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Author(s): Tome, Carlos

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Experimental and numerical characterization of local stresses associated with twinning in HCP

C. N. Tomé[1]

Collaborators: M. Arul Kumar[1], Y. Liu[2], R.J. McCabe[1], B. Clausen[1], L. Capolungo[1], W. Liu[3], J. Tischler[3], J. Wang[4]

[1]Materials Sc and Tech Div, Los Alamos National Laboratory, Los Alamos, NM, USA

[2] Shanghai Jiao Tong University, Shanghai, China

[3] Argonne Photon Source, Argonne National Laboratory, Argonne, IL, USA

[4]University of Nebraska-Lincoln, Lincoln, NE, USA

BES-DOE Project FWP 06SCPE401

"Dilatational and shear transformations in HCP metals: interfacial defects and collective interactions"

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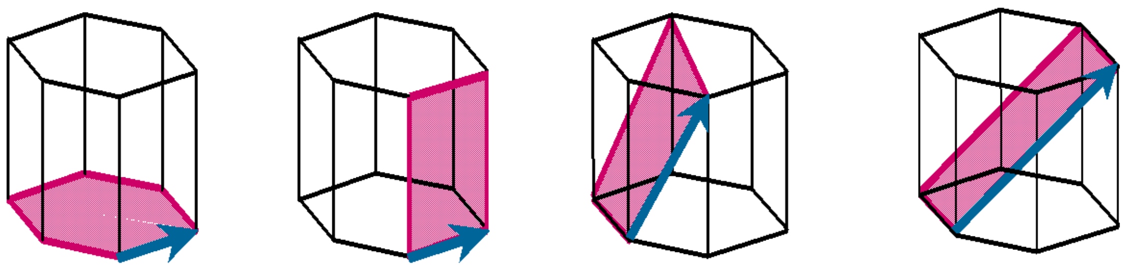
Plasticity of hexagonal materials

Several slip and twin modes with different activation threshold and high anisotropy

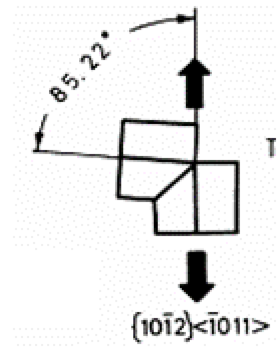


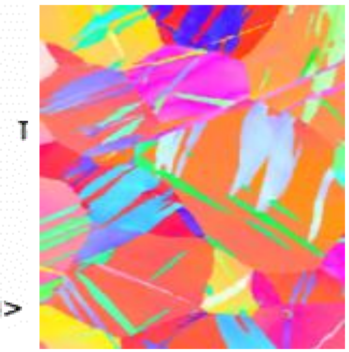
$(0001)\langle 11\bar{2}0\rangle$ **Basal slip**

$(10\bar{1}0)\langle 11\bar{2}0\rangle$ **Prismatic slip**

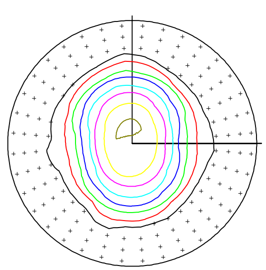
$(11\bar{2}2)\langle 11\bar{2}3\rangle$ **Pyramidal slip**

$(10\bar{1}2)\langle 10\bar{1}1\rangle$ **Tensile twin**

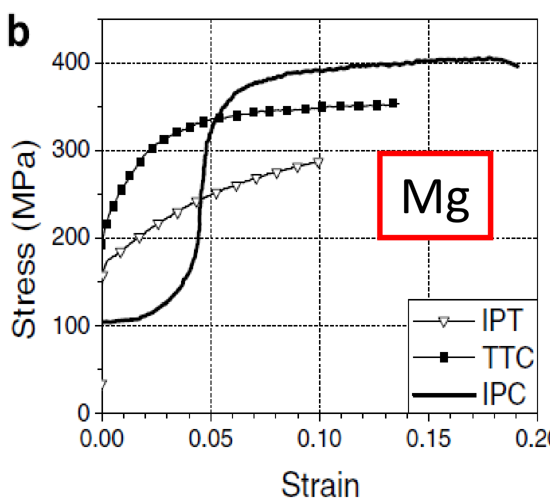


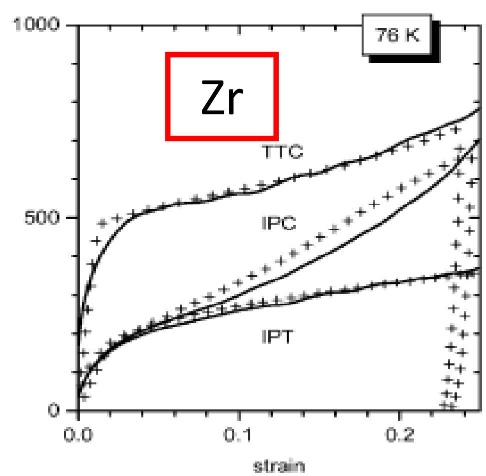


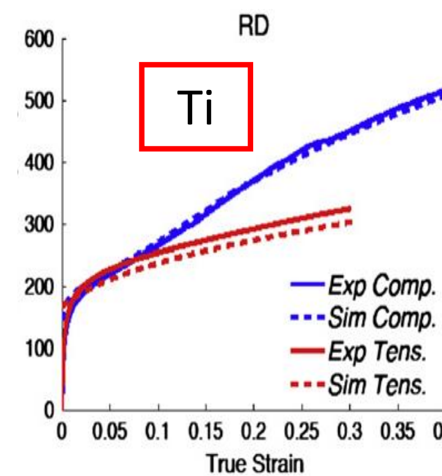
Twinning affects texture, hardening, anisotropy



rolling texture

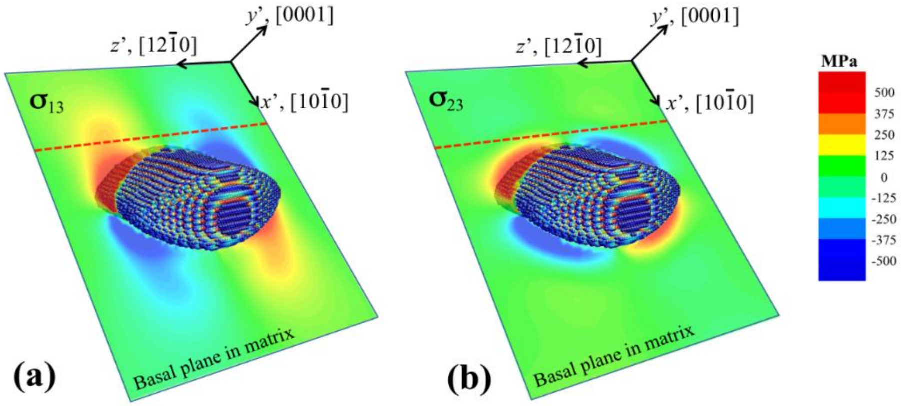






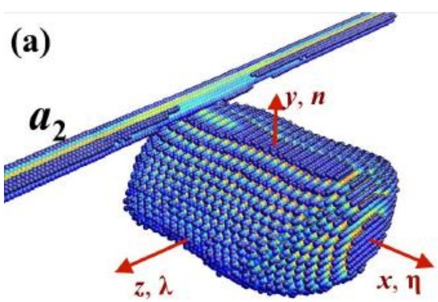
Stress field of 3D twins

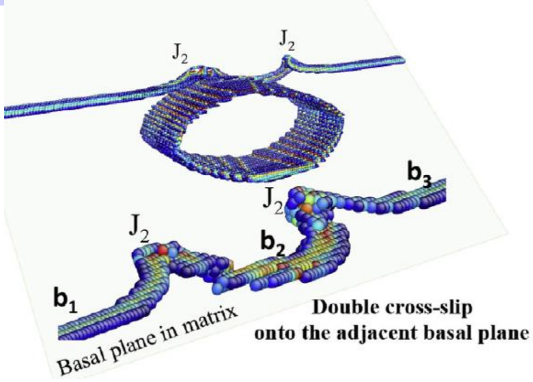
MD simulation of twin shear transformation and interaction with dislocations
(Gong et al, Acta Materialia 2018)

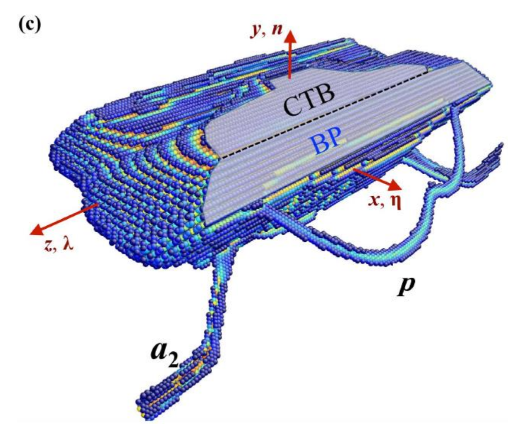


Shear stress induced by twin in the glide plane of <a> mixed dislocation

Reaction between twin and <a>-type mixed dislocation → (1) easy lateral growth of twin; (2) local stress at the interface facilitates dislocation reactions



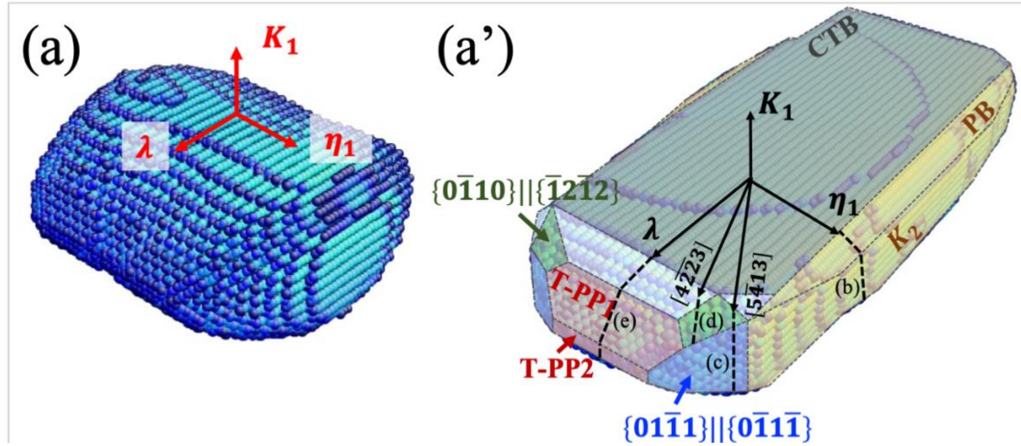


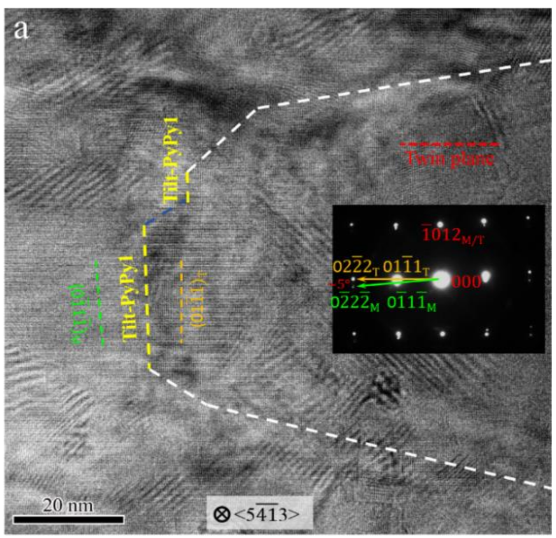


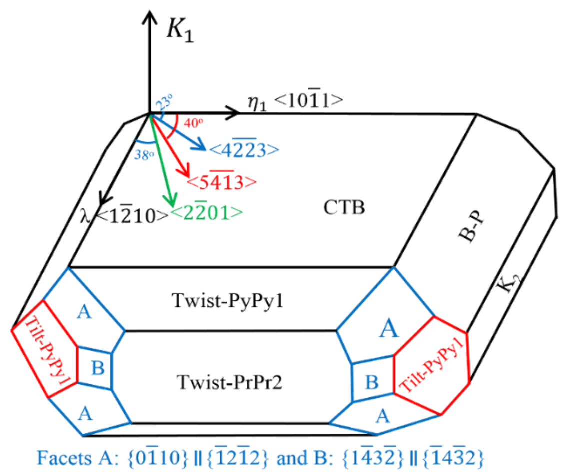
Talk by M. Gong et al – Wednesday 2:30 pm – Room 302C

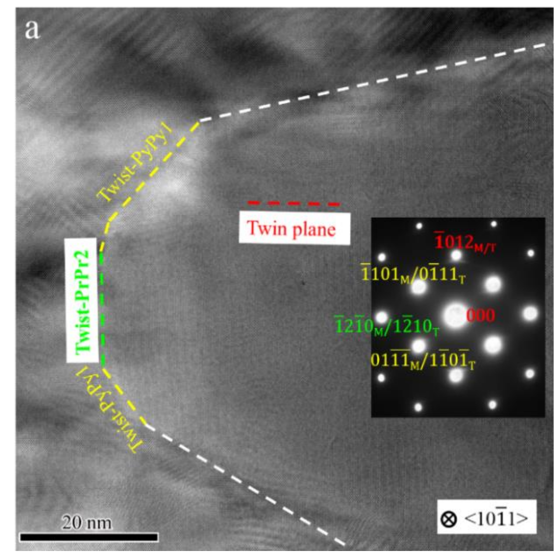
Stress as driving force for twin growth

Twins grow in 3 dimensions via combined motion of low energy facets









HRTEM of $\{10\bar{1}2\}$ twin boundaries viewed along a $\langle 5\bar{4}13\rangle$ direction

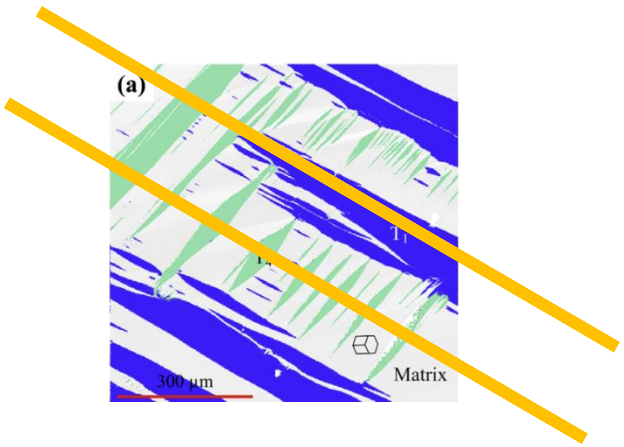
HRTEM of $\{10\bar{1}2\}$ twin boundaries viewed along a $\langle 10\bar{1}1\rangle$ direction

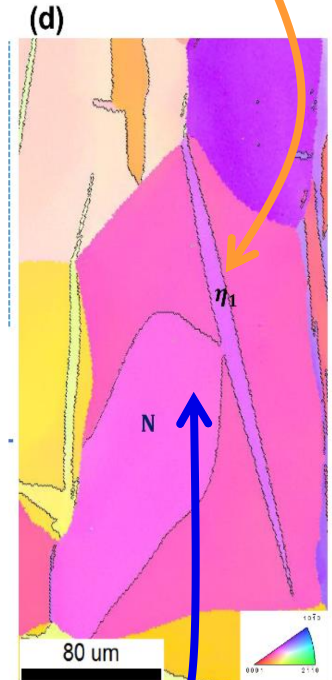
S. Wang et al , "Characterizing facets in {10-12} twin" , under preparation

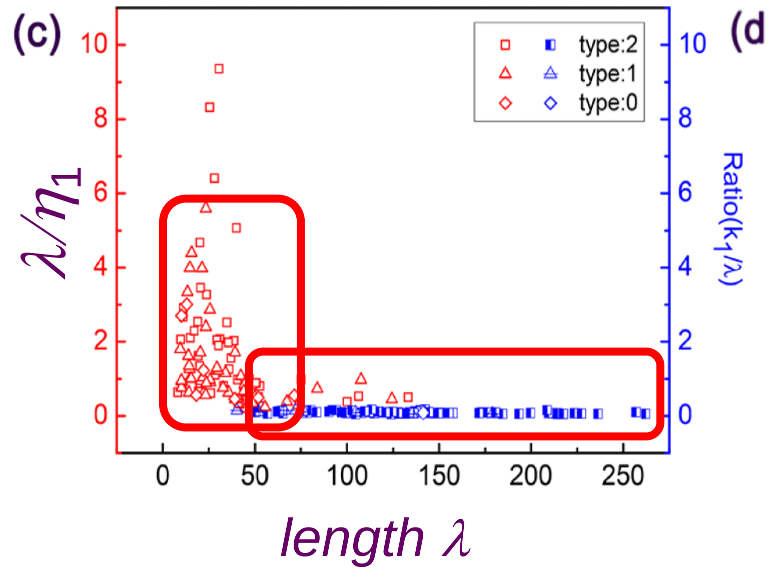
3D: forward, normal & lateral growth of twins in Mg

Twin viewed along the forward direction η_1
→ oblate shape

EBSD statistics done on 170 twins

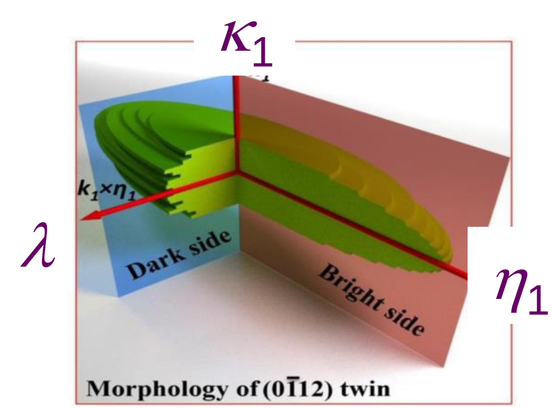






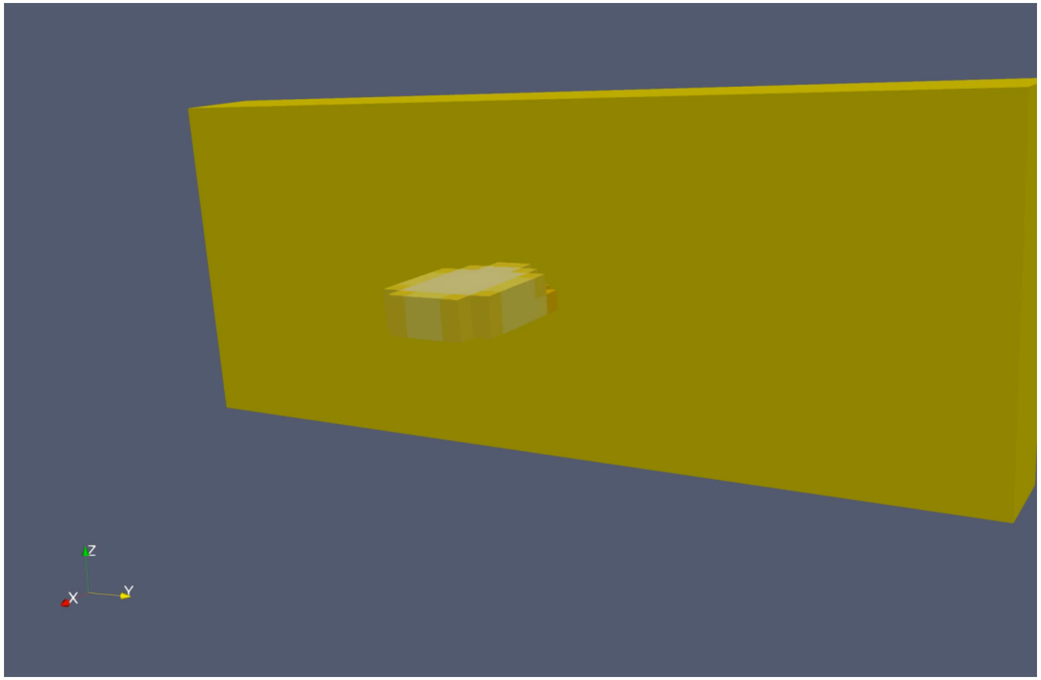
Twin sections to reveal morphology along K_1 and η_1

Twin viewed along the normal direction K_1
→ irregular shape

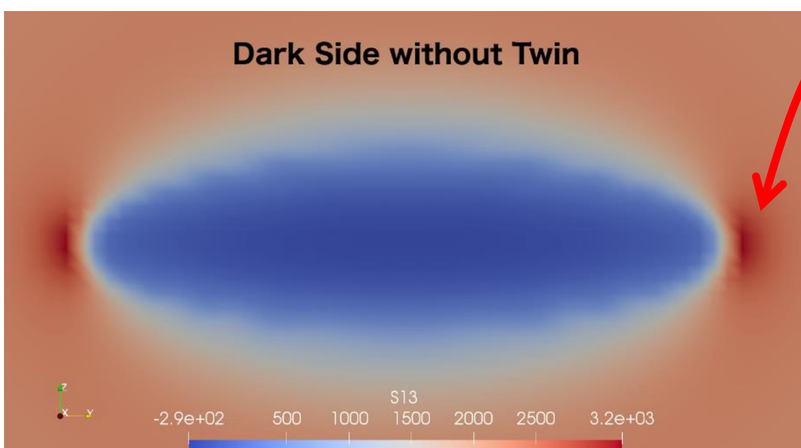


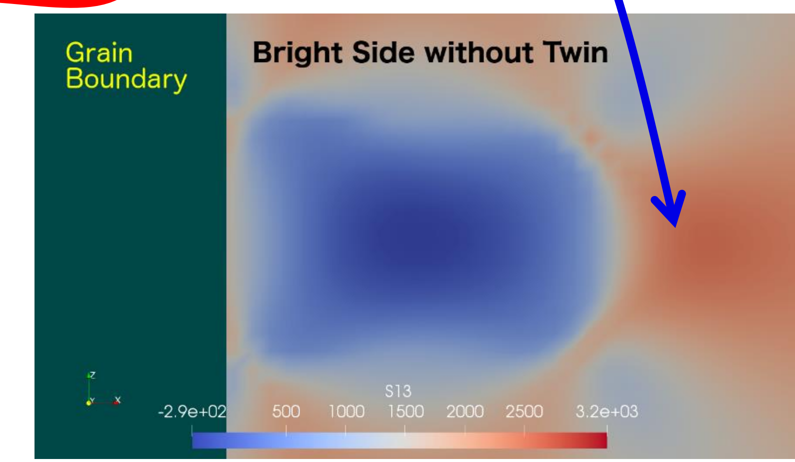
Pengzheng Tang et al., "3D nature of {10-12} twins in Mg", Wednesday 5:00 pm, Room 302A

Twin growth & transformation-induced shears (Mg)



- Phase-field simulations of twin growth
- Isotropic mobility of facets assumed
- Lateral growth is faster than forward growth





John Graham, L. Capolungo, under development

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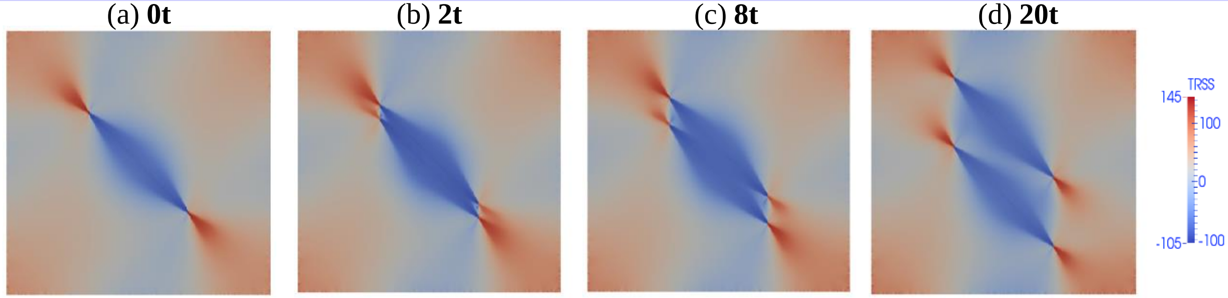
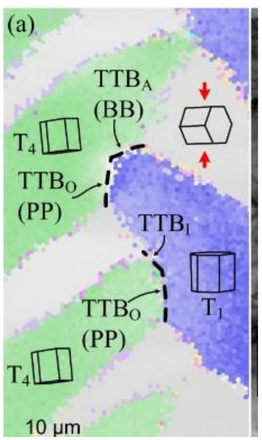
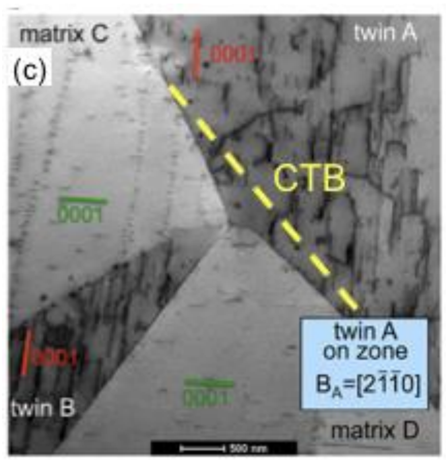
Stress field of twin (back shear stress) prevents formation of same variant neighboring twin and determines minimum separation

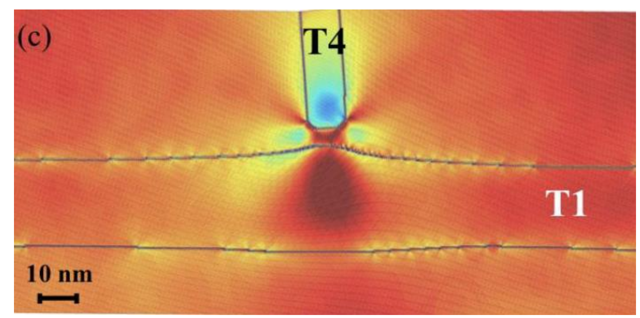


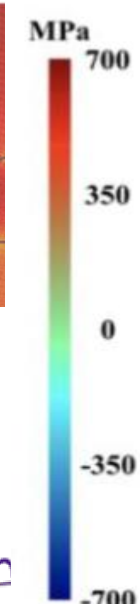
CP-FFT simulation of twin shear transformation

Stress field of twin (forward shear stress) favors attractive interaction and the formation of twin junctions









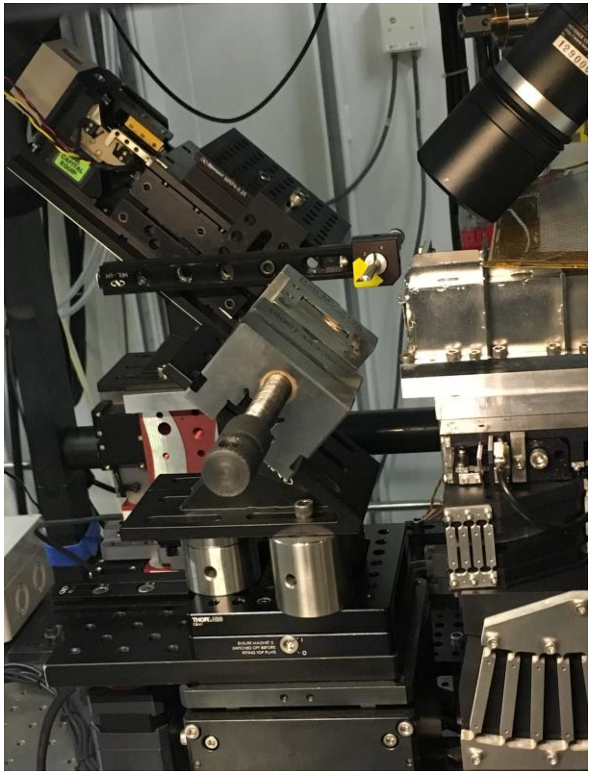
MD simulation: RSS on T1 induced by T4 favors attractive interaction

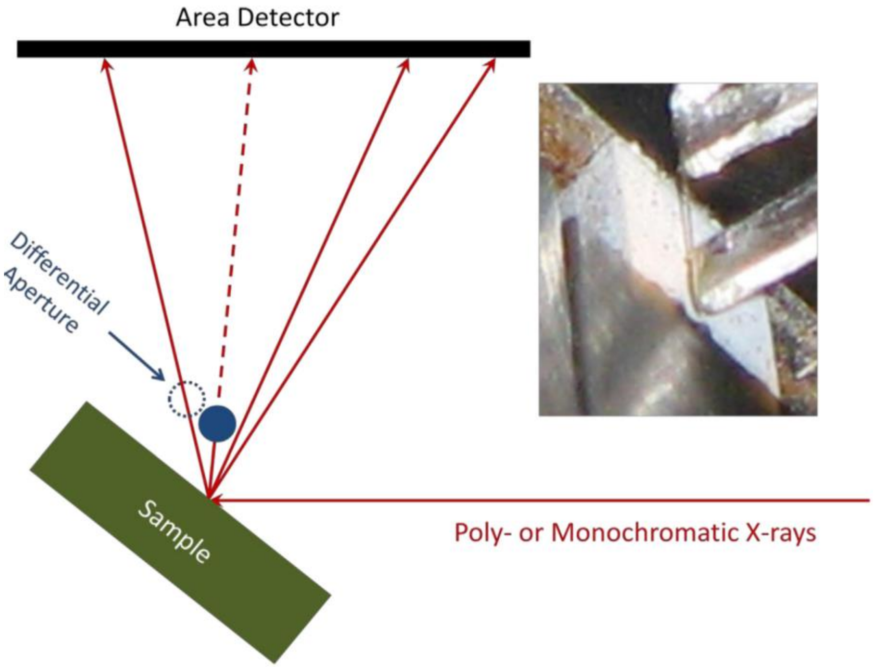
Arul Kumar et al , "… co-zone twin-twin junctions ..", Acta Materialia 168 (2019)

Twin stress measurement in HCP Mg and Ti

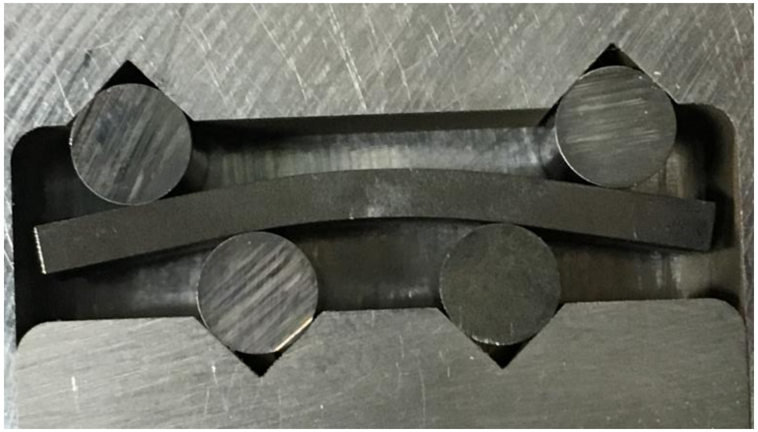
X-ray Laue diffraction in 3D at 34-ID-E beam (APS-ANL)

~0.25 µ resolution



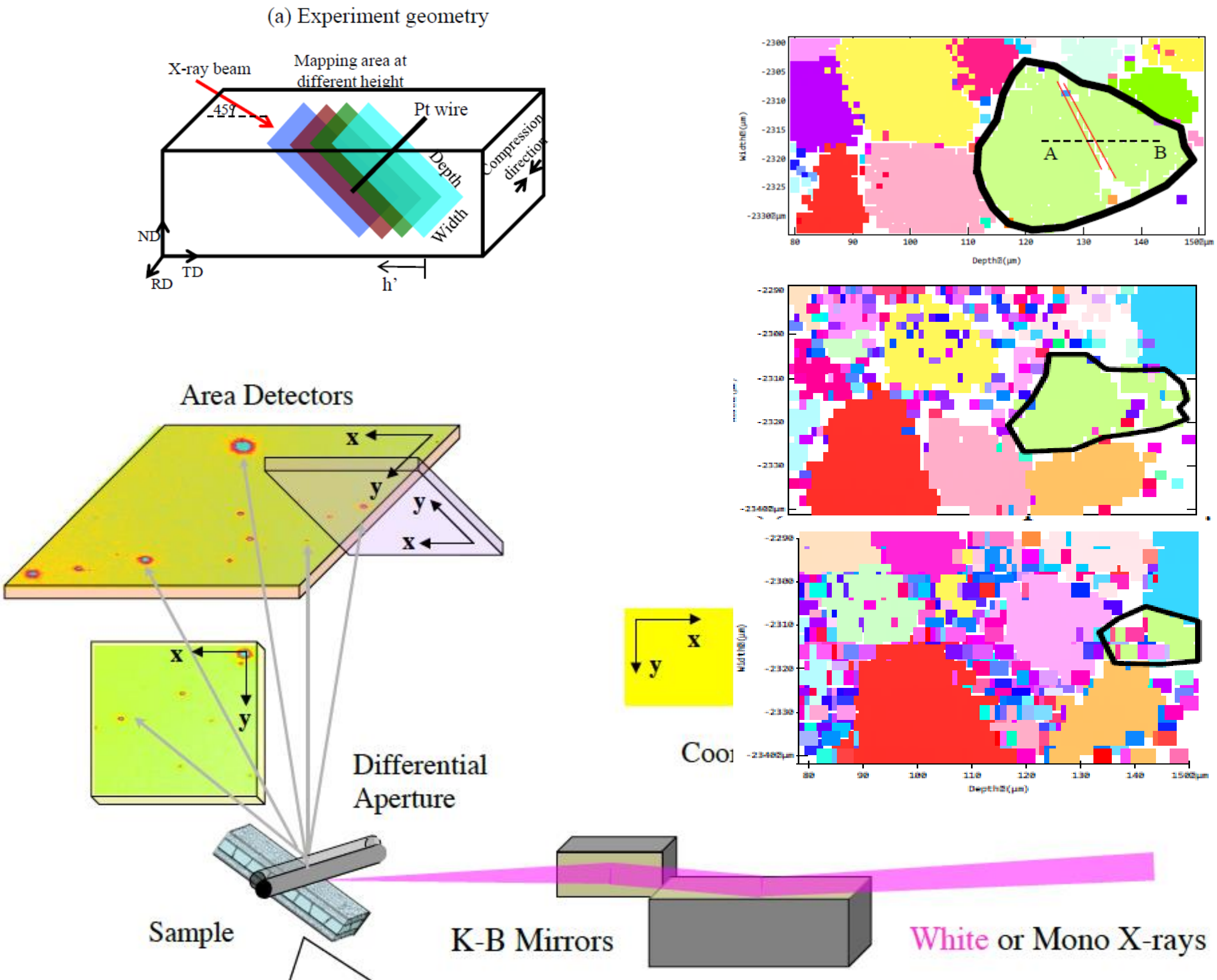


Mg



Ti

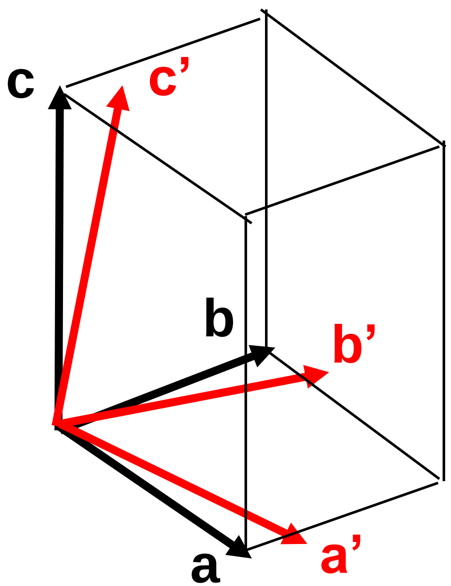
X-ray Laue diffraction in 3D at 34-ID-E beam (APS-ANL)



Calculating local stress

X-ray diffraction gives the 3 vectors (a', b', c') of the distorted cell, one for each X-ray frequency

They relate to the undistorted ones (a, b, c) through the distortion tensor *U*



$$X_i' = (I_{ij} + U_{i,j}) X_j$$

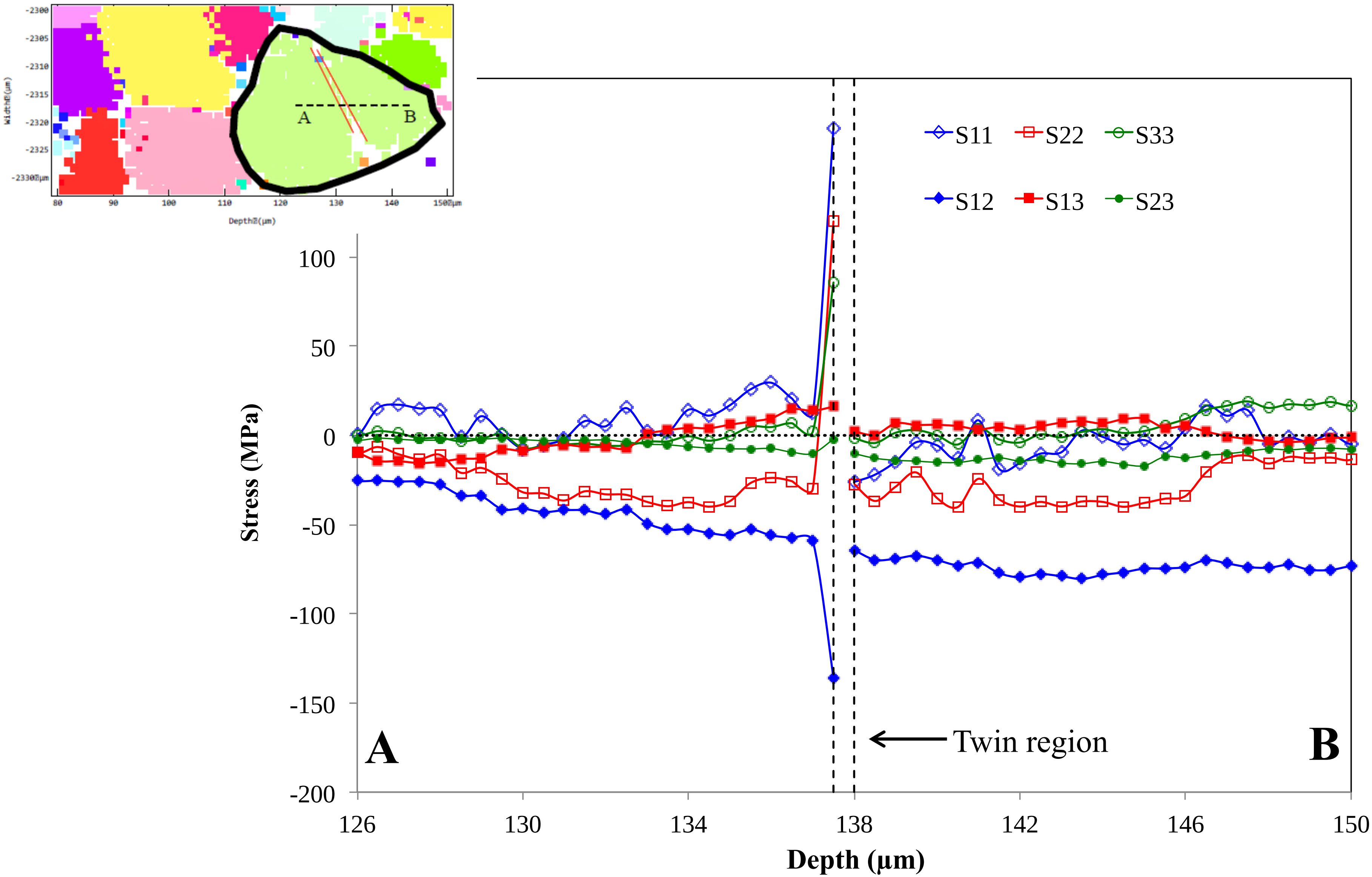
$$X_i' = a_i', b_i', c_i' \qquad U_{i,j} = \frac{\partial U_i}{\partial X_j} \qquad X_j = a_j, b_j, c_j$$

9 equations with 9 unknowns $U_{i,j}$
give elastic strain and stress tensors

$$\varepsilon_{ij}^{elastic} = \frac{U_{i,j} + U_{j,i}}{2}$$

$$\sigma_{ij} = C_{ijkl}\, \varepsilon_{kl}^{elastic}$$

Stress components along line A-B

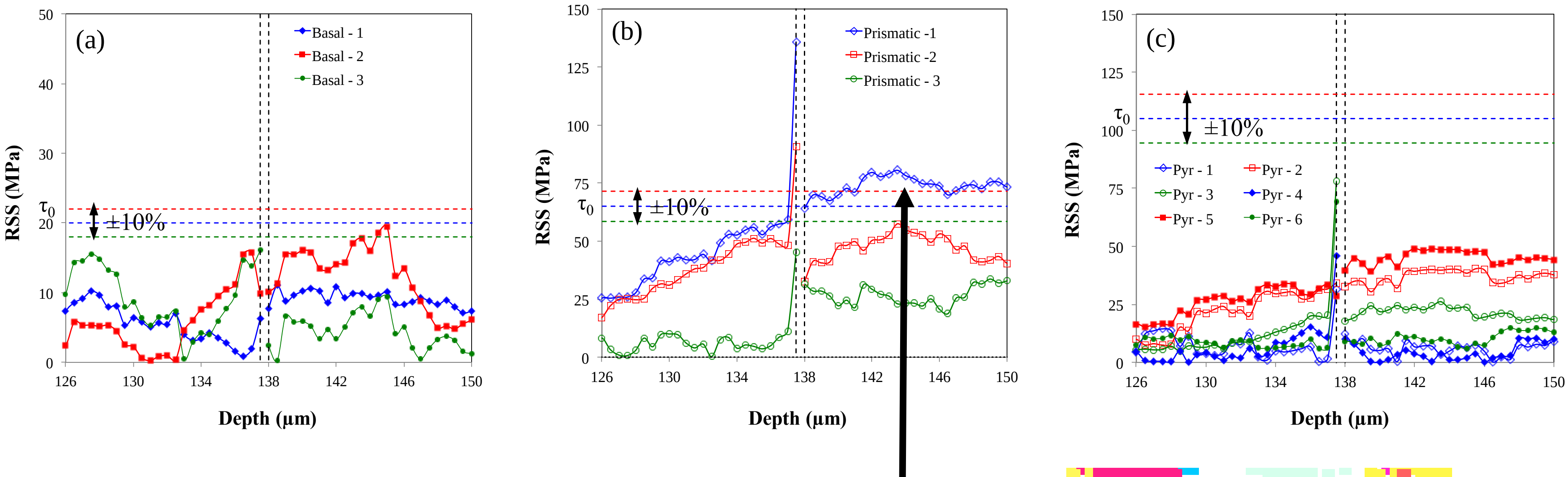


Mg: resolved shear stress on slip systems along line A-B

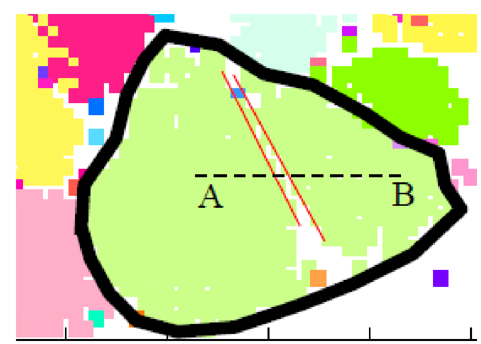
3 basal planes
τ_0 ~ 20MPa

3 prism planes
τ_0 ~ 65MPa

6 pyramidal planes
τ_0 ~ 105MPa



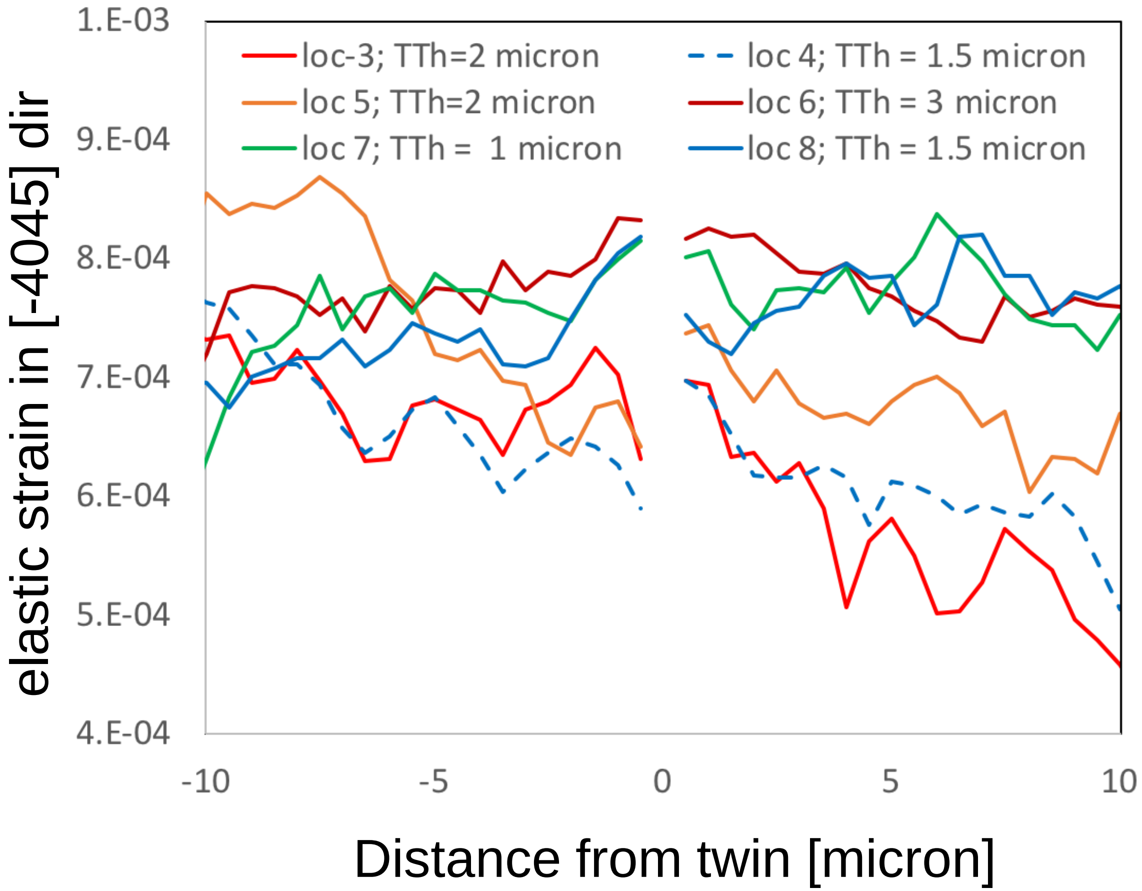
RSS on one prism system exceeds the initial CRSS of τ_0 ~ 65MPa
… but only on one side of the twin !

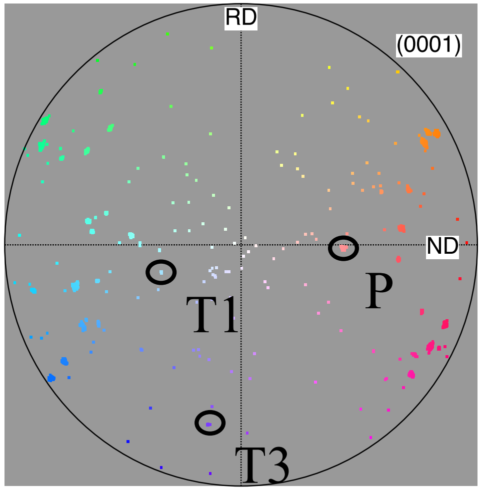


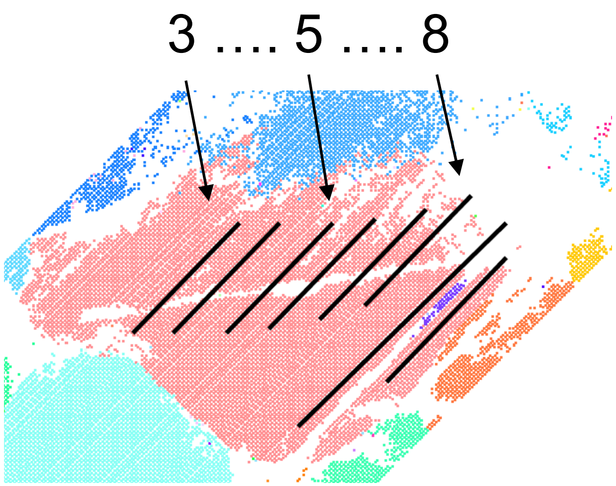
Twin partitions the grain: one side remains elastic and the other deforms plastically !

Ti twin: elastic strain profiles for (-4 0 4 5) planes

Variation between lines indicates stress inhomogeneity in the grain!

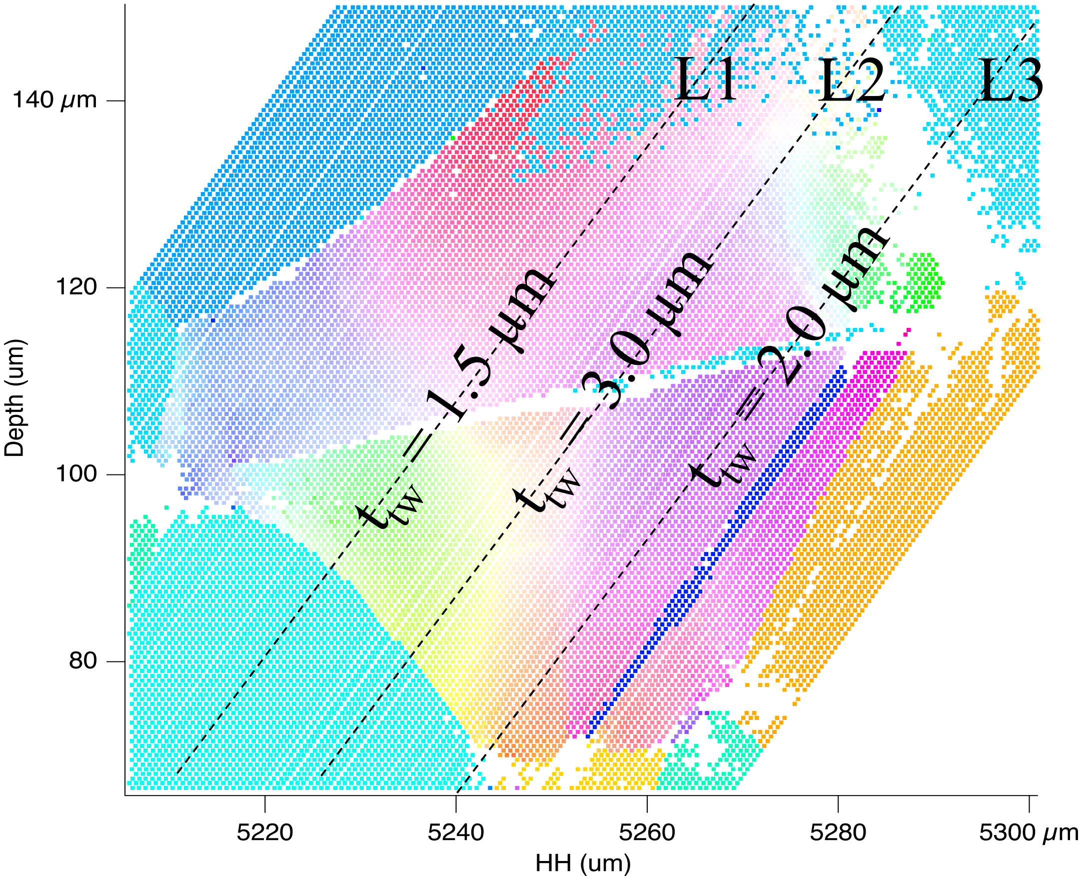


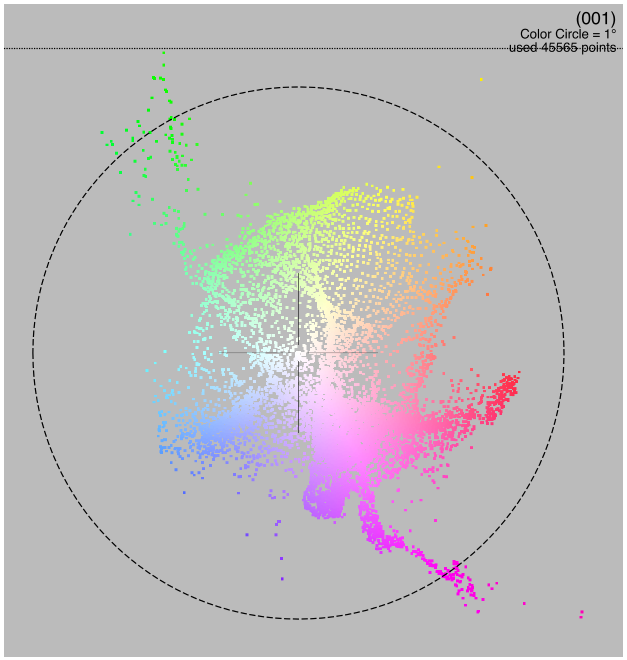




Grain size:
~100(RD) , 50(TD) , 50(ND)

Ti grain: intragranular misorientation map





Circle corresponds to 1° misorientation

Intragranular misorientation suggests inhomogeneity in local plastic activity, local hardening and, as a consequence inhomogeneity in local stress

Mg: high-resolution scan TEM *

TWIN-ASSOCIATED STRESSES AT THE NANO-SCALE

- Can we characterize them?
- What can we learn?

Nano-beam electron diffraction (NBED)

- characterizes point-to-point diffraction pattern and calculates the strain from each diffraction pattern
- was applied to obtain strain field with ~5 nm spatial resolution.
- technique had to be adapted for applicability in HCP Mg, and was validated against PP measurements.

Peak Pair (PP)

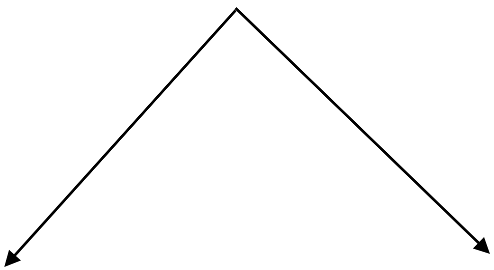
- measures the displacement of the atoms in real space from the perfect lattice position (Å resolution)

* Experiments performed at Molecular Foundry (Lawrence-Berkeley Nat Lab)

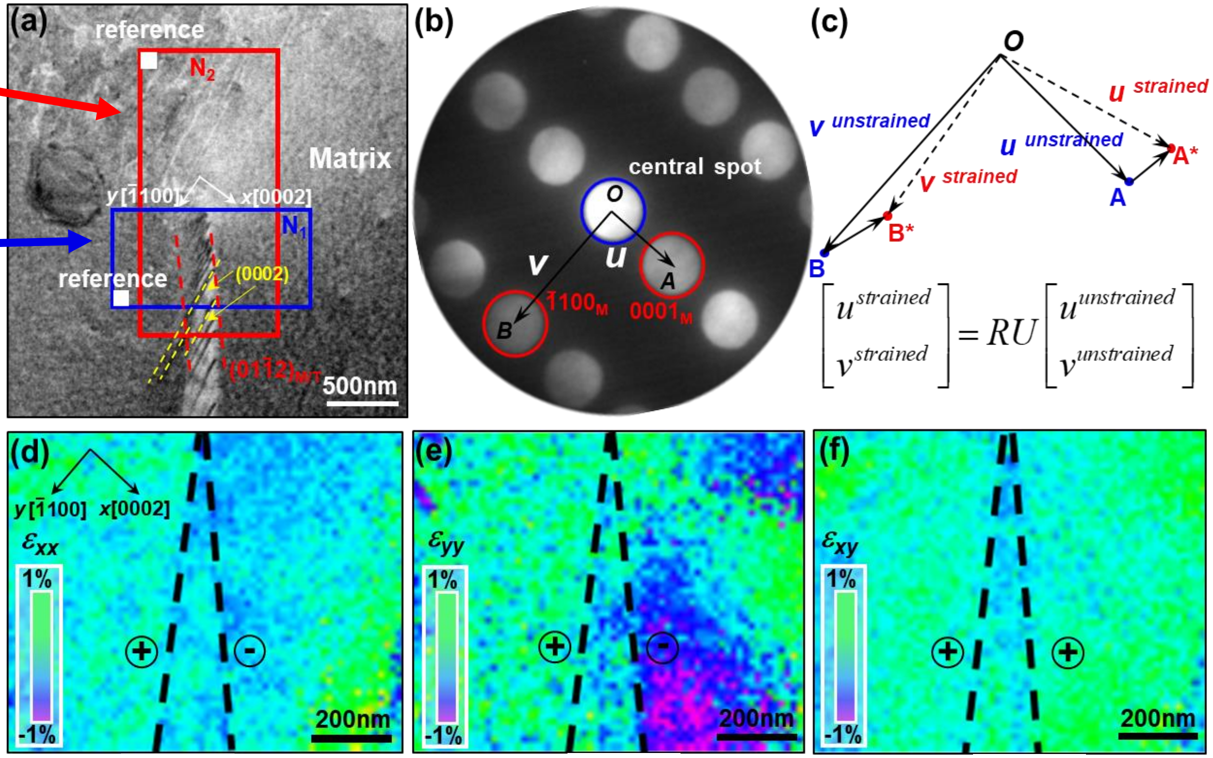
Mg: NBED results near (10-11) twin interface

Zone #2: twin tip region

Zone #1: (10-11) twin interface region



Y [-1100]   X [0002]

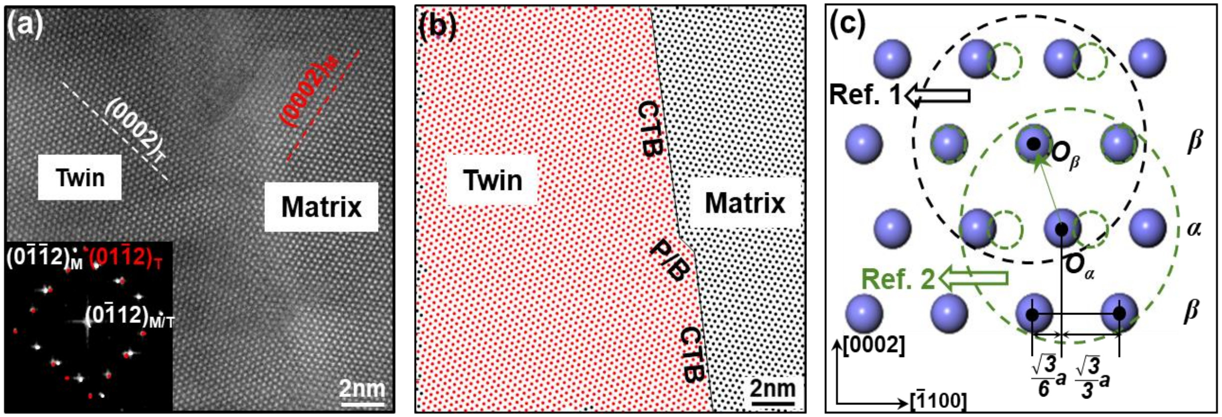


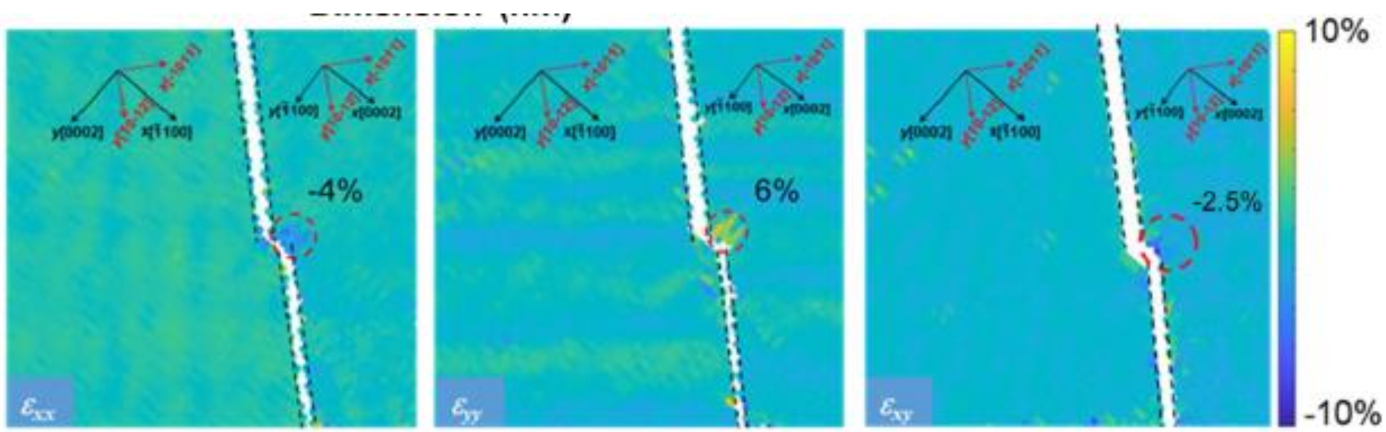
$$\begin{bmatrix} u^{strained} \\ v^{strained} \end{bmatrix} = RU \begin{bmatrix} u^{unstrained} \\ v^{unstrained} \end{bmatrix}$$

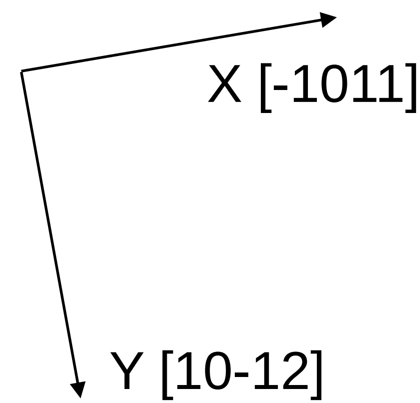
ε_{xx} ε_{yy} ε_{xy}

- The strain components ε_{xx} and ε_{yy} on different sides of the twin are of opposite sign
- The reference axes do not highlight the shear parallel to the twin interface

Mg: Peak-Pair results near (10-11) twin interface







ε_{xx} ε_{yy} ε_{xy}

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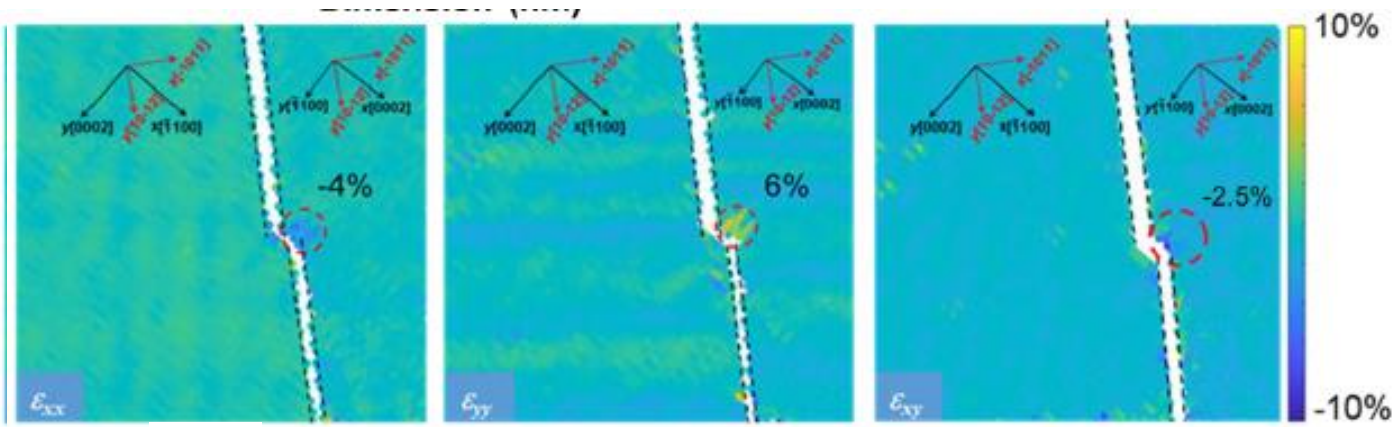
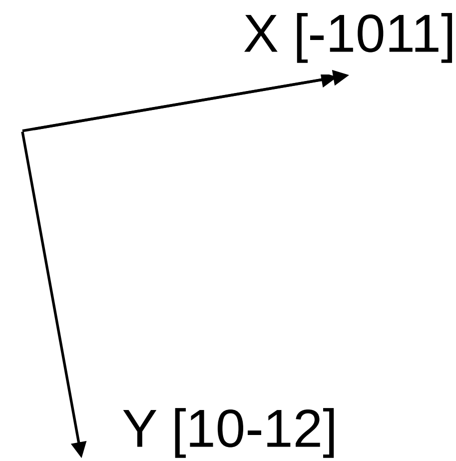
Mg: Peak-Pair results near (10-11) twin interface

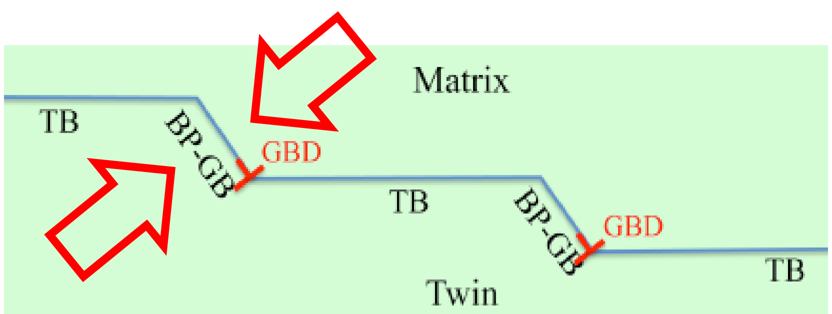


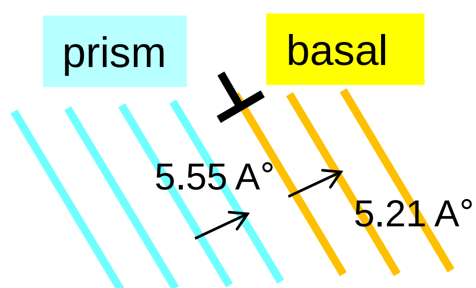
ε_{xx} ε_{yy} ε_{xy}



In this reference system, ε_{xx} ~ -4% and ε_{yy} ~ +6% at the Basal-Prism step

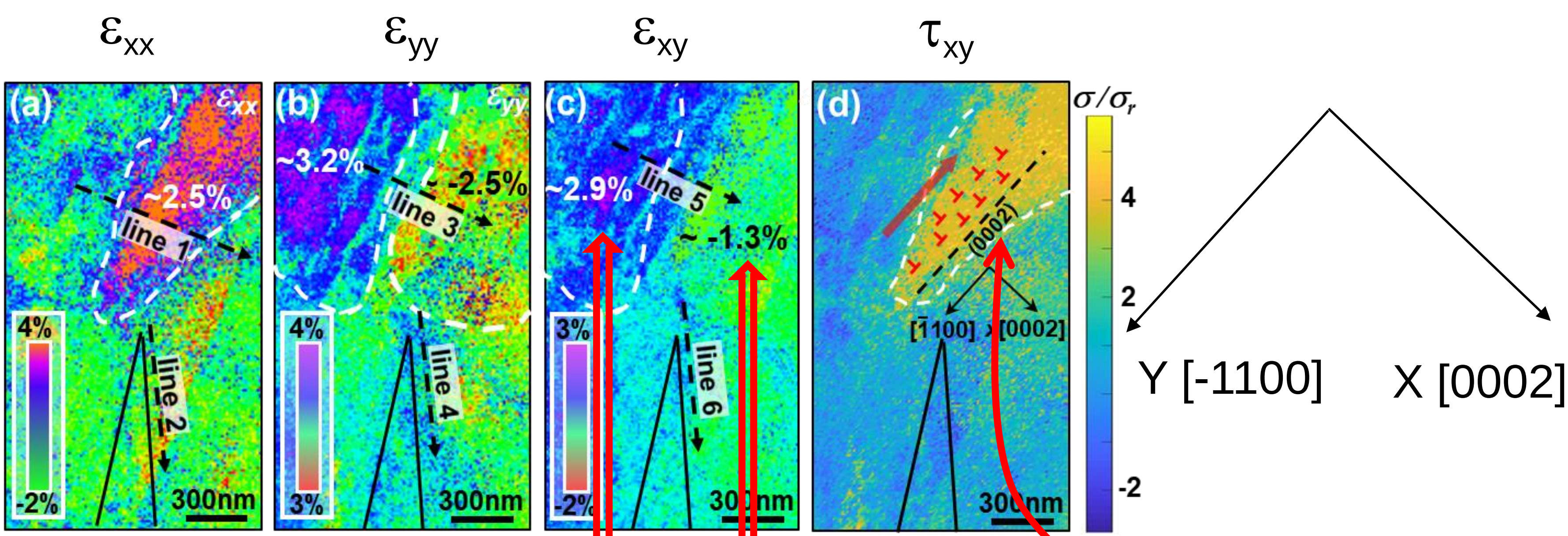
→ consistent with difference in lattice parameters across BP interface





6% difference

Mg: NBED results near twin tip

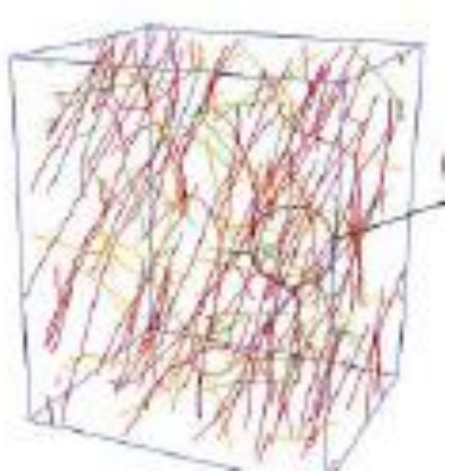


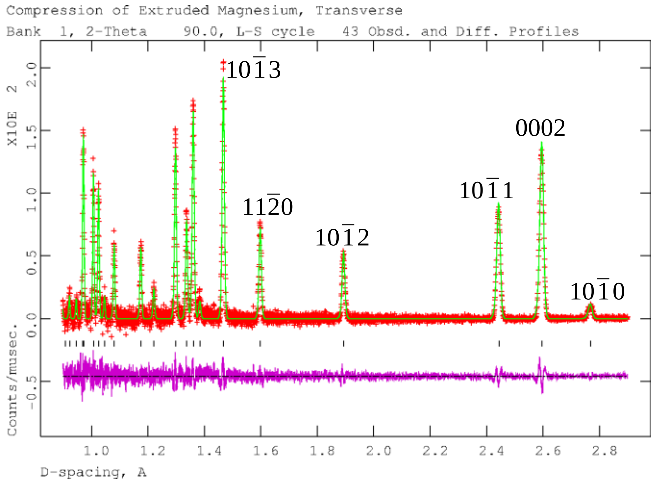
- The shear strain component ε_{xy} shows an asymmetry (2.9% vs -1.3%) on lobes ahead of the twin tip
- This asymmetry would be consistent with stress relaxation due to emission of basal dislocations ahead of the twin tip

OVERALL: The elastic strain field in the vicinity of the twin tip is extremely inhomogeneous

Can we link local twin stresses with macroscopic response ?

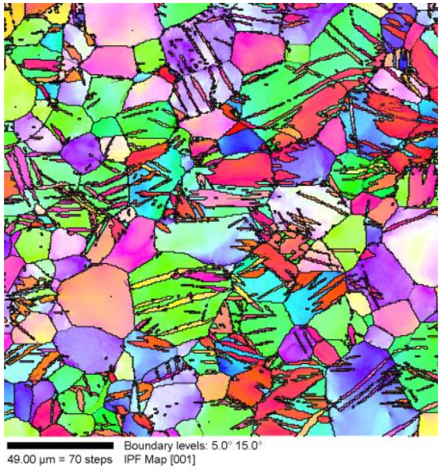
- The standard deviation of lattice strain (SDLS) is a stochastic quantity derived from peak broadening measurements
- Peak Profile Analysis correlates SDLS with dislocation density via contrast factors

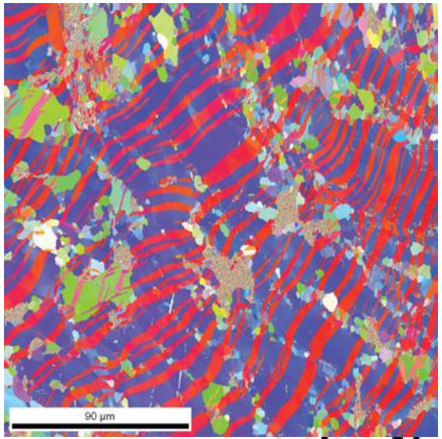




$$SDLS = \sqrt{\sum_s \frac{\rho^s b^{s2}}{8\pi} C^{(k)s}}$$

Can we develop a similar formalism for addressing the stress distributions associated with twinning structures ?





SUMMARY

- Stress fields associated with twins interact with other stress fields (applied, from other twins, from dislocations) to determine twin-facet mobility
- MD and Continuum Plasticity provide a (very simplified) nano-scale and sub-micron scale measure of local stress
- HR-STEM and X-ray diffraction provide experimental access to both scales, but show large local fluctuations
- A statistical approach is likely the only way for linking local and macroscopic mechanical response.