Nonconvex Plasticity and Microstructure

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In collaboration with: S. Conti, E. Guerses, P. Hauret, J. Rimoli,

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Dedicated to Giulio Maier

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Classical (convex) plasticity

- Plasticity's early development focused on establishing the elastic limit of materials → yield surface, elastic domain (Tresca, Coulomb, Föppl, Voigt, Huber, Mohr, Hencky, Prandtl, von Mises, Timoshenko...)
- The flow theory was formalized by Bishop, Nadai, Hill, Drucker, Prager...
- Structural plasticity was developed in parallel (Maier, Martin, Ponter, Symonds...)
- Heavy emphasis was placed on ensuring existence and uniqueness of solutions of the rate problem...

Crystal plasticity – Deformation theory

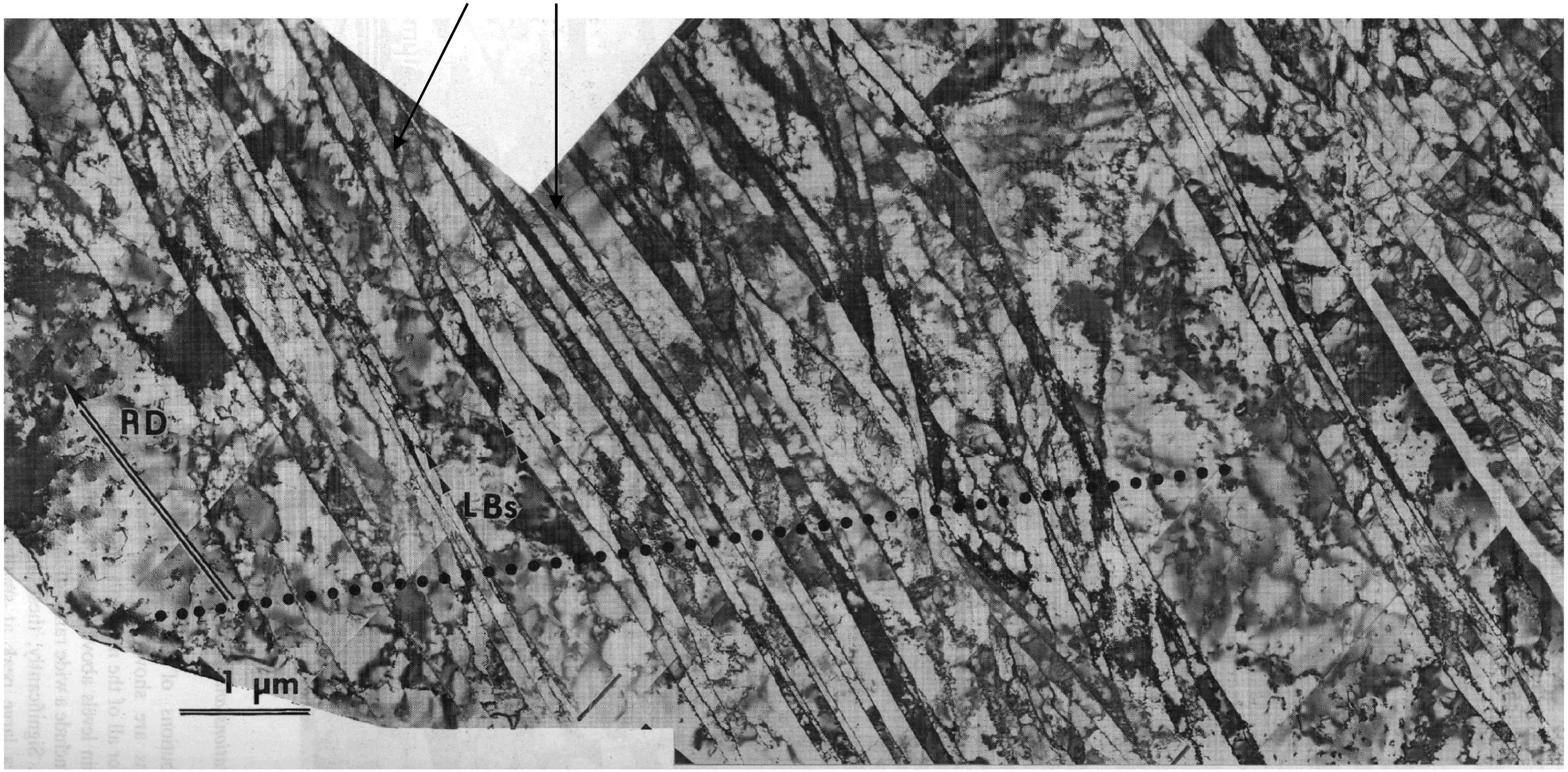
- Pseudo-energy density: $W(F) = \inf_{paths} \int P \cdot \dot{F}\, dt$
- Variational problem: $\inf_{y \in Y} \int_\Omega W(\nabla y)\, dx +$ forcing terms
- Linearized kinematics: $\epsilon^p(\gamma) = \sum_\alpha \gamma^\alpha \text{sym}(s^\alpha \otimes m^\alpha)$
- Rate-independent behavior, monotonic loading:

$$W(\epsilon) = \inf_{\gamma \geq 0} \{W^e(\epsilon(u) - \epsilon^p(\gamma)) + W^p(\gamma)\}$$

- Drucker's postulates: $W(\epsilon)$ convex!
- Convexity $\Rightarrow$ minimizer (if it exists) is **unique**!

Dislocation structures

Dislocation walls



Lamellar dislocation structure in 90% cold-rolled Ta

(DA Hughes and N Hansen, Acta Materialia, 44 (1) 1997, pp. 105-112)

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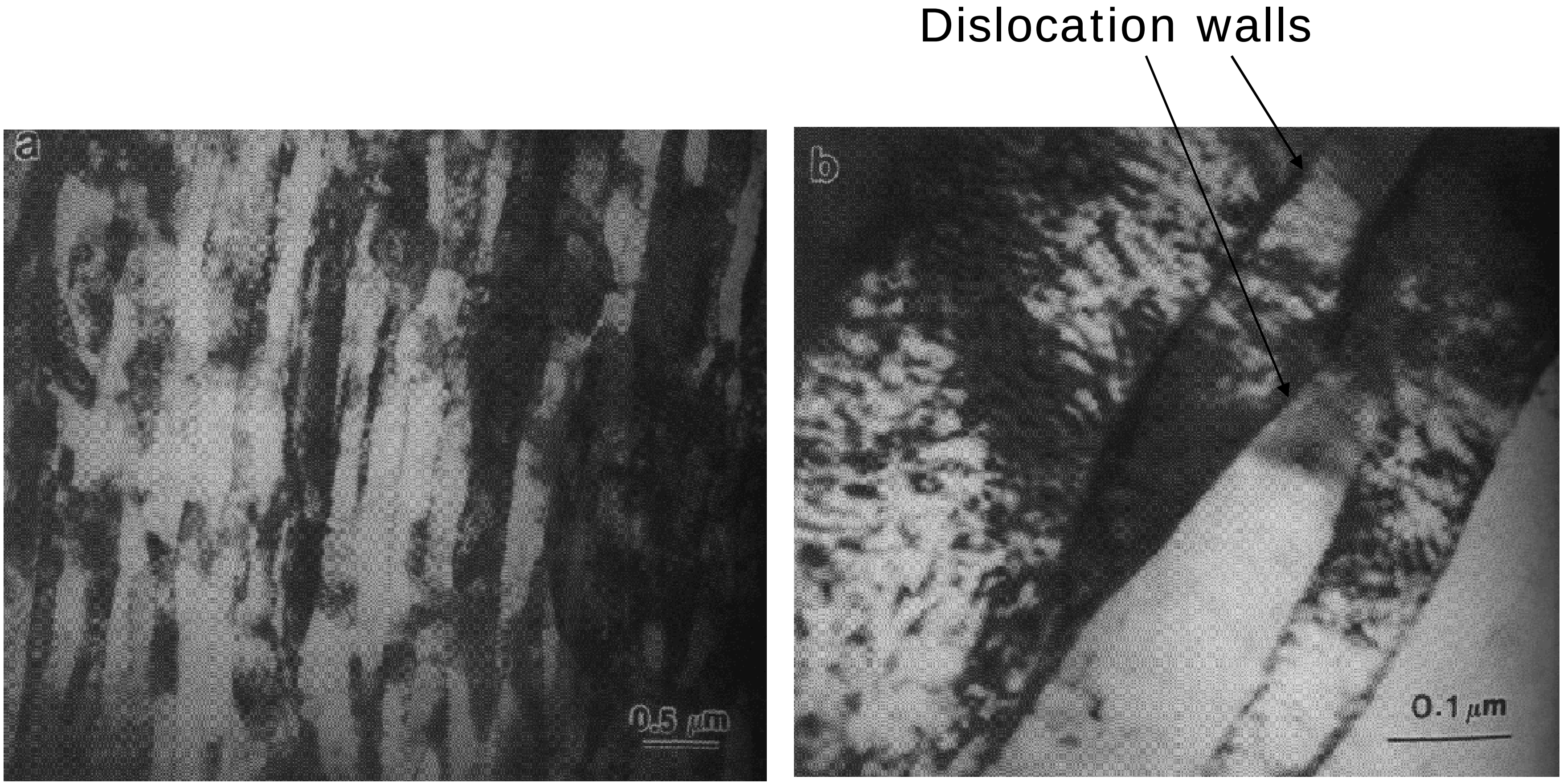
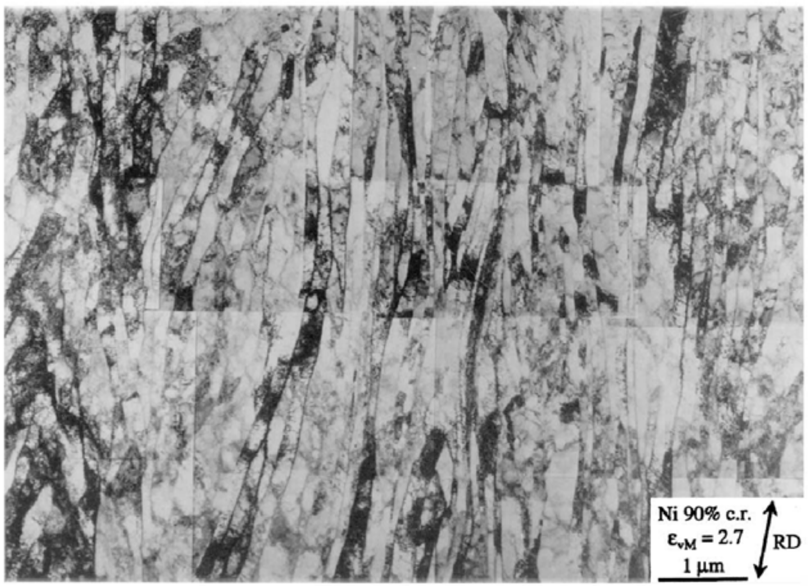
Dislocation structures

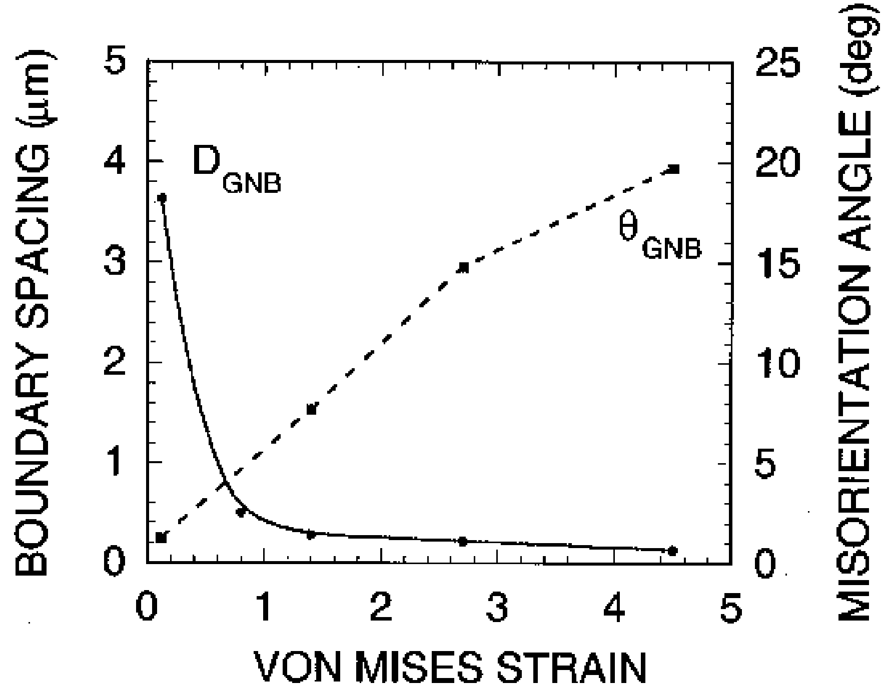


Lamellar structures in shocked Ta
(MA Meyers et al., Metall. Mater. Trans., 26 (10) 1995, pp. 2493-2501)

Dislocation structures – Scaling laws



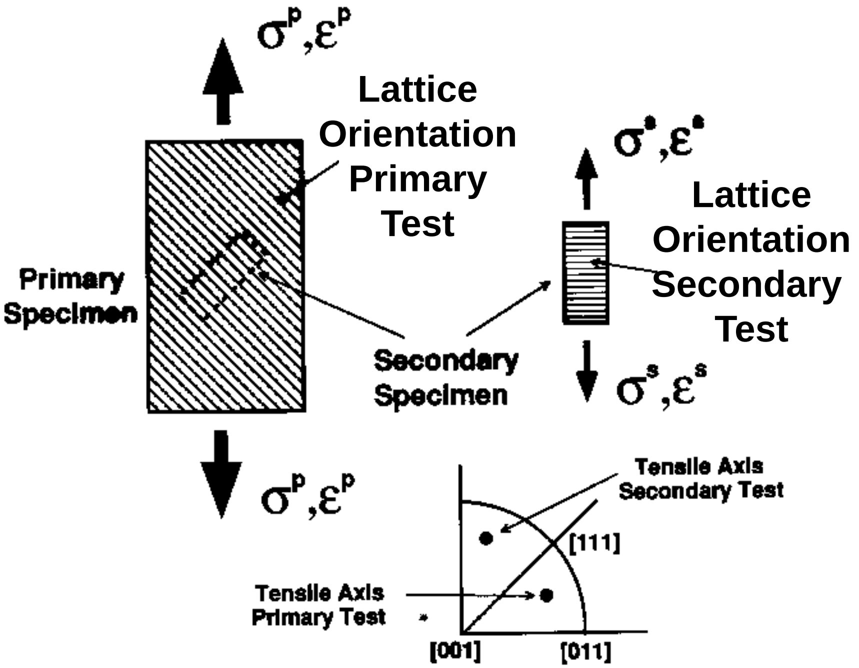
Pure nickel cold rolled to 90%
Hansen *et al.* Mat. Sci. Engin. A317 (2001).

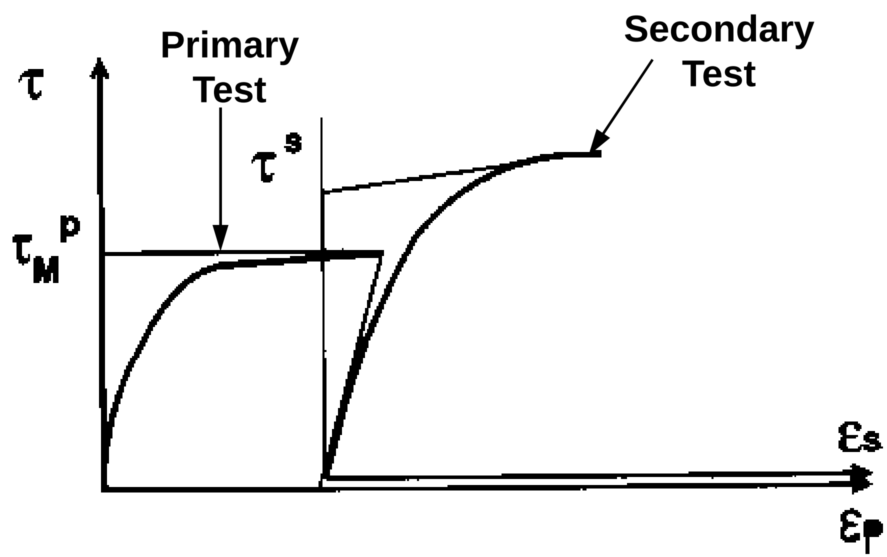


Lamellar width and misorientation angle as a function of deformatation
Hansen *et al.* Mat. Sci. Engin. A317 (2001).

Scaling of lamellar width and misorientation angle with deformation

Non-convexity - Strong latent hardening



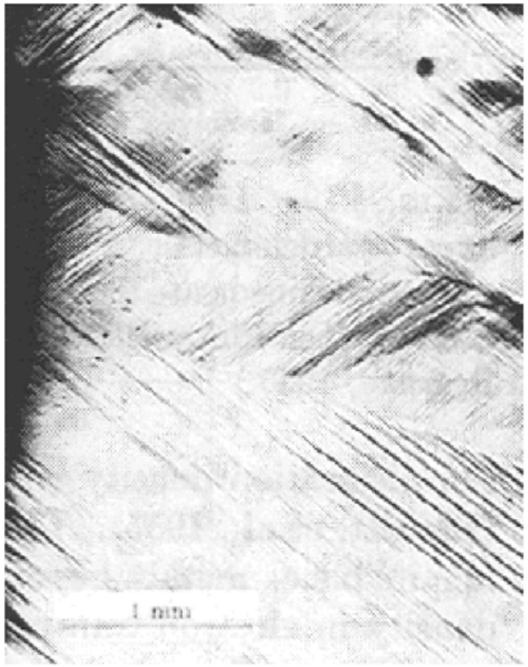


Latent hardening experiments

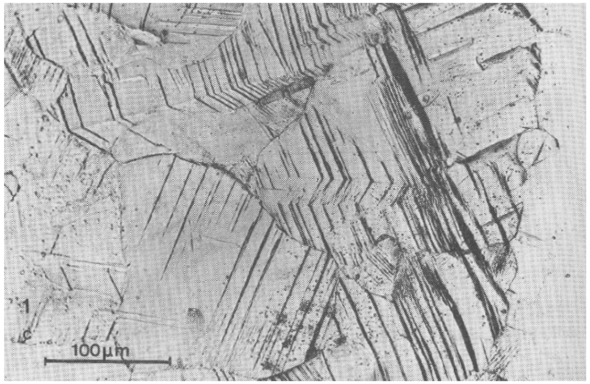
UF Kocks, *Acta Metallurgica*, **8** (1960) 345

UF Kocks, *Trans. Metall. Soc. AIME*, **230** (1964) 1160

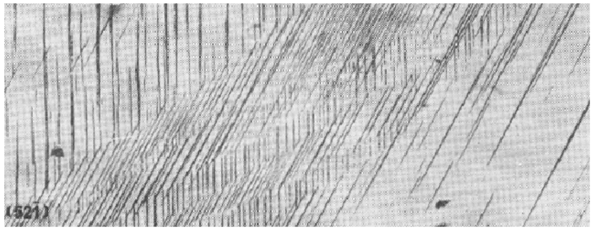
Non-convexity - Strong latent hardening



(Saimoto, 1963)



(Ramussen and Pedersen, 1980)

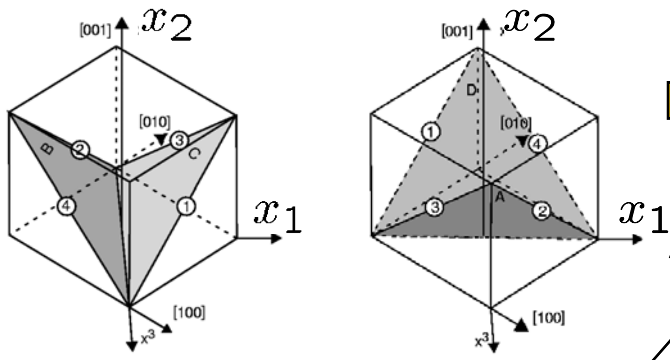


(Jin and Winter, 1984)

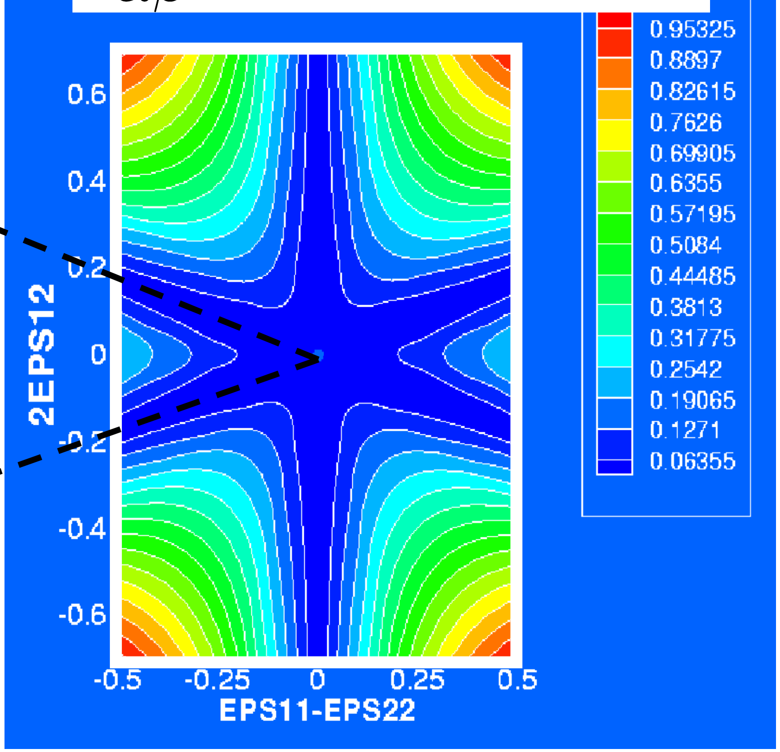
- **Latent hardening**: *"These results prove the reality of latent-hardening, in the sense that the slip lines of one system experience difficulty in breaking through the active slip lines of the other one"* (Piercy, G. R., Cahn, R. W., and Cottrell, A. H., *Acta Metallurgica*, **3** (1955) 331-338).

Non-convexity - Strong latent hardening

- Linear hardening: $W^p = \tau_0 \sum_\alpha \gamma^\alpha + \sum_\alpha \sum_\beta h_{\alpha\beta} \gamma^\alpha \gamma^\beta$
- Example: FCC crystal deforming on $(1\bar{1}0)$-plane



$h_{\alpha\beta} > h_{\alpha\alpha}, \quad \beta \neq \alpha$



$W(\nabla u)$

$\beta^p \in \gamma s \otimes m + so(3)$

(Single slip)

- $W(\nabla u)$ non-convex!

(Ortiz and Repetto, *JMPS*, **47**(2) 1999, p. 397)

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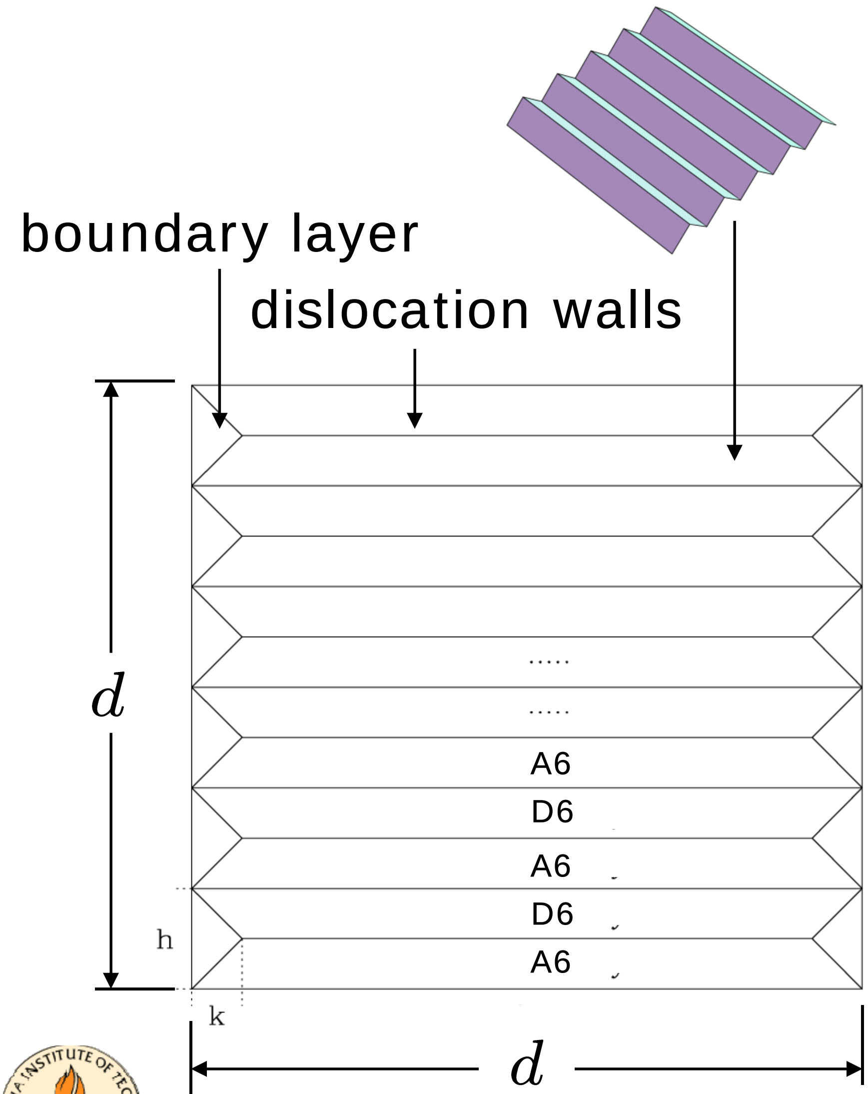
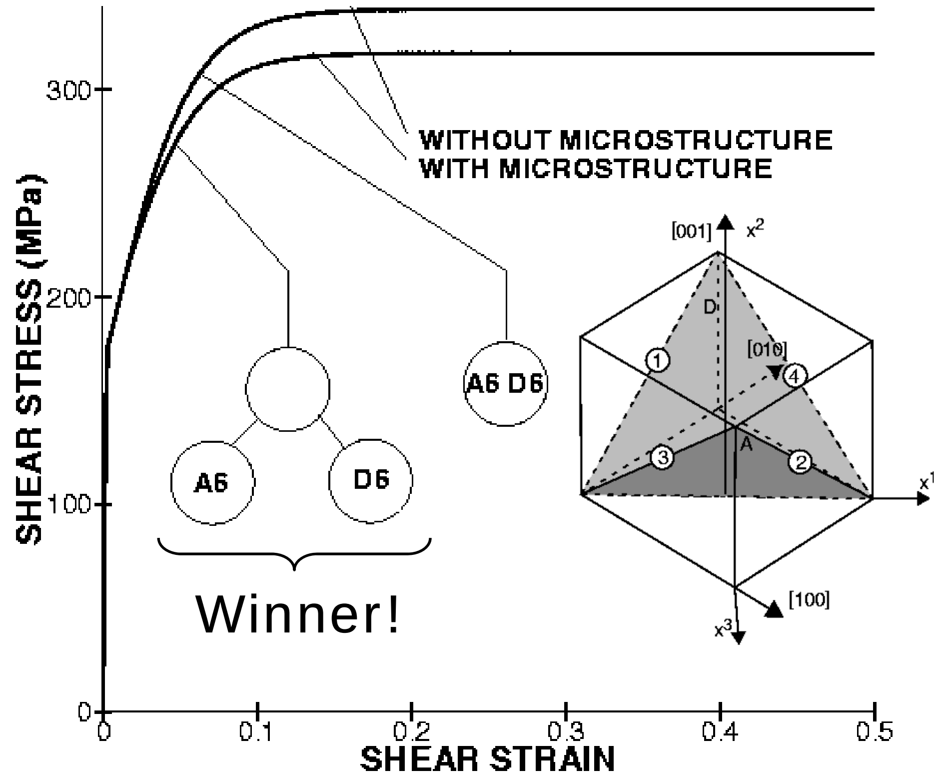
Non-convexity - Strong latent hardening





FCC crystal deformed in simple shear on (001) plane in [110] direction

(M Ortiz, EA Repetto and L Stainier *JMPS*, **48**(10) 2000, p. 2077)

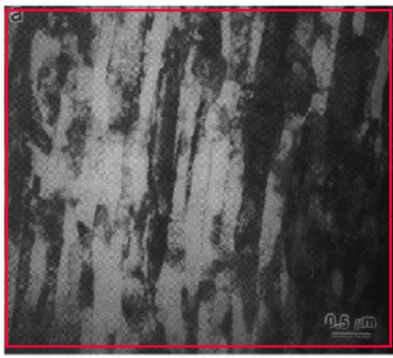
Non-convexity and microstructure

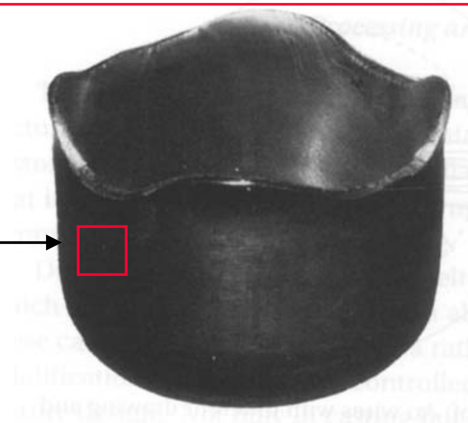
- Classical convex plasticity is ill-suited for describing subgrain dislocation structures in a continuum setting...
- Strong latent hardening and geometrical softening render the variational problem of crystal plasticity non-convex...
- Microstructures beat uniform multiple slip in general...
- How to build microstructure into finite element calculations?

Separation of scales - Relaxation

$$F(u) = \int_\Omega W(\nabla u)\,dx \quad \Rightarrow \quad m_X(F) = \inf_{u \in X} F(u)$$

$u = Ax$





$$QW(A) = \inf_{v \in W_0^{1,\infty}(E)} \frac{1}{|E|} \int_E W(A + \nabla v)\,dx$$

$$sc^- F(u) = \int_\Omega QW(\nabla u)\,dx$$

$$m_X(F) = \inf_{u \in X} sc^- F(u)$$

Relaxation of the constitutive model

Relaxed problem

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Separation of scales - Relaxation

- The relaxed problem is much nicer than the original one, can be solved, e.g., by finite elements
- The relaxed and unrelaxed problems deliver the same macroscopic response (e.g., force-displacement curve)
- All microstructures are accounted for by the relaxed problem (no physics lost)
- All microstructures can be reconstructed from the solution of the relaxed problem (no loss of information)

Relaxation and enhanced elements

- Let:
  - $\mathcal{T}_h \equiv$ triangulation of Ω, $\quad T \in \mathcal{T}_h$
  - $E \subset W_0^{1,\infty}(T; \boldsymbol{R}^n) \equiv$ local enrichment (bubbles).
- Enhanced elements:

$$\inf_{u \in X_h} \left(\sum_{T \in \mathcal{T}_h} \inf_{v \in E} \int_T W(\nabla u + \nabla v)\, dx \right)$$

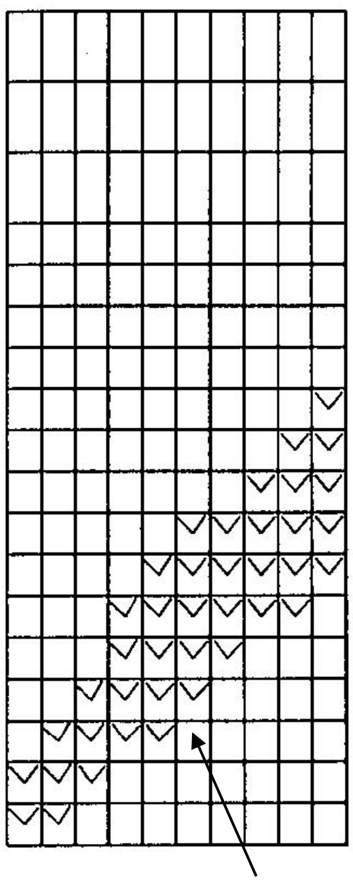
- Partially relaxed constitutive equations:

$$EW(F) \equiv \inf_{v \in E} \frac{1}{|T|} \int_T W(F + \nabla v)\, dx$$

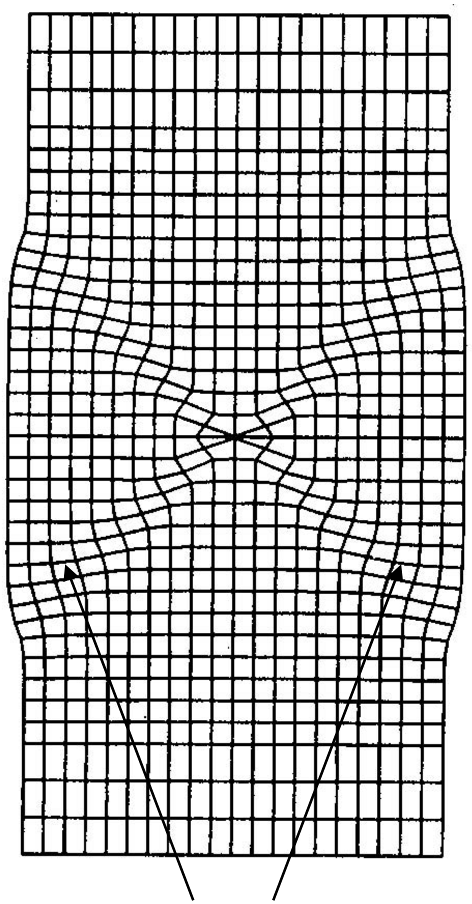
- Partially relaxed problem: $\boxed{\inf_{u \in X_h} \int_\Omega EW(\nabla u)\, dx}$

Relaxation and enhanced elements

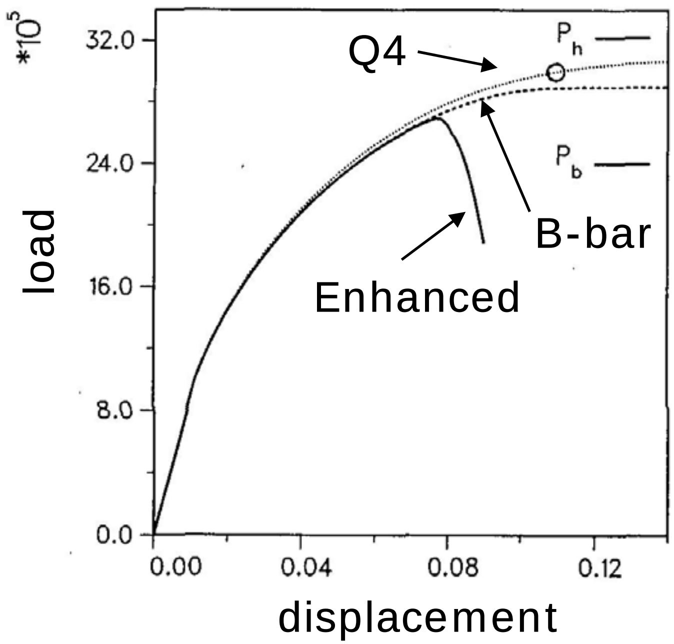
- Example: Localization elements.



Embedded strain discontinuities



Shear bands



Ortiz, Leroy and Needleman, *CMAME*, **61** (2): 189-214 (1987)

Relaxation and enhanced elements

- Effect of element enhancement/enrichment in microstructure problems:
  - *Partially relax the constitutive relations*
  - *Solve partially relaxed problem with original elements*
- In general: $EW(F) \gg QW(F)$, unless enrichment is carefully tailored to specific material microstructures
- Always: $EW(F) \geq QW(F)$ relaxation provides the optimal element enhancement!

Relaxation – Fast multiscale models

- **Fast Multiscale Models**: Use explicitly relaxed constitutive relation (when available) to represent sub-grid behavior
- Much faster than concurrent multiscale calculations (on-the-fly generation of sub-grid microstructures, e.g., by sequential lamination)
- Finite elements are equipped with optimal microstructures, exhibit optimal effective behavior
- Optimal element enhancement!

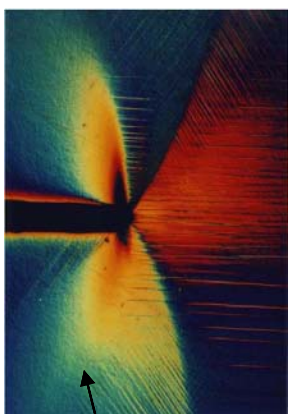
Crystal plasticity – Exact relaxation

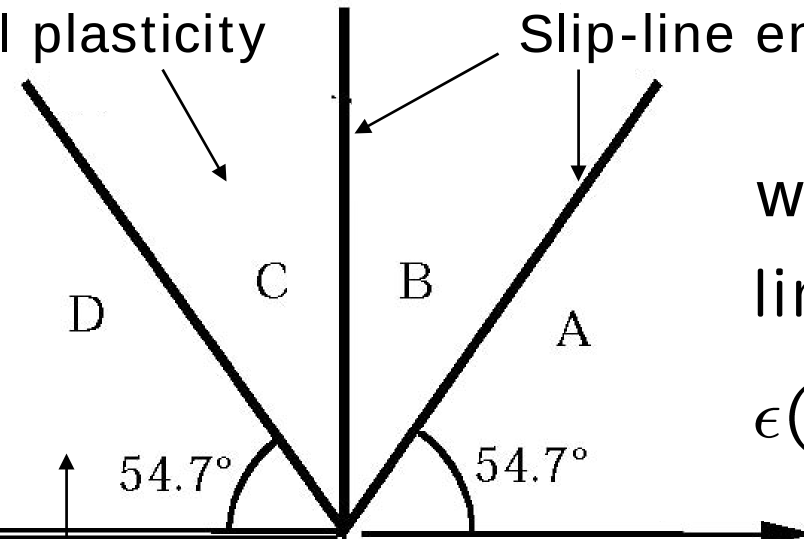
- Relaxation of small-strain crystal plasticity (S Conti and M Ortiz, *ARMA*, **176** (2005) 147):

$$\underbrace{\int_\Omega W^{**}(\mathcal{E}u)dx}_{\text{Ideal plasticity}} + \int_\Omega \underbrace{W^\infty\left(\frac{E_s u}{|E_s u|}\right)}_{\text{Slip-line energy}} d|E_s u|$$

Ideal plasticity

Slip-line energy





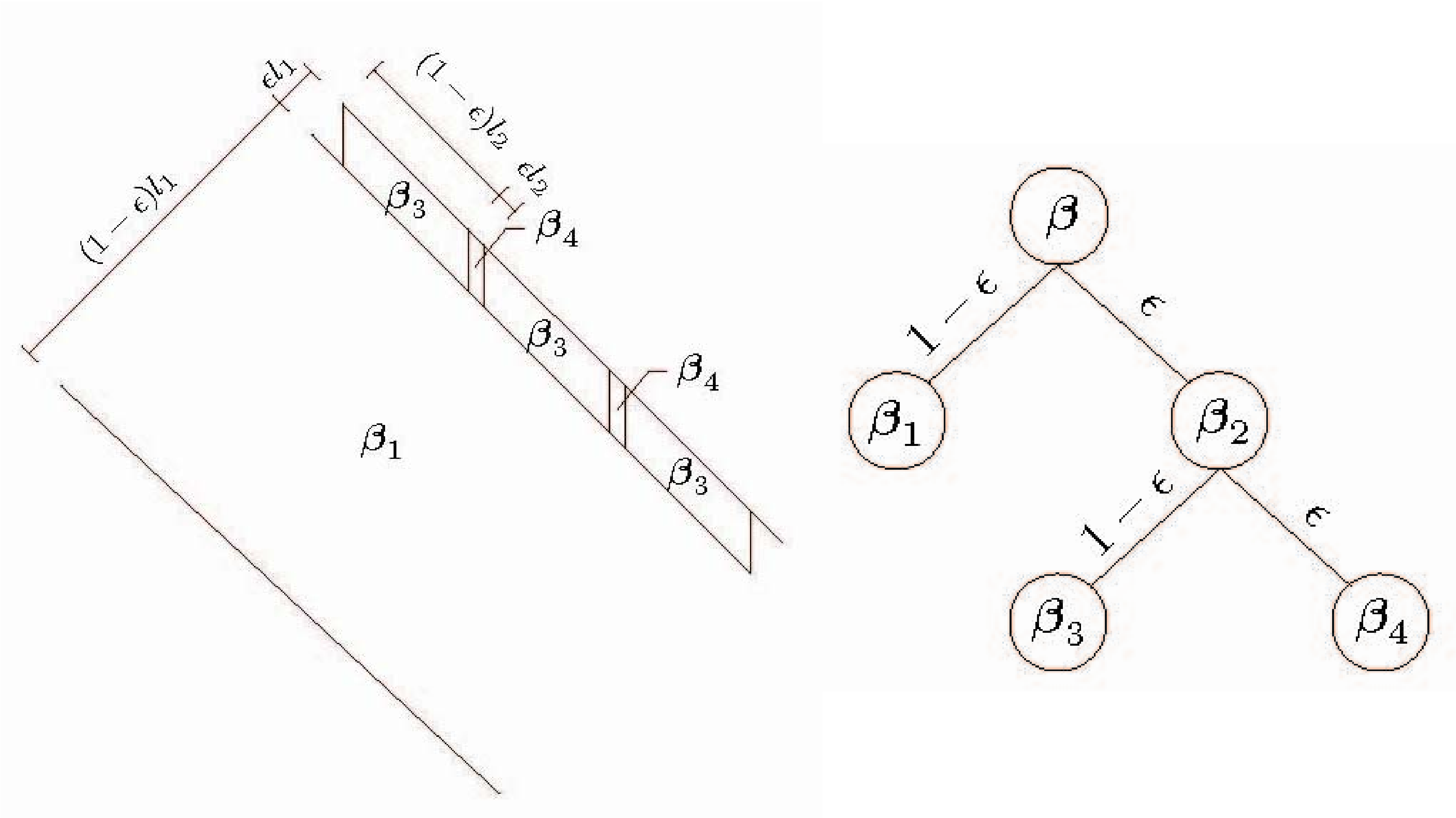
where: $W^\infty(A) = \lim_{t\to\infty} W^{**}(tA)/t$,

$\epsilon(u) = \mathcal{E}u dx + E_s u$

(Rice, *Mech. Mat*., 1987)

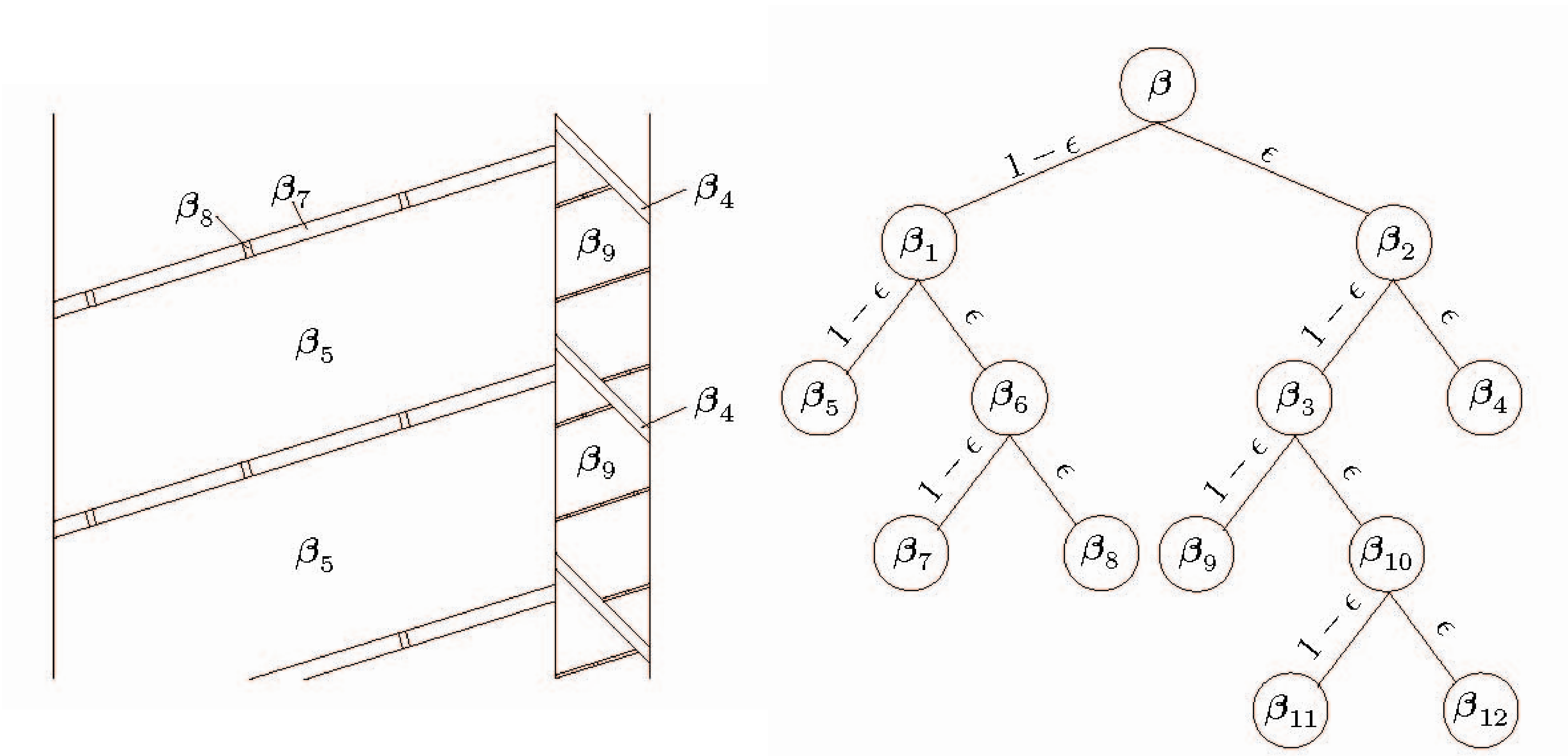
(Crone and Shield, *JMPS*, 2002)

Crystal plasticity – Exact relaxation



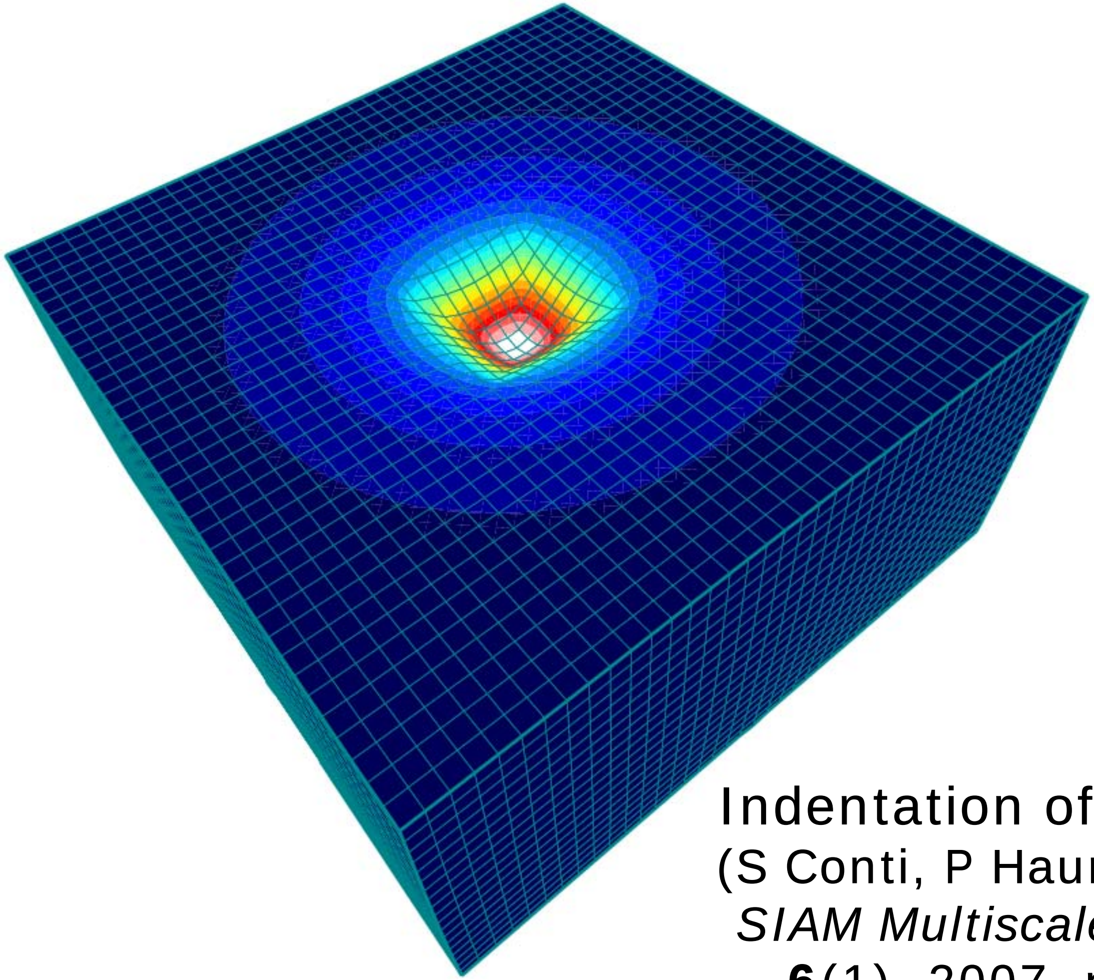
Optimal microstructure construction in double slip
(Conti and Ortiz, ARMA, 2004)

Crystal plasticity – Exact relaxation



Optimal microstructure construction in triple slip
(Conti and Ortiz, ARMA, 2004)

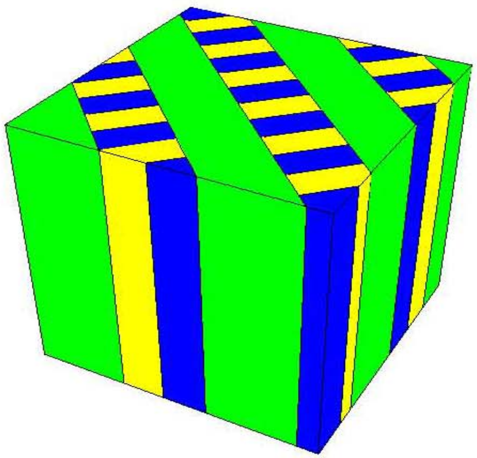
Relaxation – Fast multiscale models

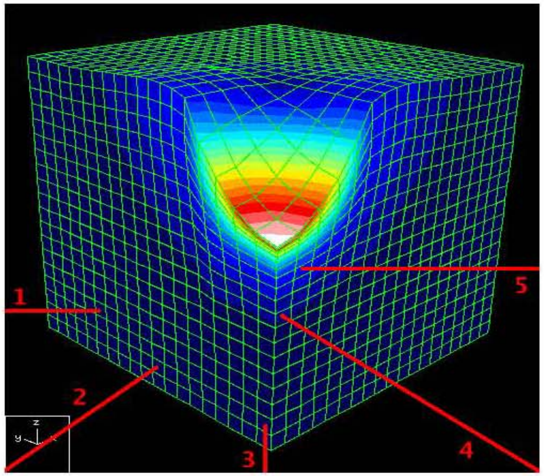


Indentation of [001] copper
(S Conti, P Hauret and M Ortiz, *SIAM Multiscale Model. Simul*. **6**(1), 2007, pp. 135–157)

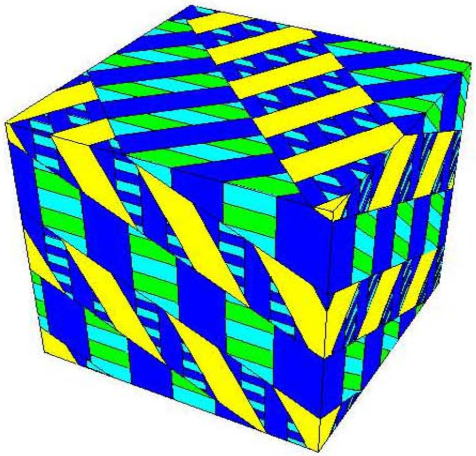
Relaxation – Fast multiscale models

rank 2/2, $|\gamma|_\infty$ = 0.0025

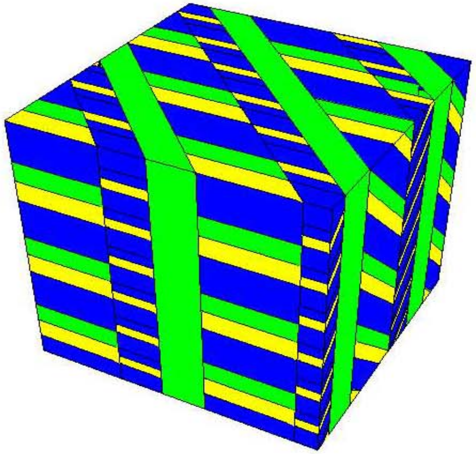




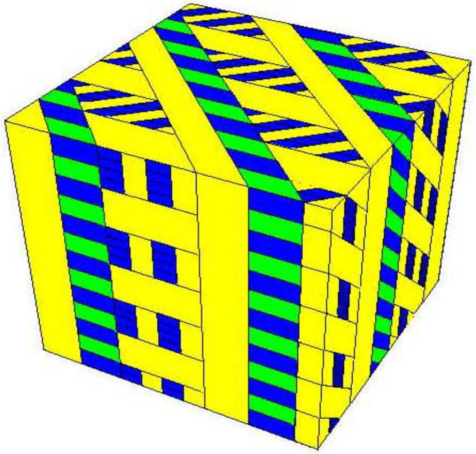
rank 4/14, $|\gamma|_\infty$ = 0.43



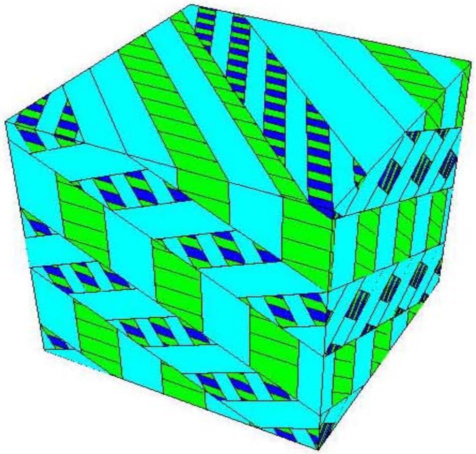
rank 4/12, $|\gamma|_\infty$ = 0.02



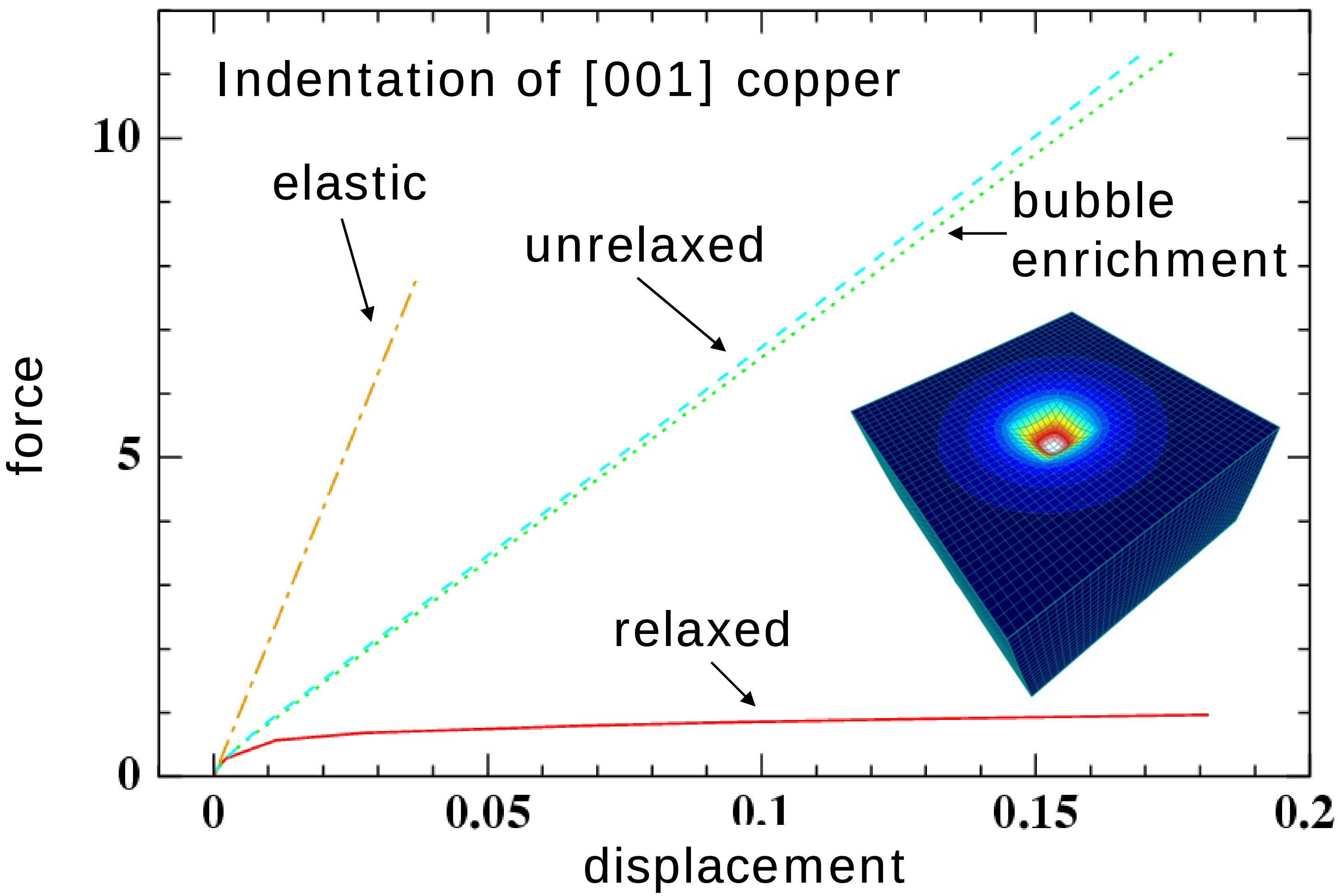
rank 4/6, $|\gamma|_\infty$ = 0.026



rank 4/16, $|\gamma|_\infty$ = 0.21



Relaxation – Fast multiscale models



(S Conti, P Hauret and M Ortiz, *SIAM Multiscale Model. Simul.* **6**(1), 2007, pp. 135–157)

High-Explosives Detonation Initiation

Detonation of high-explosive (RDX, PETN, HMX)

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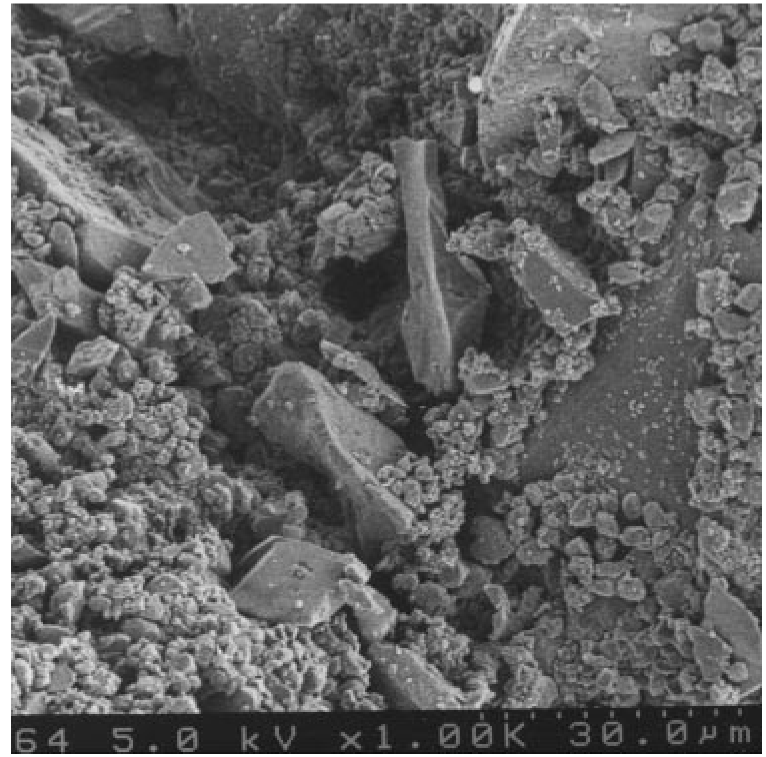
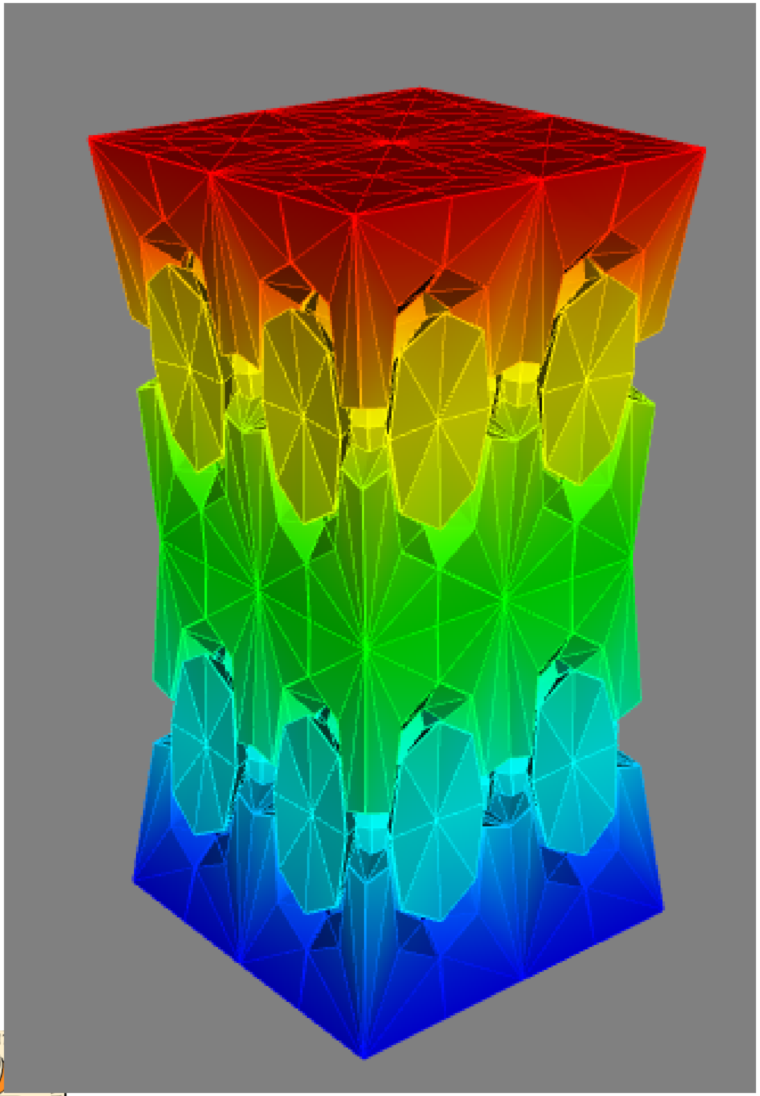
High-Explosives Detonation Initiation

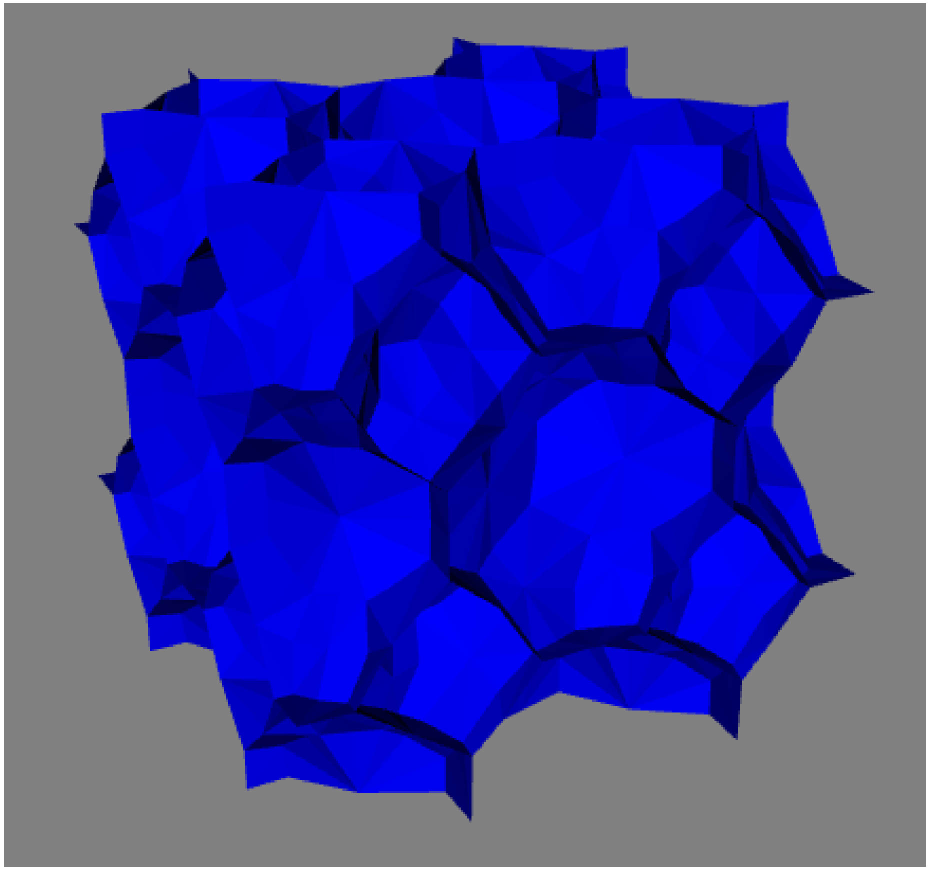
- In high explosives (HE) localized hot spots cause detonation initiation
- Some hot spots may arise as a result of localized plastic deformation
- Heterogeneity and defects act as stress risers and promote localization
- Need to predict defor-mation microstructures, extreme events! (not just average behavior)



Polycrystalline structure of high-explosive (LLNL S&TR June 1999)

High-Explosives Detonation Initiation





Polycrystal model and grain boundaries

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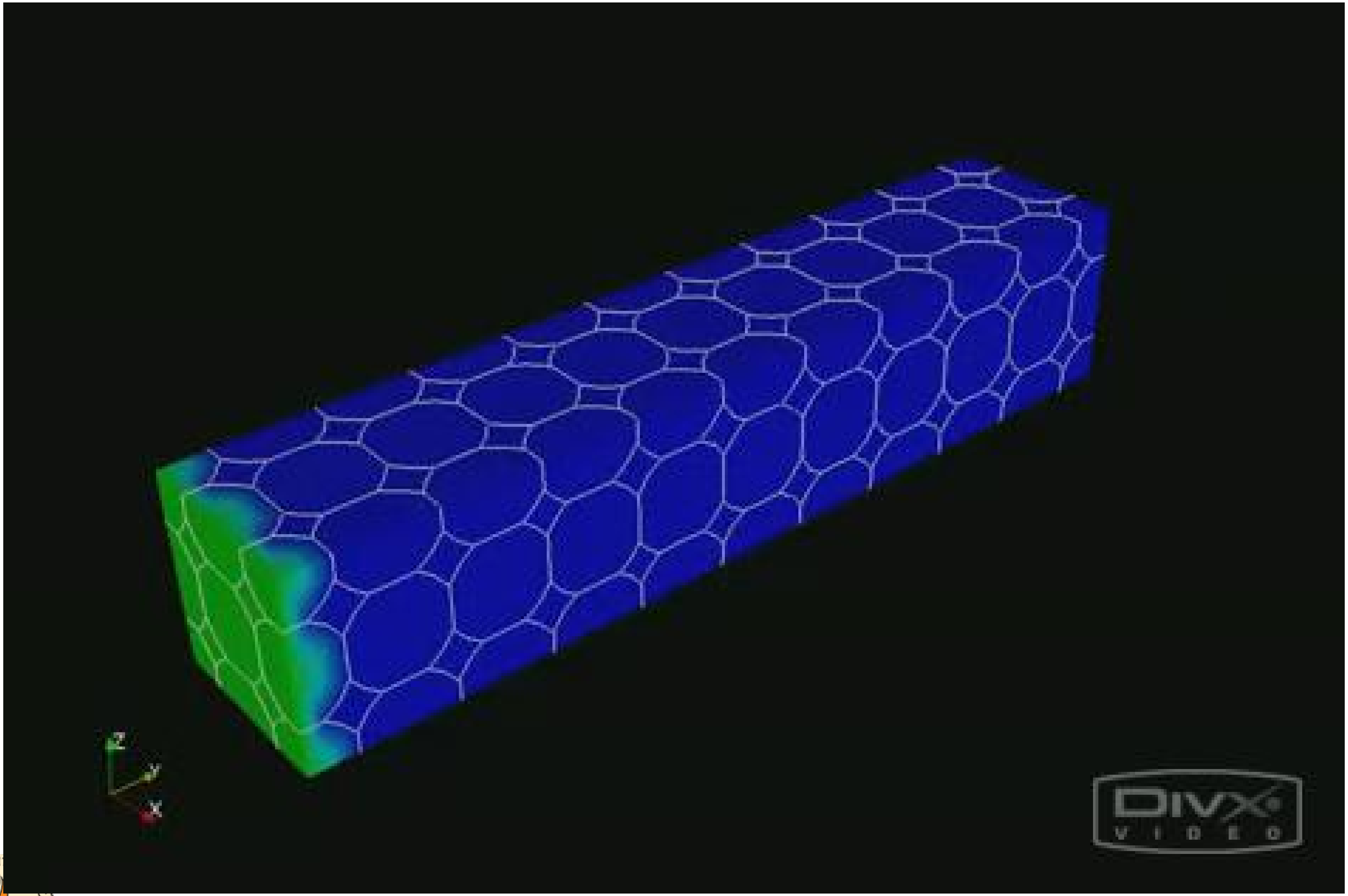
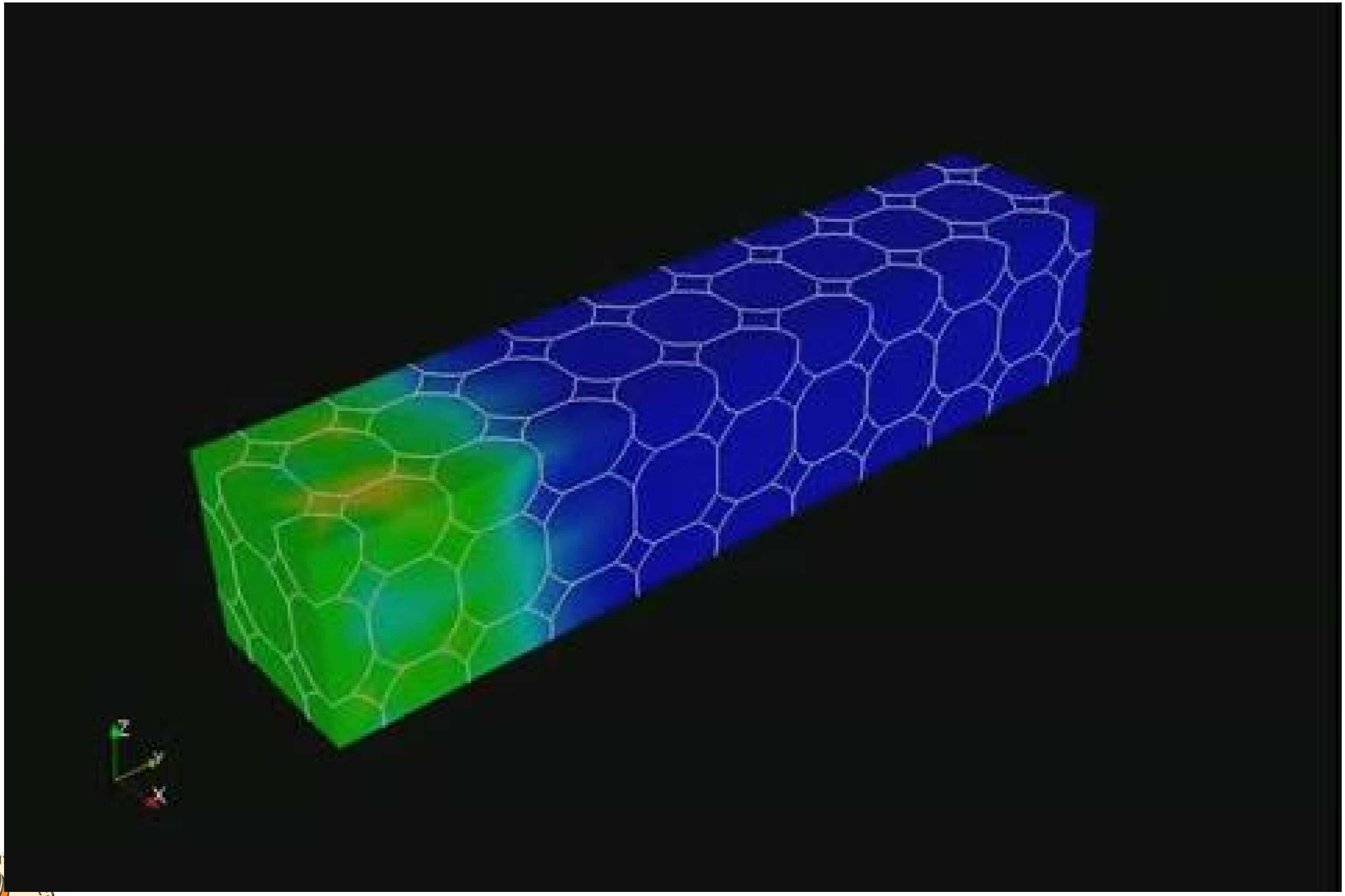


Plate impact simulation

High-Explosives Detonation Initiation



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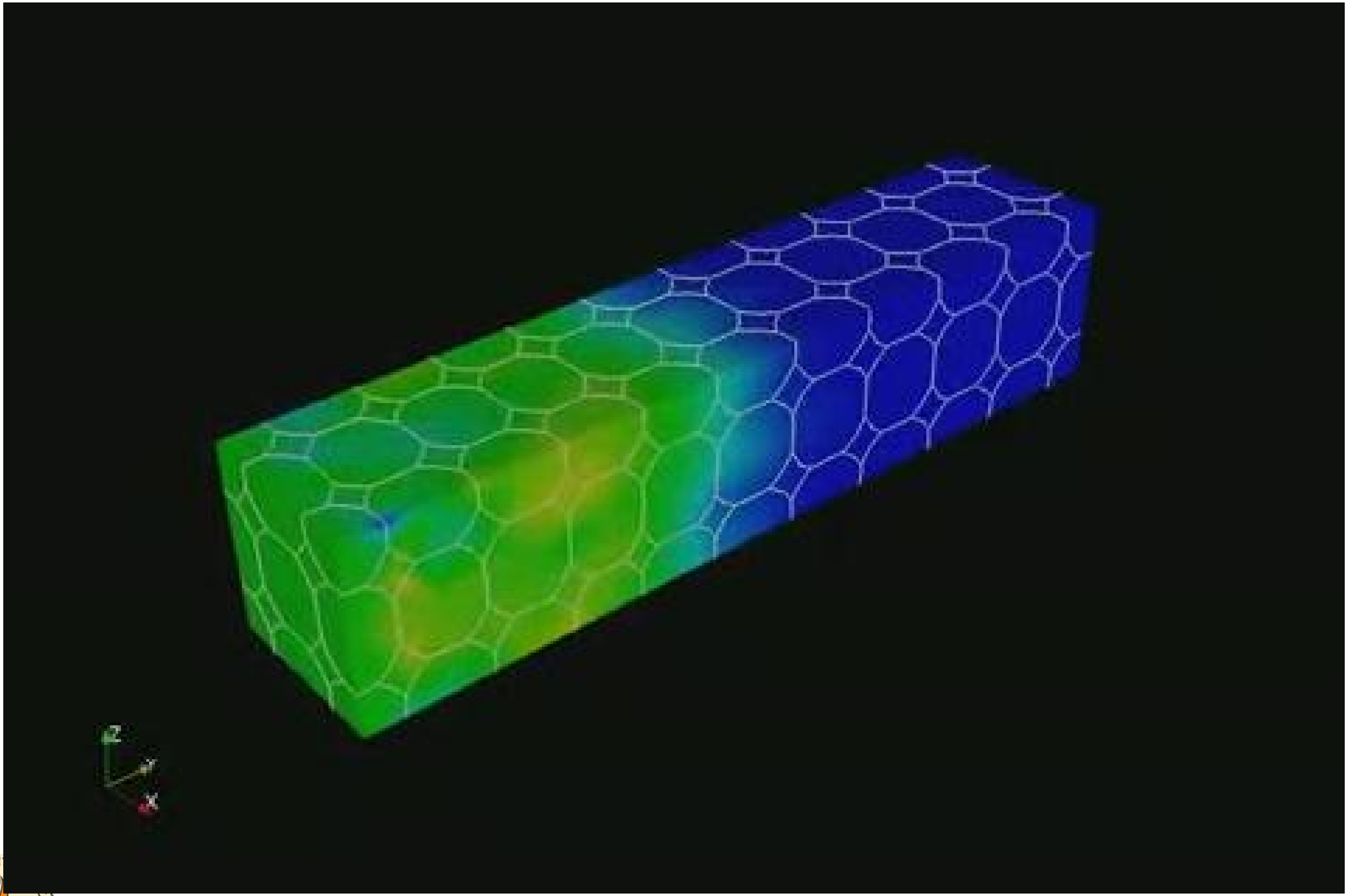

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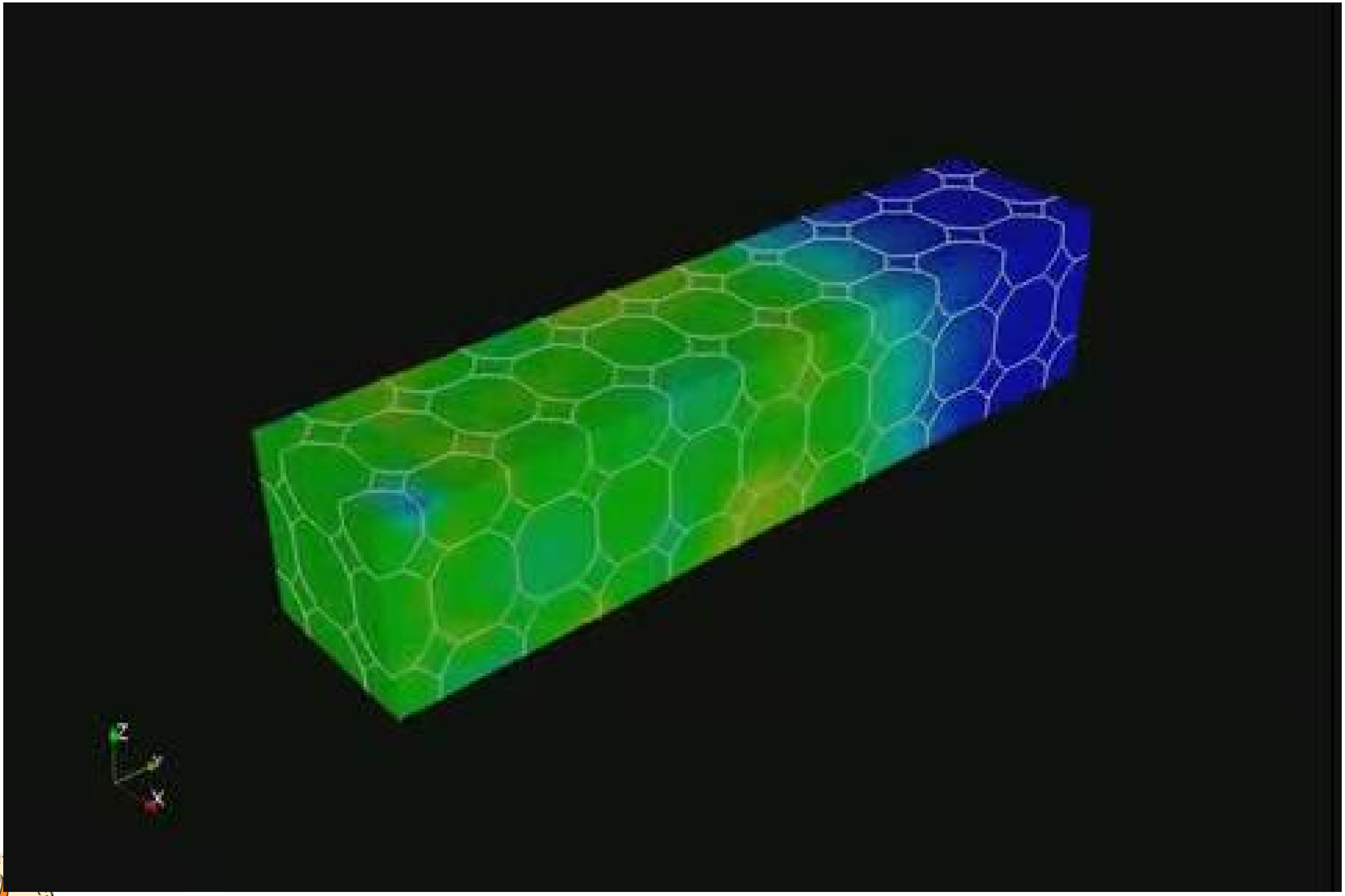

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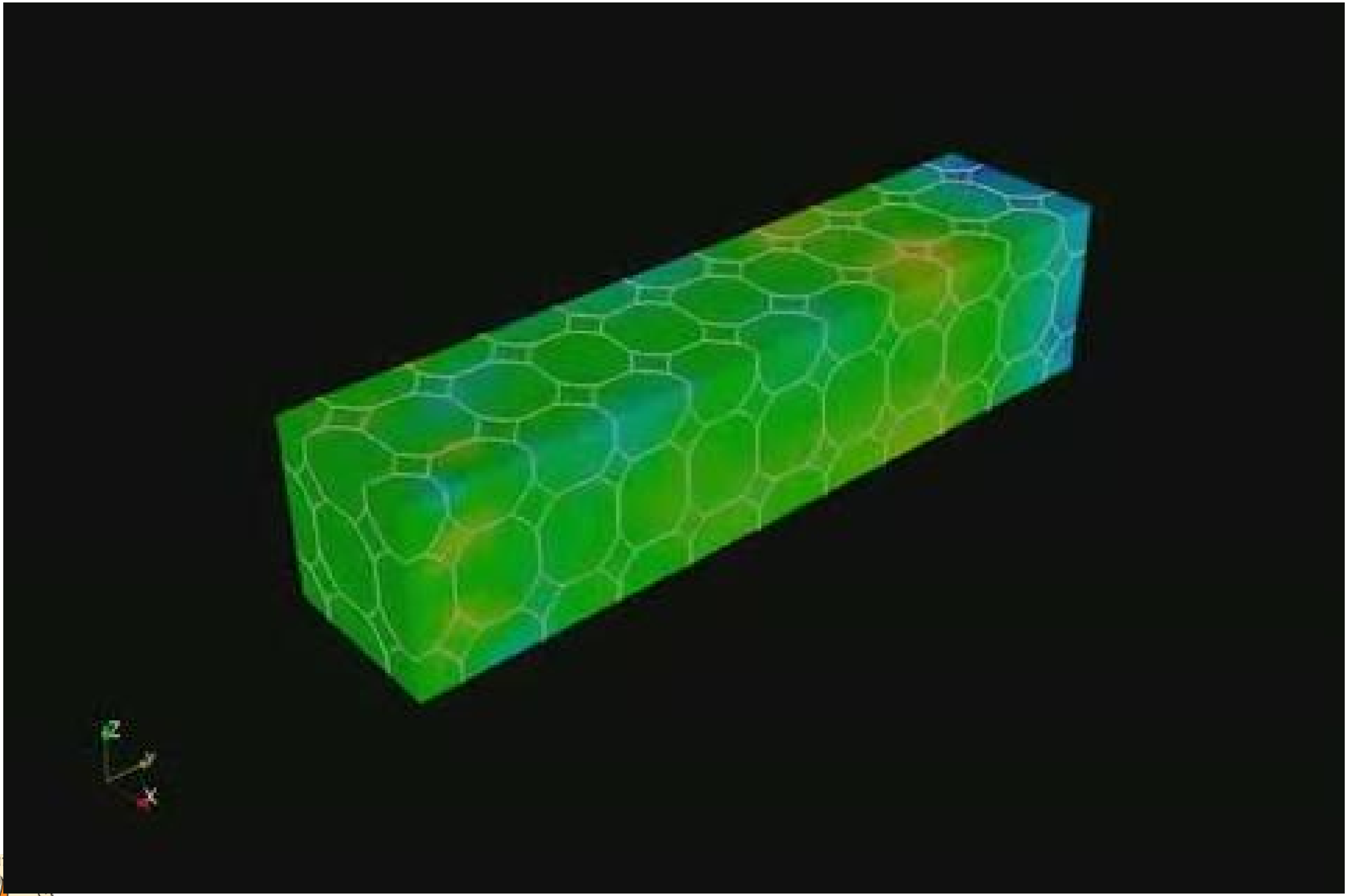

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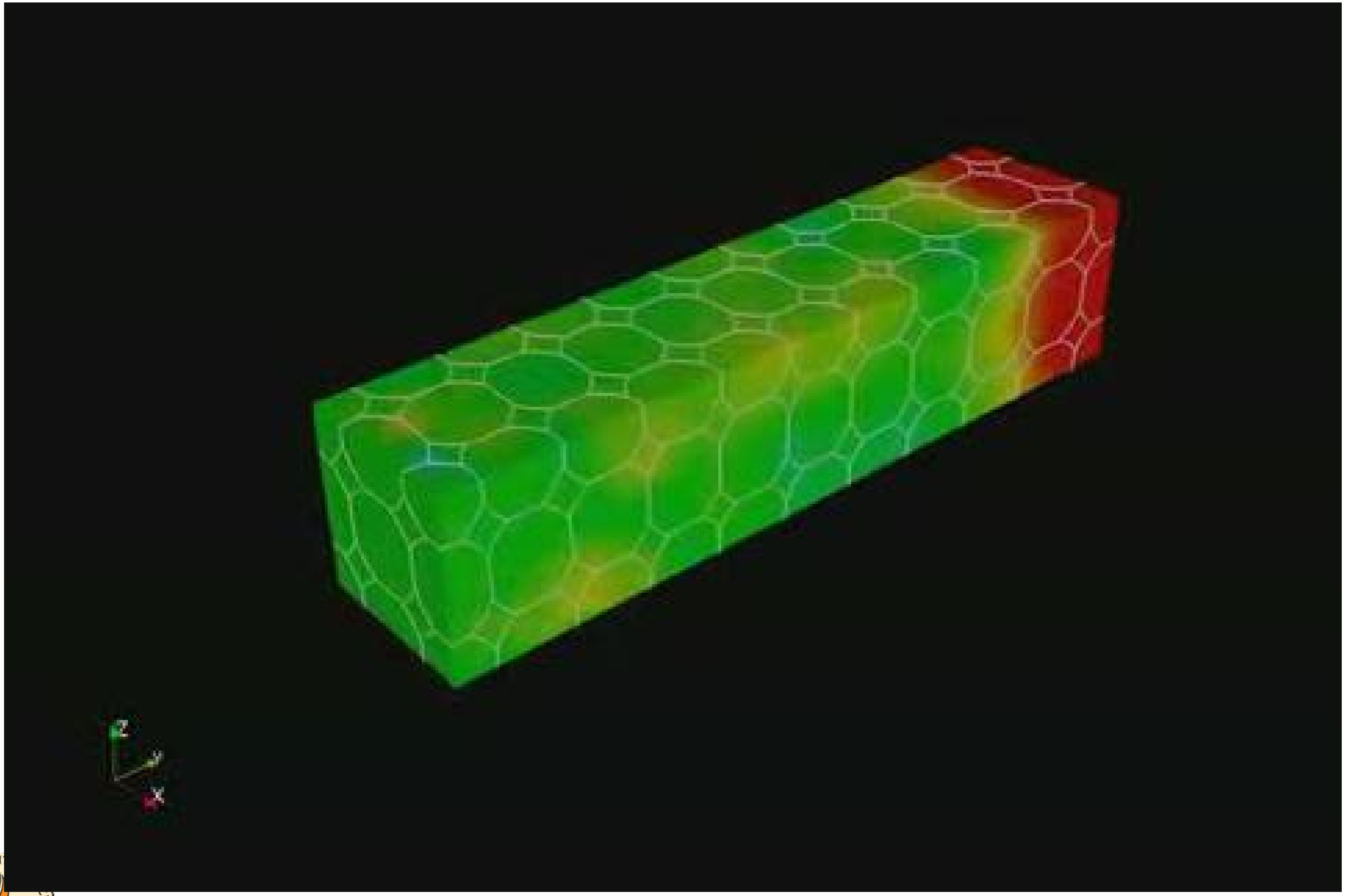

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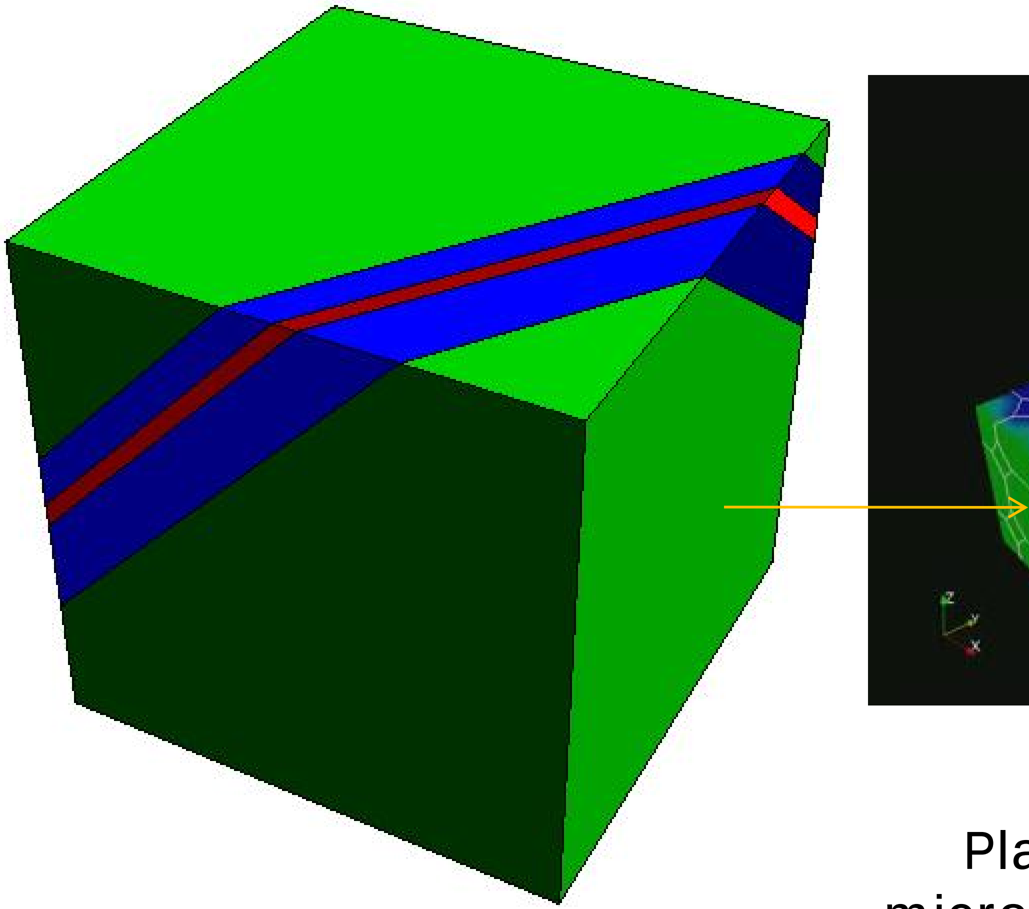

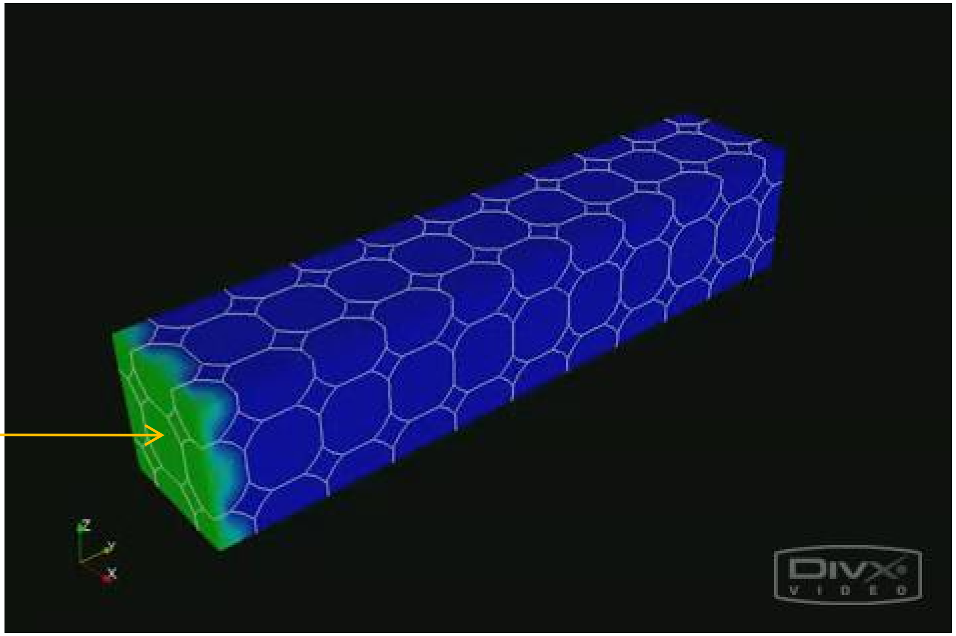

Plate impact simulation
microstructure reconstruction

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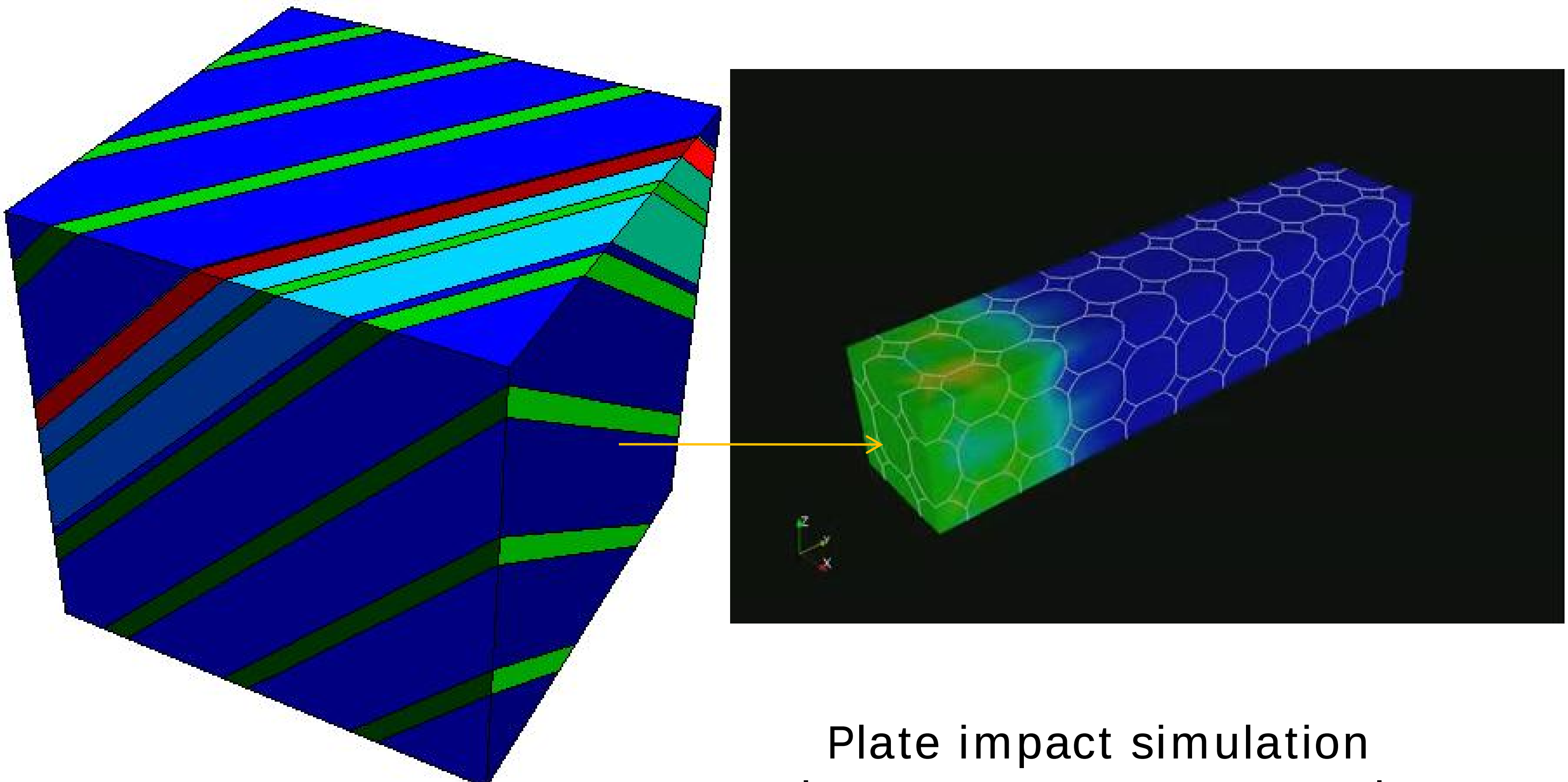

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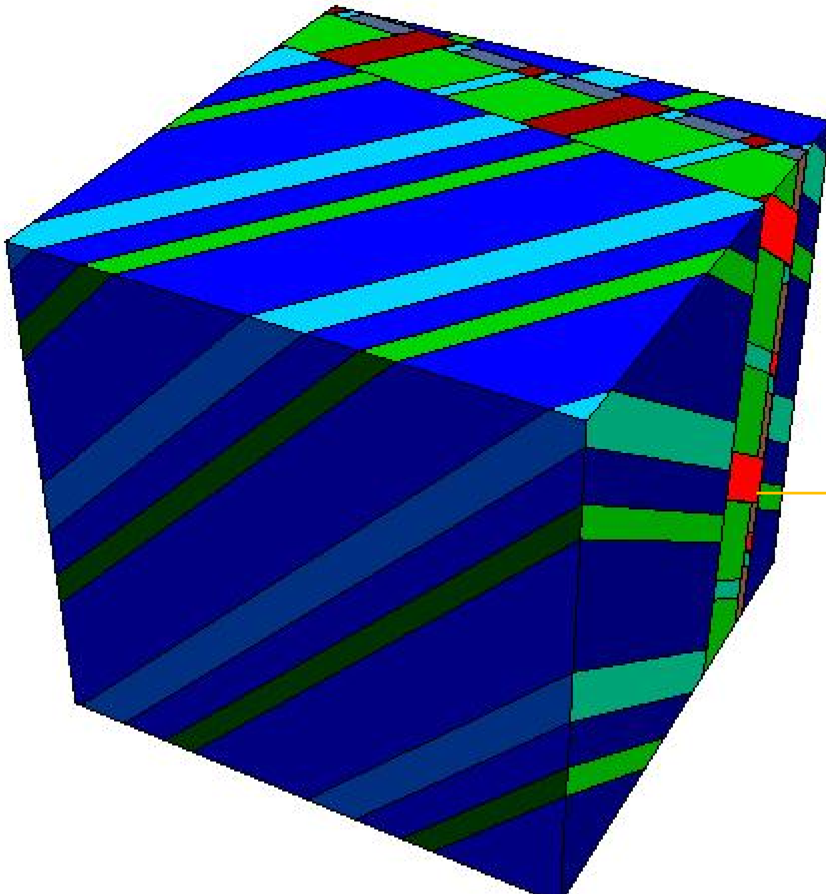

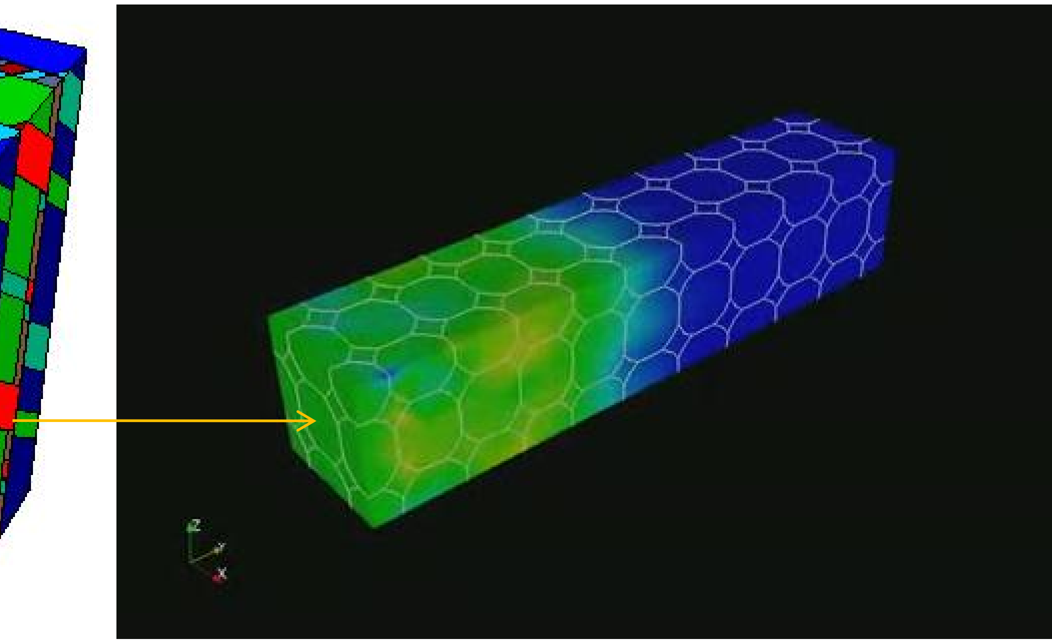

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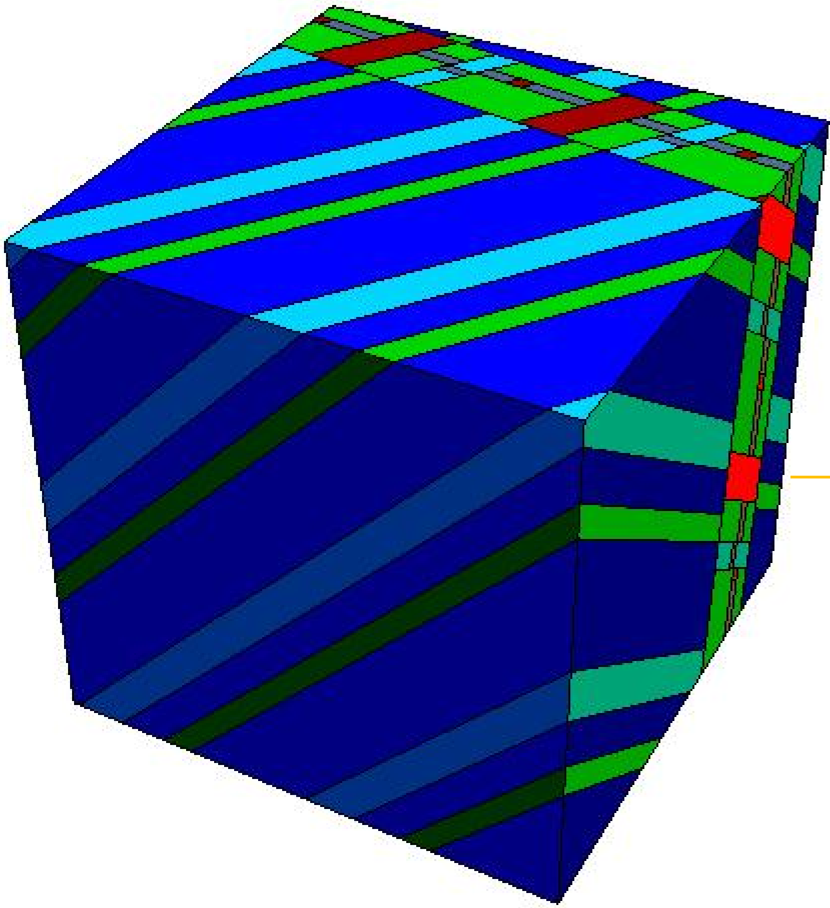

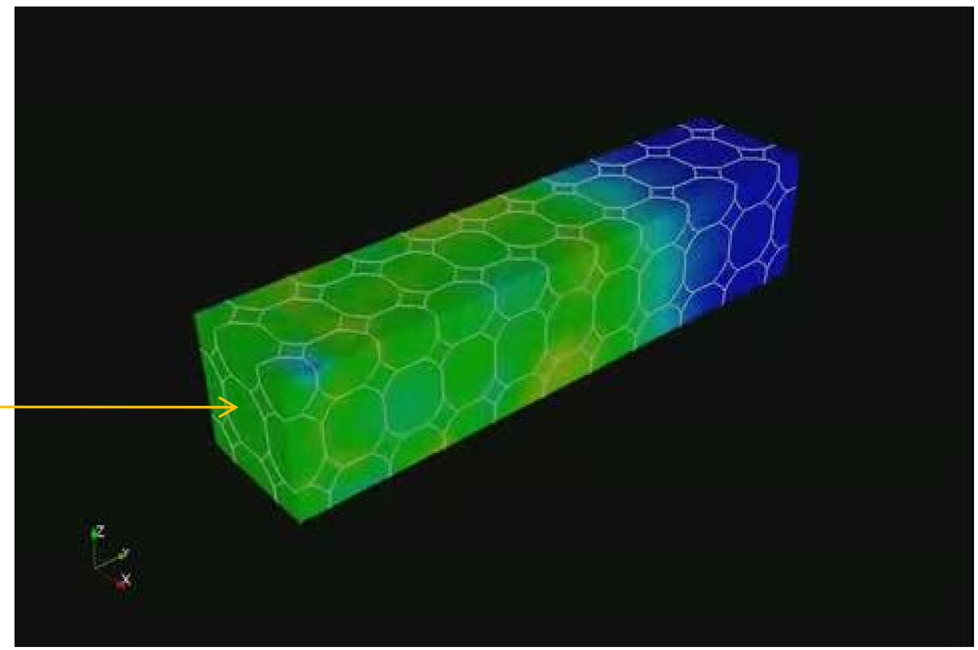

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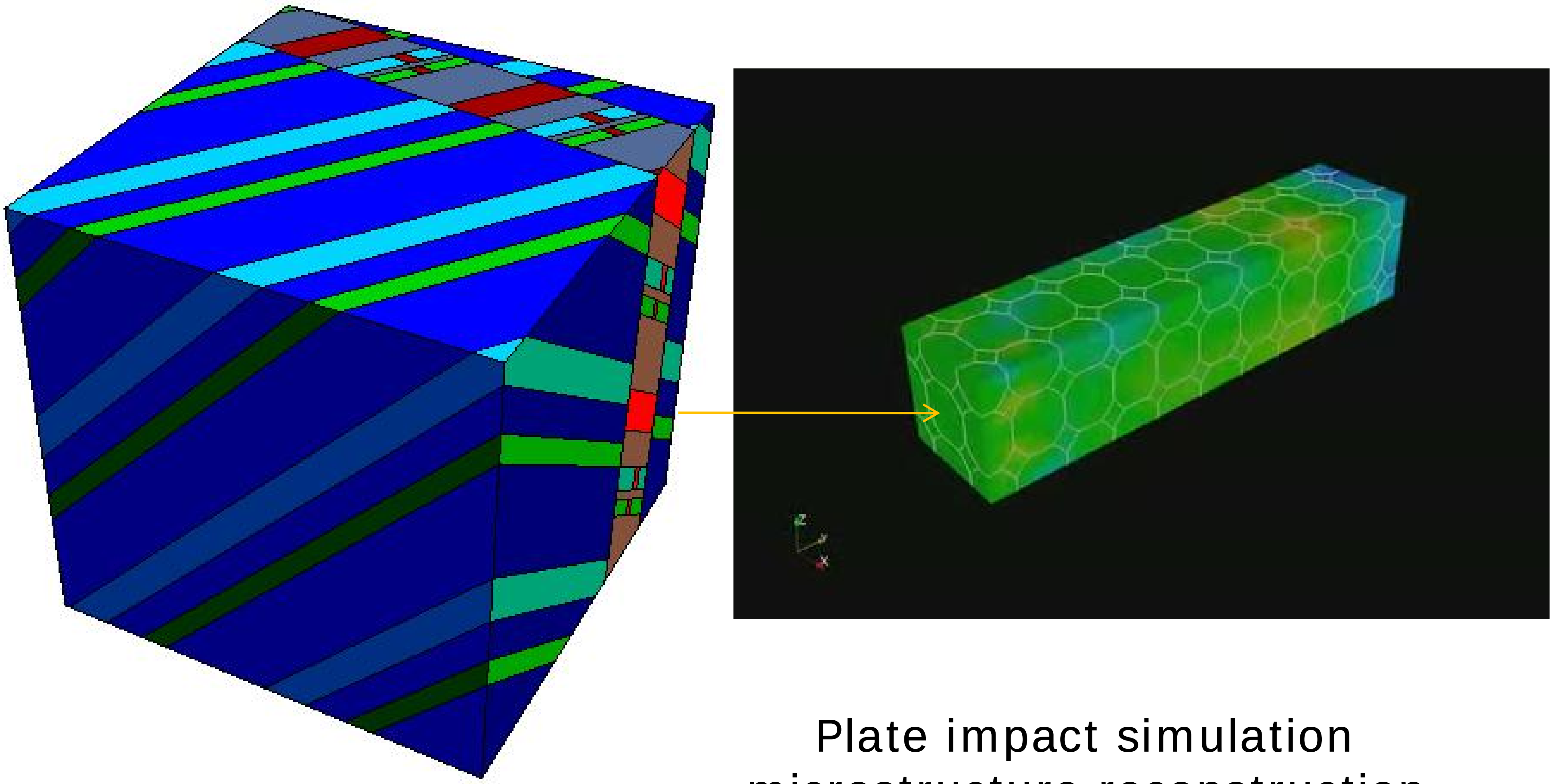

Plate impact simulation
microstructure reconstruction

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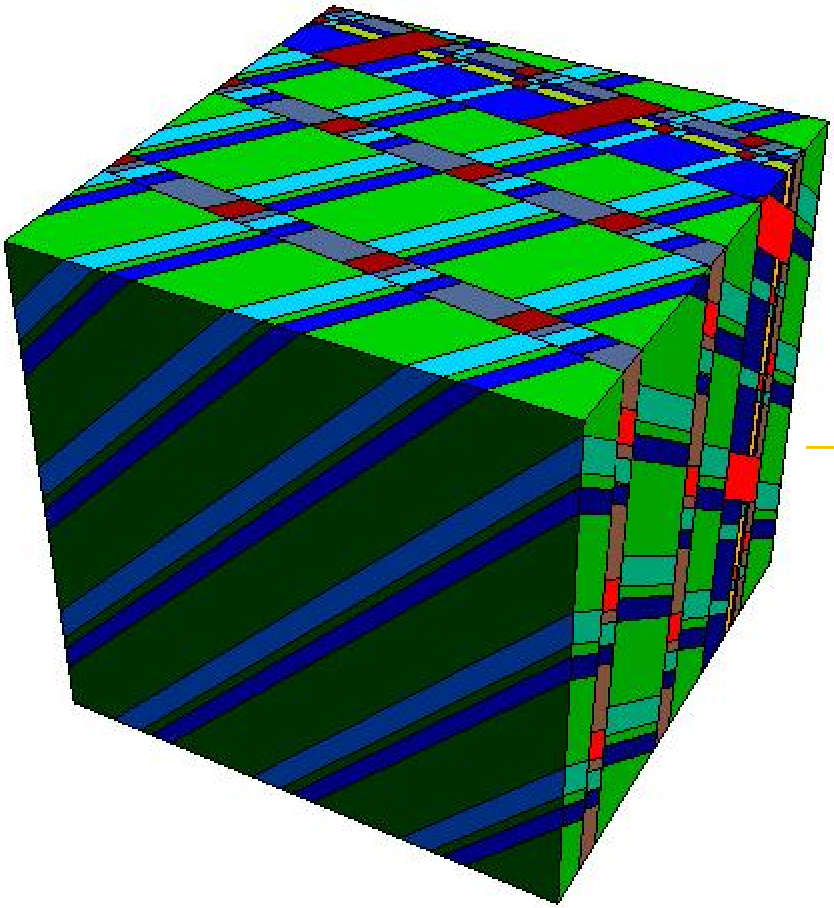

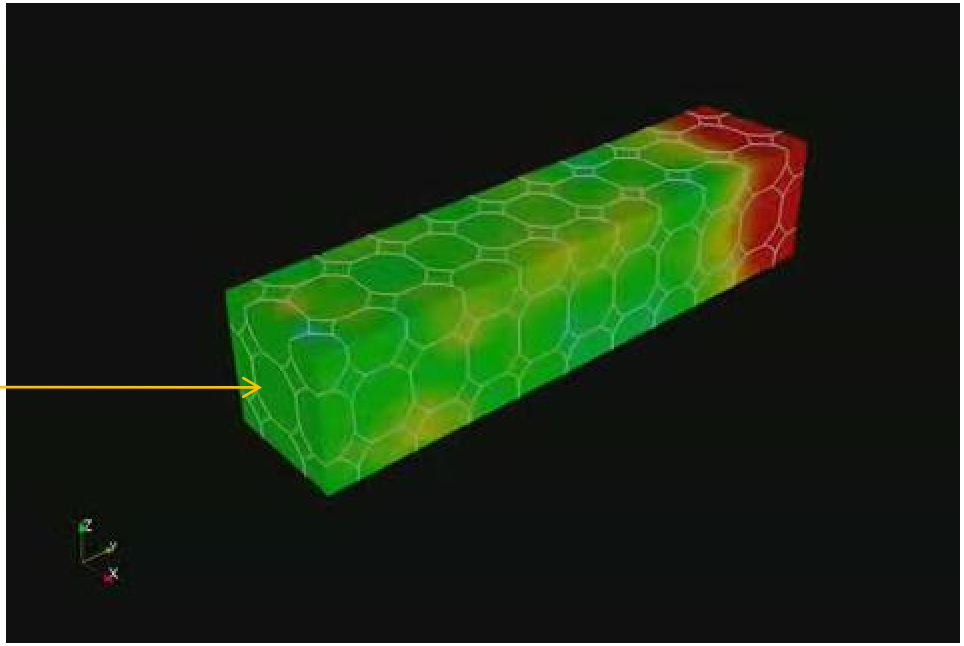

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microstructure reconstruction

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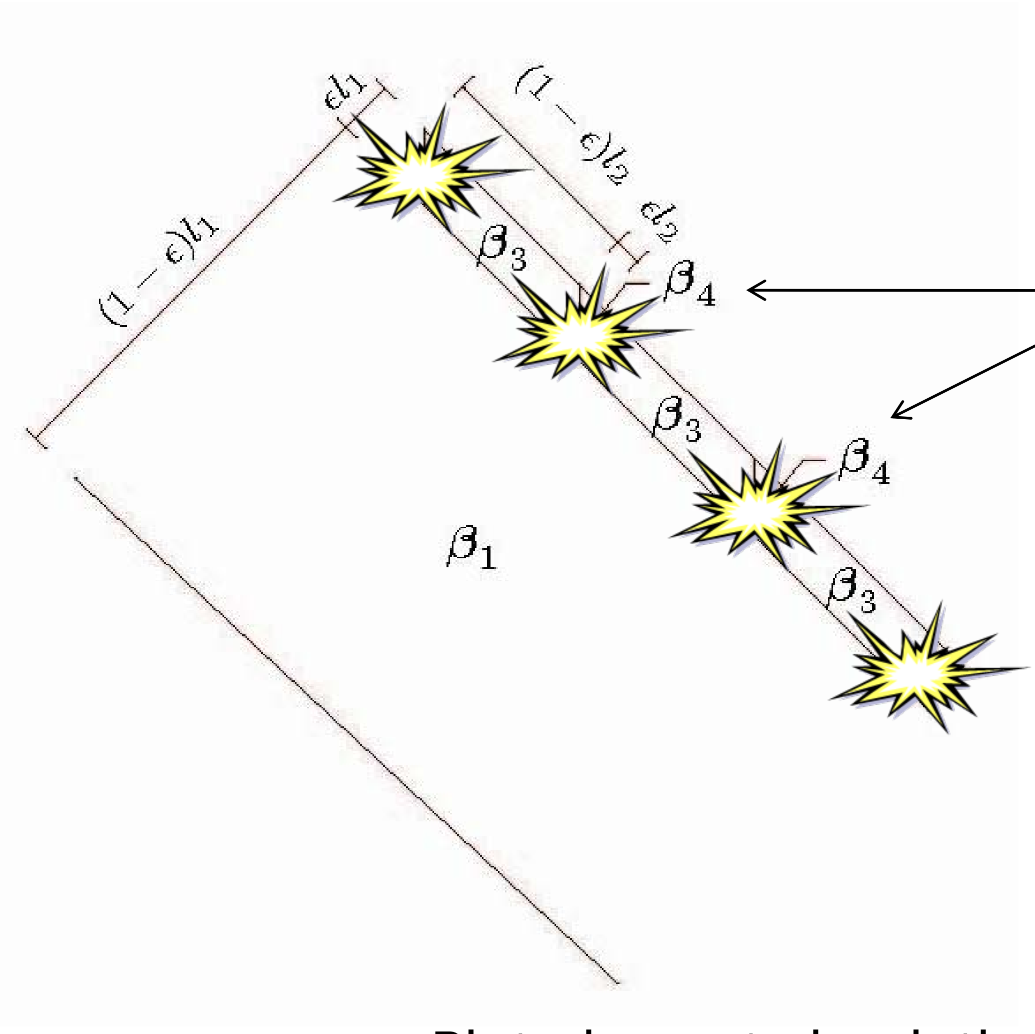

high deformation,
deformation rate,
temperature

Hot spots!

Plate impact simulation
hot spot analysis

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Convex *vs.* nonconvex-plasticity