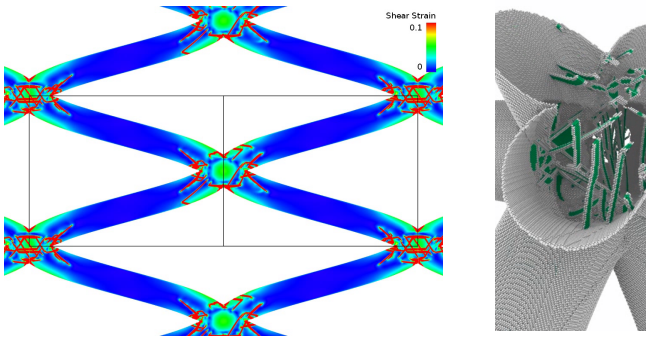

Fig. 2. (Left) Cross section through a periodic 'bcc' structure in the compressed state showing strain accumulation and dislocation activity in the nodal regions. (Right) Visualization of the dislocation defects accumulating in the material. The strut has a solid cross section, only defect atoms are displayed.

• Scaling behavior of stiffness and strength

$$\frac{\bar{E}}{E_s} = C\left(\frac{\rho}{\rho_s}\right)^n$$

$$\frac{\bar{\sigma}}{\sigma_s} = D\left(\frac{\rho}{\rho_s}\right)^m$$

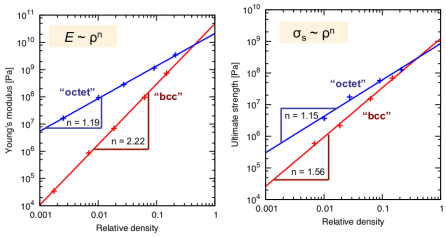

Fig. 3. Ashby plots showing the scaling behavior of elastic stiffness and strength versus density from MS simulations which is in agreement with analytical predictions, [1,2].

• Hollow tube nanolattices

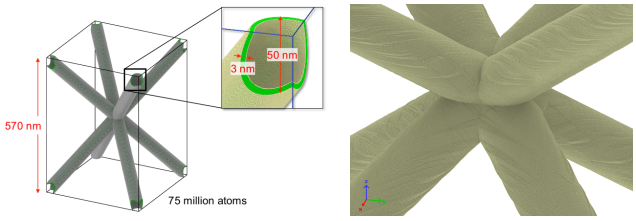

Fig. 4. (Left) A bcc unit cell of a hollow aluminum microlattice. Uniaxial compression along vertical axis has been simulated using MS. (Right) Surface wrinkles indicate deformation twinning commencing at 13% compression.

• Future challenges

The preliminary results indicate novel challenges for designing nanolattices; the question arises, which of the competing inelastic mechanisms for stress release is predominant, is it (i) dislocation-mediated plasticity as in Fig. 2, (ii) cracking or (iii) deformation twinning as in Fig. 4? How can we promote favorable inelastic mechanisms by topological and structural design and optimization? The interplay of structural mechanics dealing with struts subject to bending, buckling and folding and the material mechanics is a nontrivial challenge on the way towards a new generation of structural materials with a tailored design at the nanoscale.

• Acknowledgement

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References

[1] T. A. Schaedler et al. Science **334**, 962 (2011).
[2] L. J. Gibson, M. F. Ashby, Cellular Solids (Cambridge University Press, Cambridge, 1999).

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