Constrained sequential lamination: a sub-grid multiscale material model

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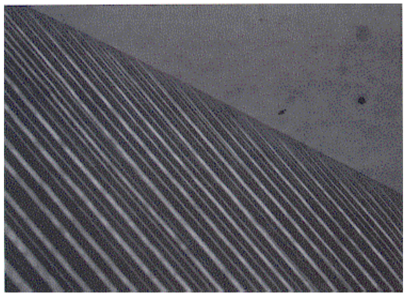
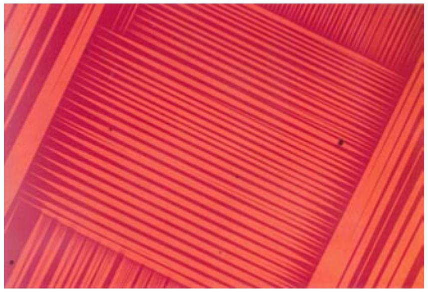
Background: Why multiscale modeling?

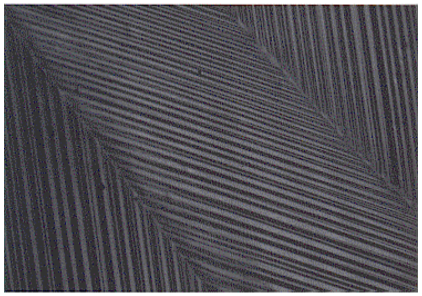
- Material behavior is often strongly influenced by the coupling of processes occurring over a range of length scales
- Some length scales and processes in solid mechanics
  - Angstrom -- electronic structure
  - Nanometers -- vacancies, dislocation cores
  - Microns -- dislocation interactions
  - Millimeters -- subgrain microstructure
- Multiscale methods incorporate effects from several scales
  - Build aggregate models $\Rightarrow$ higher fidelity
  - Direct application for some problems

Laminate introduction

- Prediction of the development of microstructures and their effect on material behavior is a key problem in the study of martensitic materials (e.g., shape memory alloys)







- Need an efficient numerical method for solving macroscopic boundary-value problems while simultaneously accounting for microstructure development

Introduction continued

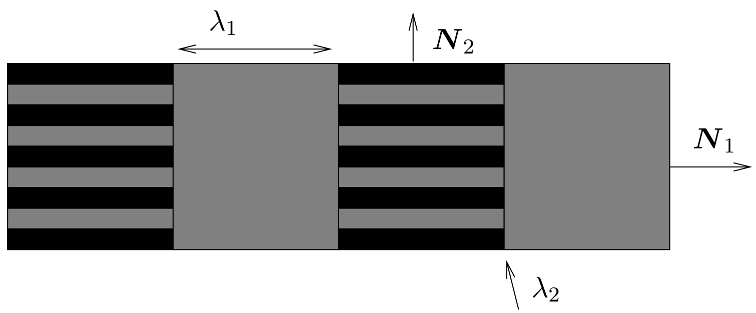
- Pose problem as energy minimization
- Such materials have several variants (or phases) ⇒ multiwell energy density
- Direct minimization results in “unrelaxed” solution
- Energy not quasiconvex
  - Infimum not attained: develop microstructures
  - Discretization must resolve microstructural details
  - Mesh biases results

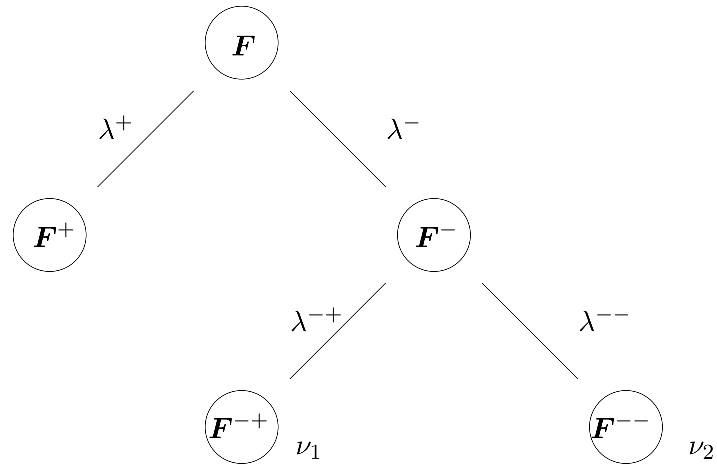
Problem formulation

- Wish to replace multiwell energy with quasiconvex envelope
  - This “relaxed” energy is well behaved
  - Require separation of length scales
  - No general algorithm is known
- Compute *partial* relaxation using the concept of sequential lamination and rank-one convexification

Sequential laminates

- Layered mixture of variants described by a binary tree





- For a given graph, material completely described by:
  - Average deformation gradient **F**
  - Polarization, normal, proportion {**a**, **N**, λ} and well number at each leaf

Lamination algorithm overview

- Formulate energy in terms of graph variables
- Include model of interfacial energy
  - Estimate of length scale
  - Eliminate runaway refinement
- Optimize laminate by minimizing energy with respect to:
  - Graph variables: {**a**, **N**, λ} and well number of each leaf
  - Graph topology
- Resulting laminate is in static and configurational equilibrium

Laminate evolution

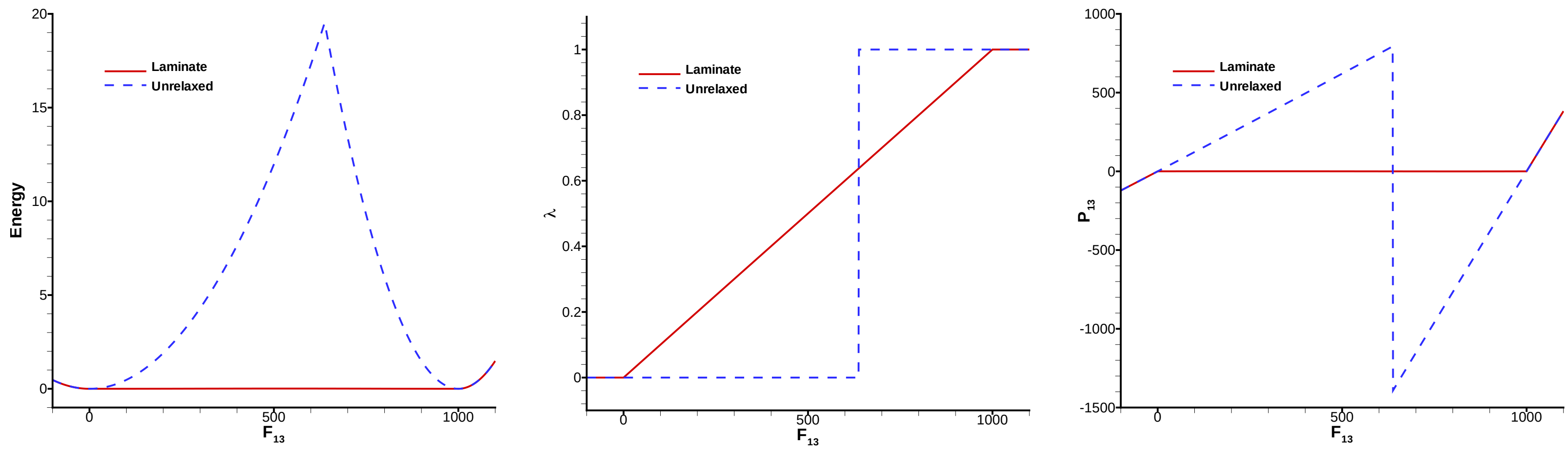
- Full rank-one convexification follows from consideration of **all** possible graphs
- Not feasible: use natural dynamics to visit important states
  - Graph must be “stable” (no zero volume fractions)
  - New graph accessible through pruning and branching

    Prune: remove null subtrees

    Branch: add two children if it reduces energy ⇒ driving force for branching
- Process of continuation: may not deliver absolute rank-one convexification, but provides a simple model of metastability and hysteresis

Example: martensite-martensite transition

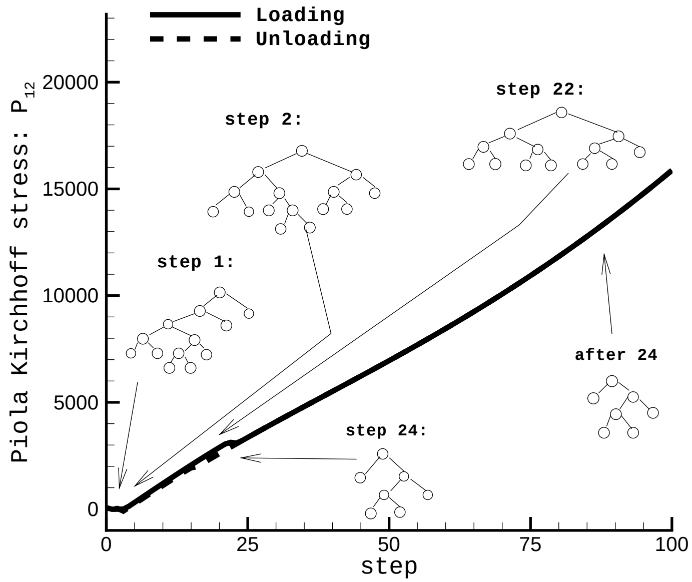
- Load from one transformation stretch to another to illustrate simple mixing between two wells

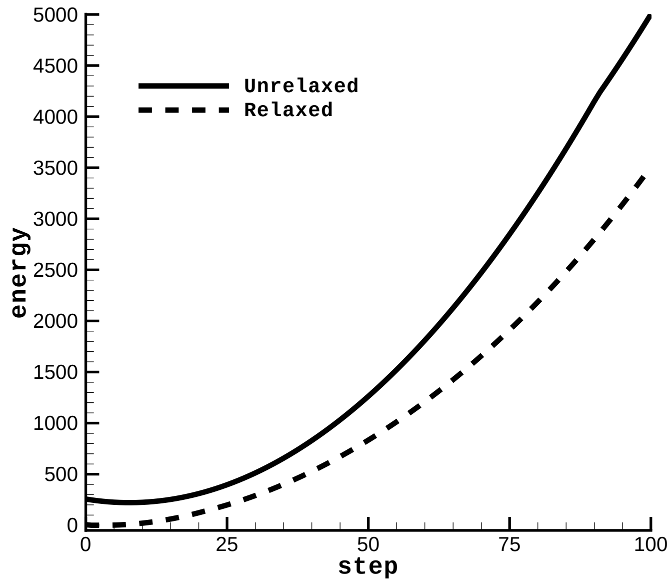


- Smooth transitions
- Fully relaxes energy and stress

Example: simple shear

- Load in simple shear
- Exclude austenitic well: forced to develop microstructure in initial configuration



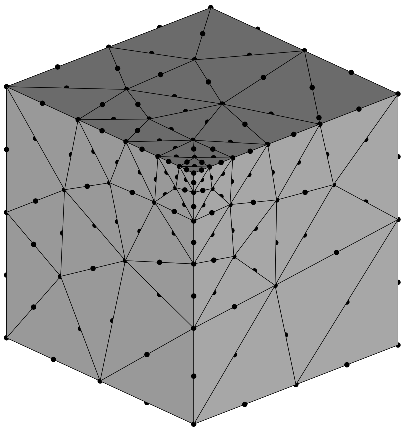


Finite element implementation

- Laminate model applied in parallel at mesh integration points providing stress and energy given deformation gradient
- Solution by energy minimization using dynamic relaxation followed by preconditioned conjugate gradient iteration

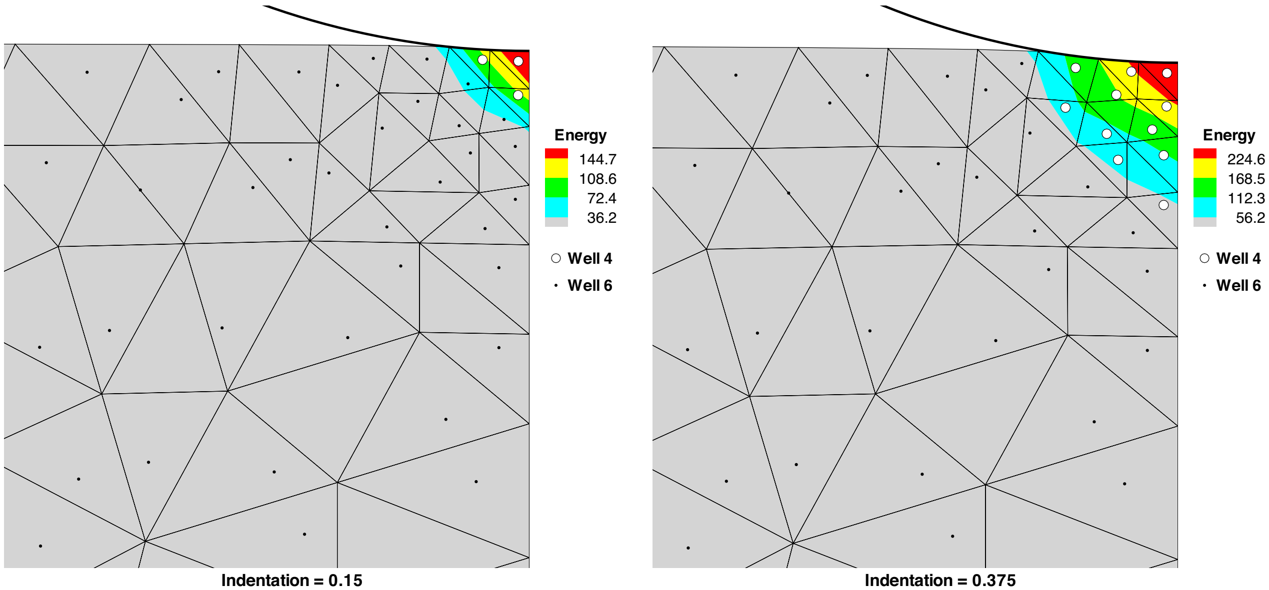
Finite Element Example Calculation

- Quasistatic indentation of Cu-Al-Ni by spherical indenter
- Quarter model of 20 mm region under a 15 mm radius indenter with 254 nodes and 105 ten-node finite strain quadratic elements
- Contact modeled by a penalty method



Finite element unrelaxed solution

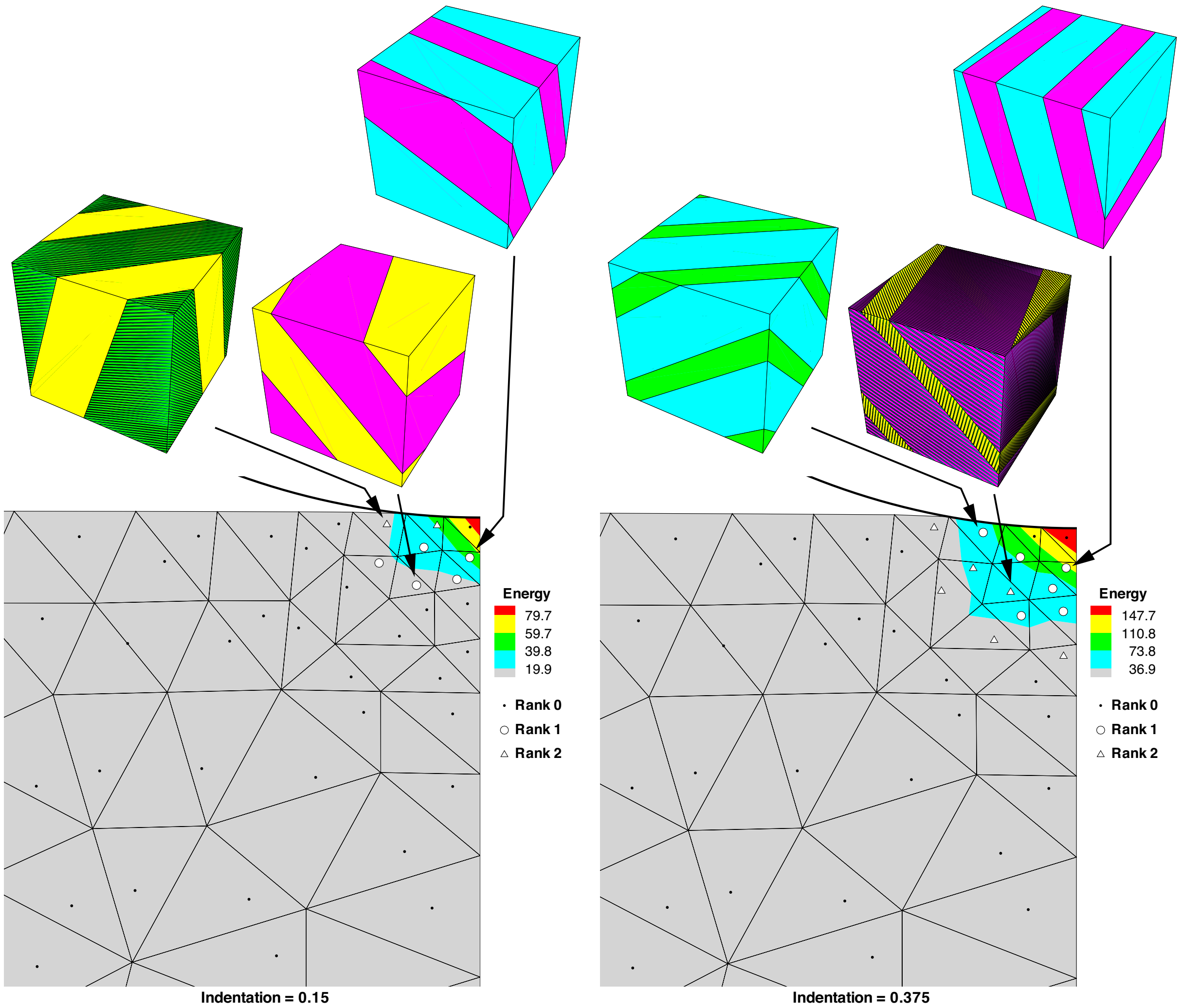
- Baseline for comparison



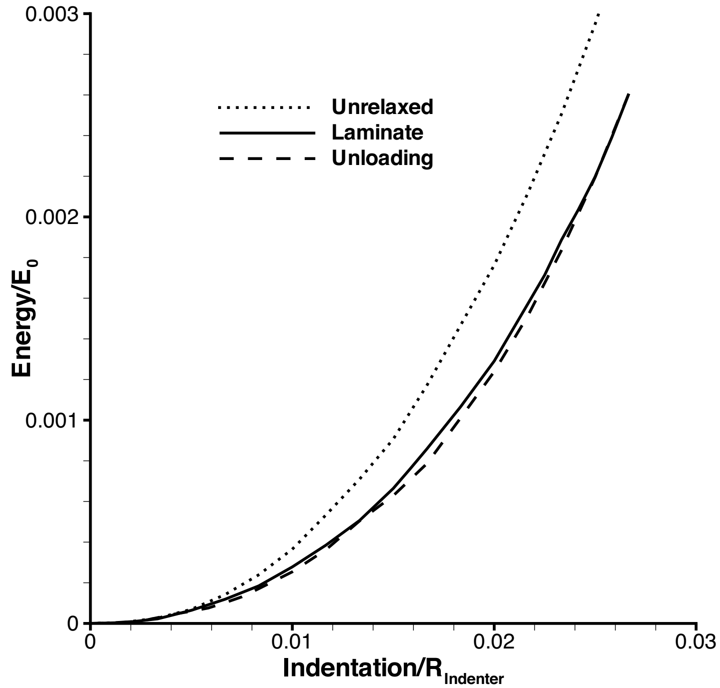
- Activate one martensitic well under indenter
- Fineness of variant arrangement limited by mesh

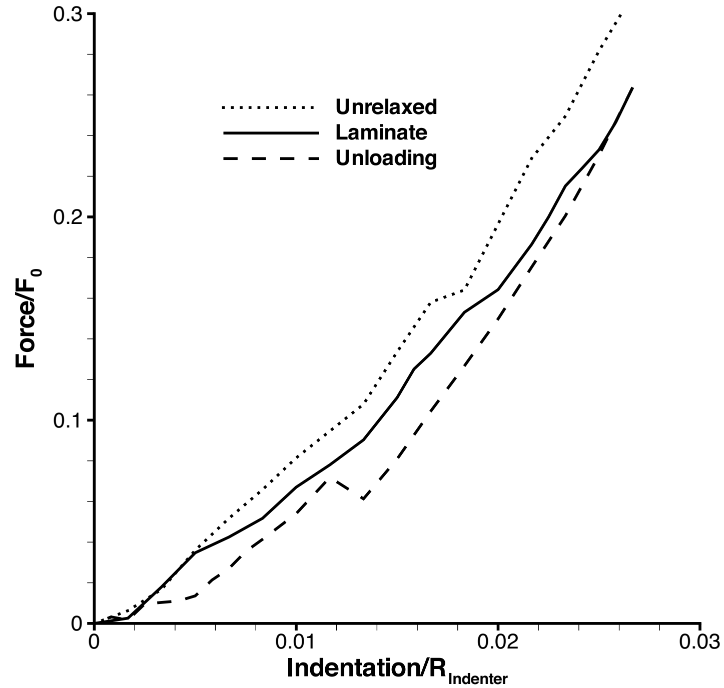
Finite element relaxed solution

- Develop rank 1 and 2 laminates
- De-twinning observed under indenter



Finite element results: energy & force

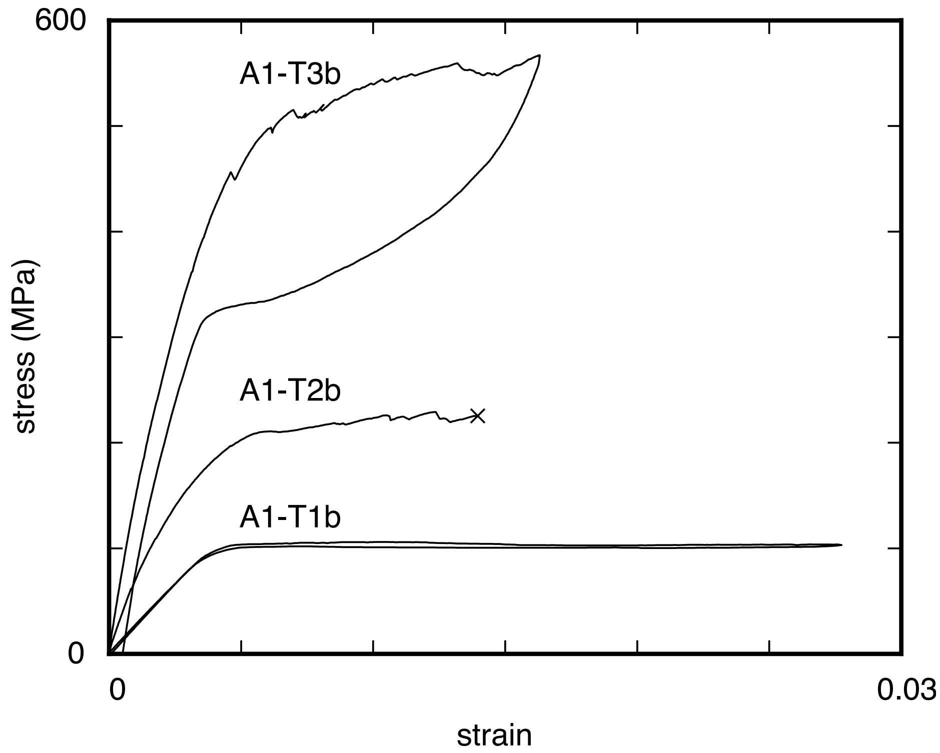


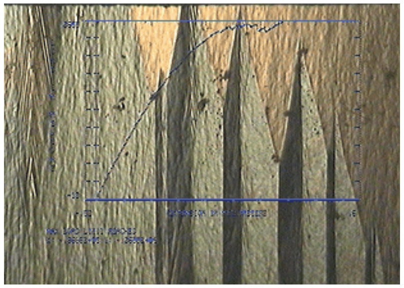


- Laminates produce softer response
- Unloading exhibits path-dependent nature of algorithm

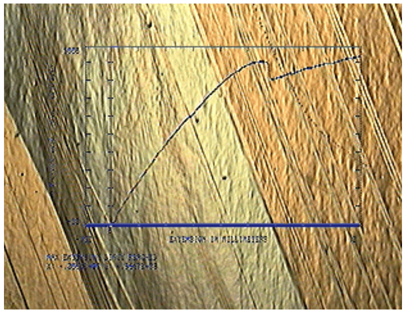
Experimental results

- T. Shield tension test experiments at several crystal orientations





A1-T3b



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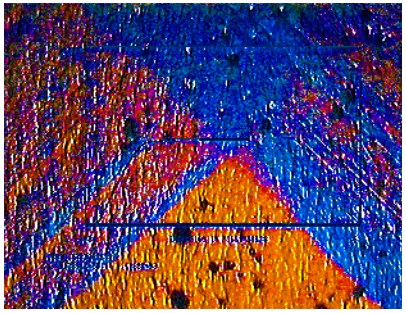
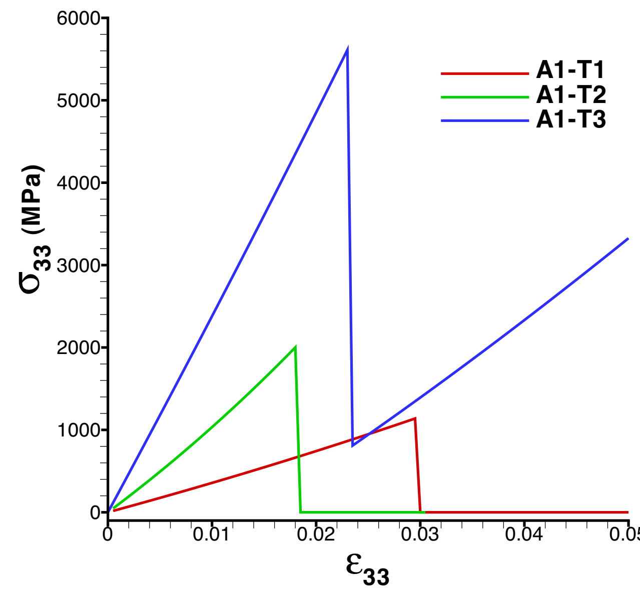
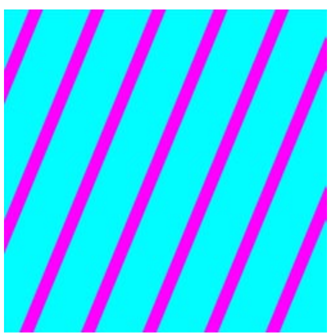


A1-T1b

Experimental validation: single point

- “Single point” laminate calculations
- Sensitive to boundary conditions
- Similar microstructures obtained
- Significantly higher transformation stresses





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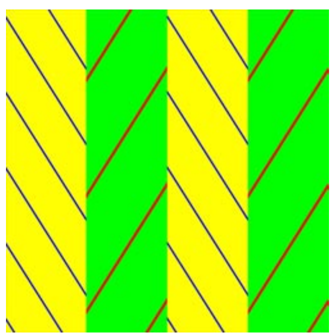

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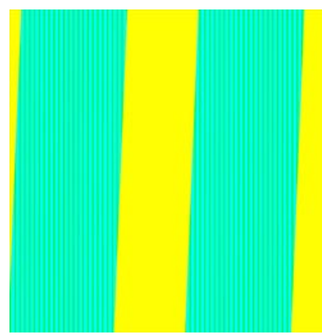
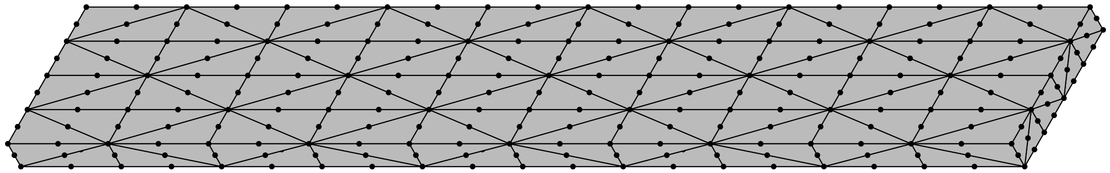


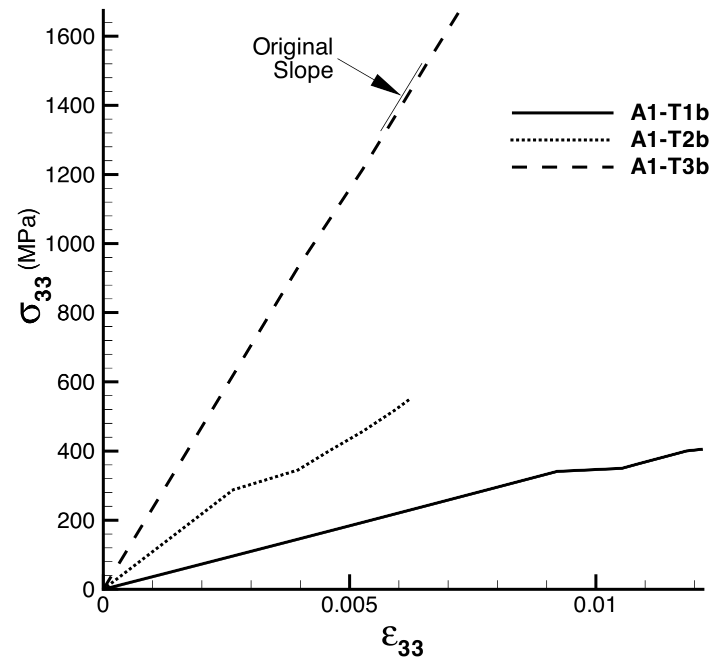
A1-T3b

Validation: finite elements

- Finite element simulation of test specimen



- Unambiguous boundary conditions
- Reduction in transformation stress, with significant softening observed



Conclusions and future work

- Demonstrated practical algorithm for partially relaxing multiwell energies through sequential lamination
- Demonstrated application of laminate model at the subgrid level of a finite element simulation
- Model produces microstructures similar to those obtained experimentally
- Can be extended to more accurately model real materials
  - Model of nucleation to reduce transformation stress
  - Replace equilibrium with kinetic relation governing interfacial motion
  - Extend to include plasticity (add variants for each slip-system)