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Boundary motion coupled with tensile and compressive deformation: TEM observation of twinning-like lattice reorientation in Mg micropillars

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Lattice Reconstruction in Mg:
Boundary Motion Coupled w/ Deformation

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ARTICLE

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Twinning-like lattice reorientation without a crystallographic twinning plane

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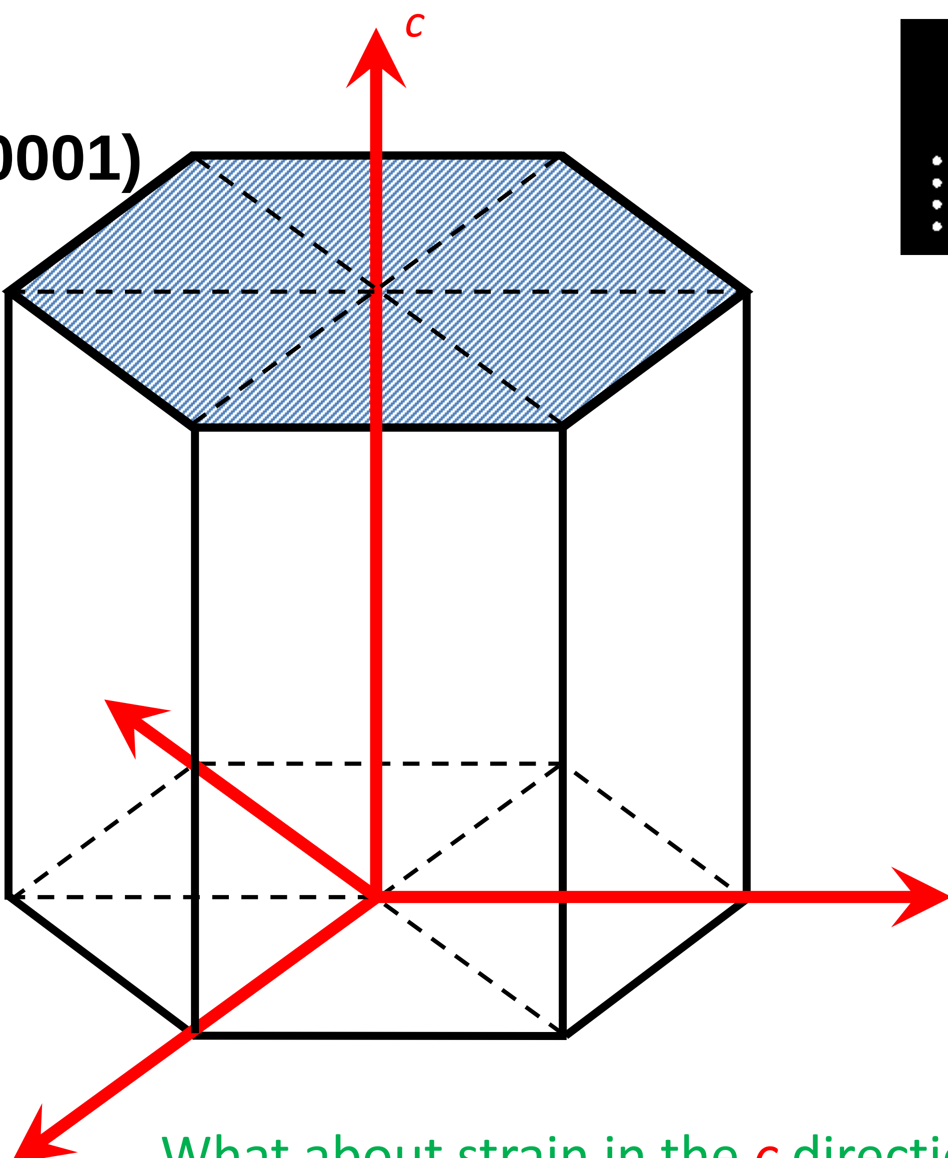
Boundary-motion-based plasticity mechanism

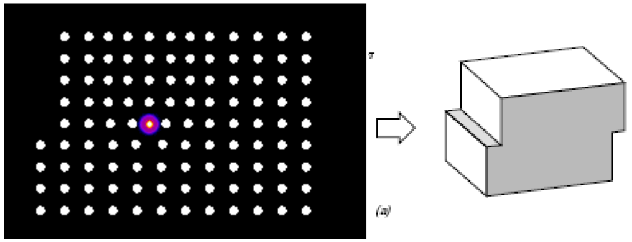
Twinning on the $\{10\bar{1}2\}$ plane is a common mode of plastic deformation for hexagonal-close-packed metals. Here we report, by monitoring the deformation of submicron-sized single-crystal magnesium compressed normal to its prismatic plane with transmission electron microscopy, the reorientation of the parent lattice to a 'twin' lattice, producing an orientational relationship akin to that of the conventional $\{10\bar{1}2\}$ twinning, but without a crystallographic mirror plane, and giving plastic strain that is not simple shear. Aberration-corrected transmission electron microscopy observations reveal that the boundary between the parent lattice and the 'twin' lattice is composed predominantly of semicoherent basal/prismatic interfaces instead of the $\{10\bar{1}2\}$ twinning plane. The migration of this boundary is dominated by the movement of these interfaces undergoing basal/prismatic transformation via local rearrangements of atoms. This newly discovered deformation mode by boundary motion mimics conventional deformation twinning but is distinct from the latter and, as such, broadens the known mechanisms of plasticity.

Q#1: Typical plasticity mechanisms in Mg ?

HCP Mg: only one set of hexagonal close packed flat planes for easy slip

Basal: (0001)





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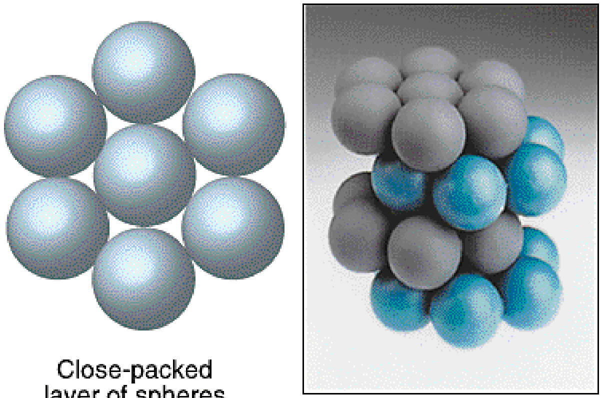


Close-packed layer of spheres

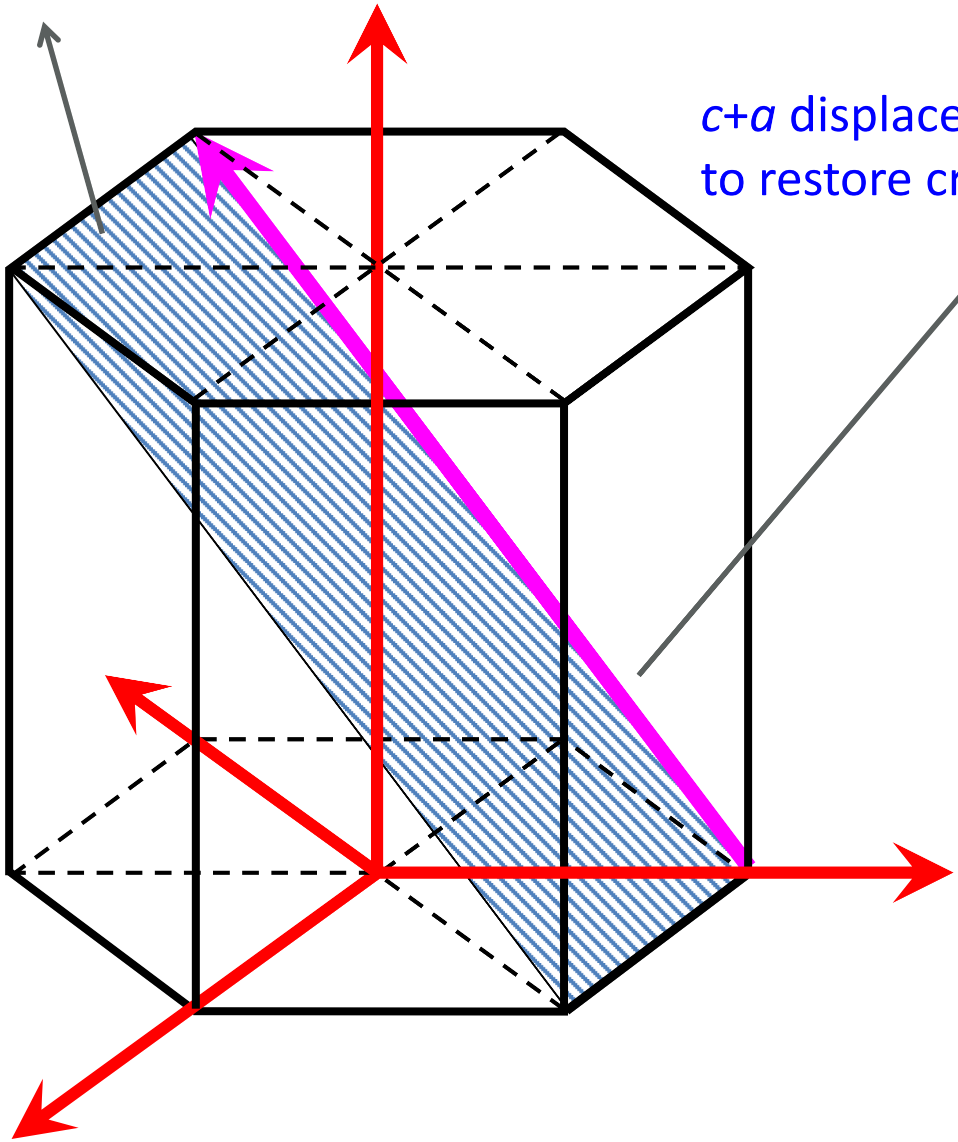
(a)

(b)

What about strain in the *c* direction ?

Need "actions" on non-close packed, corrugated (pyramidal or prismatic) planes

c+a displacements are "very long" to restore crystal registry



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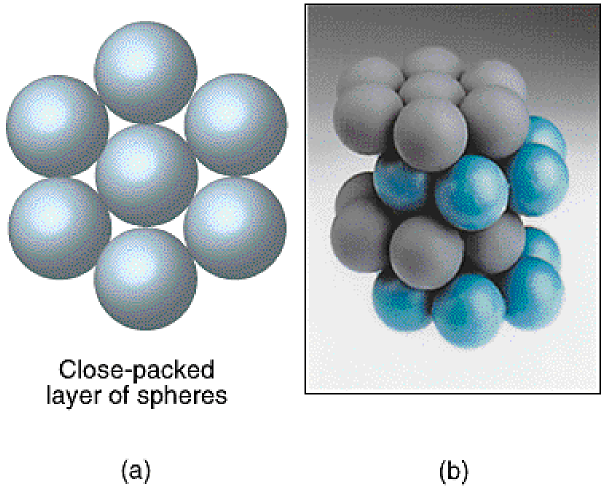
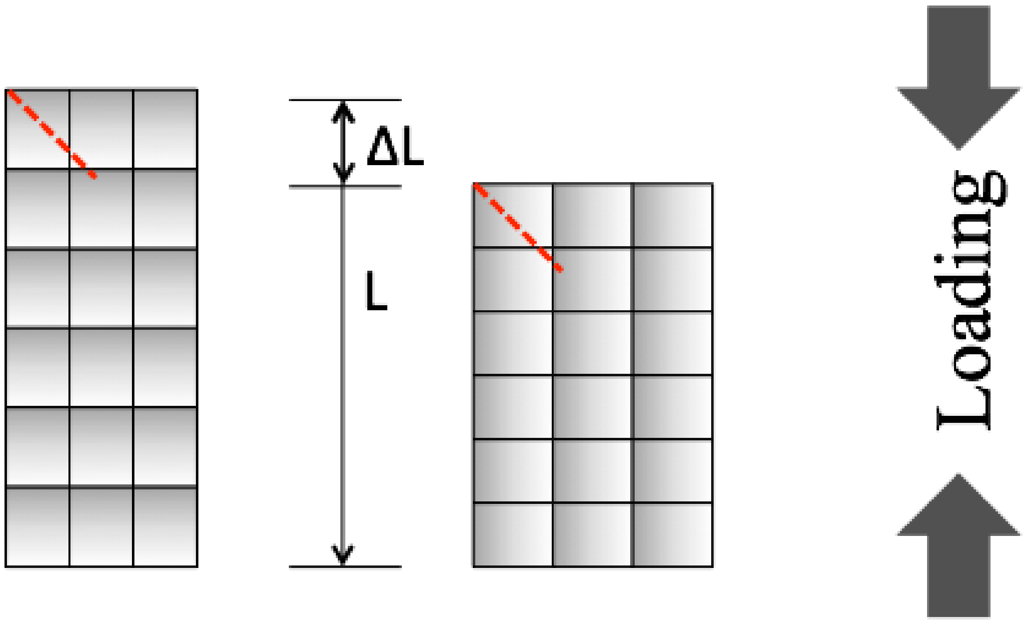


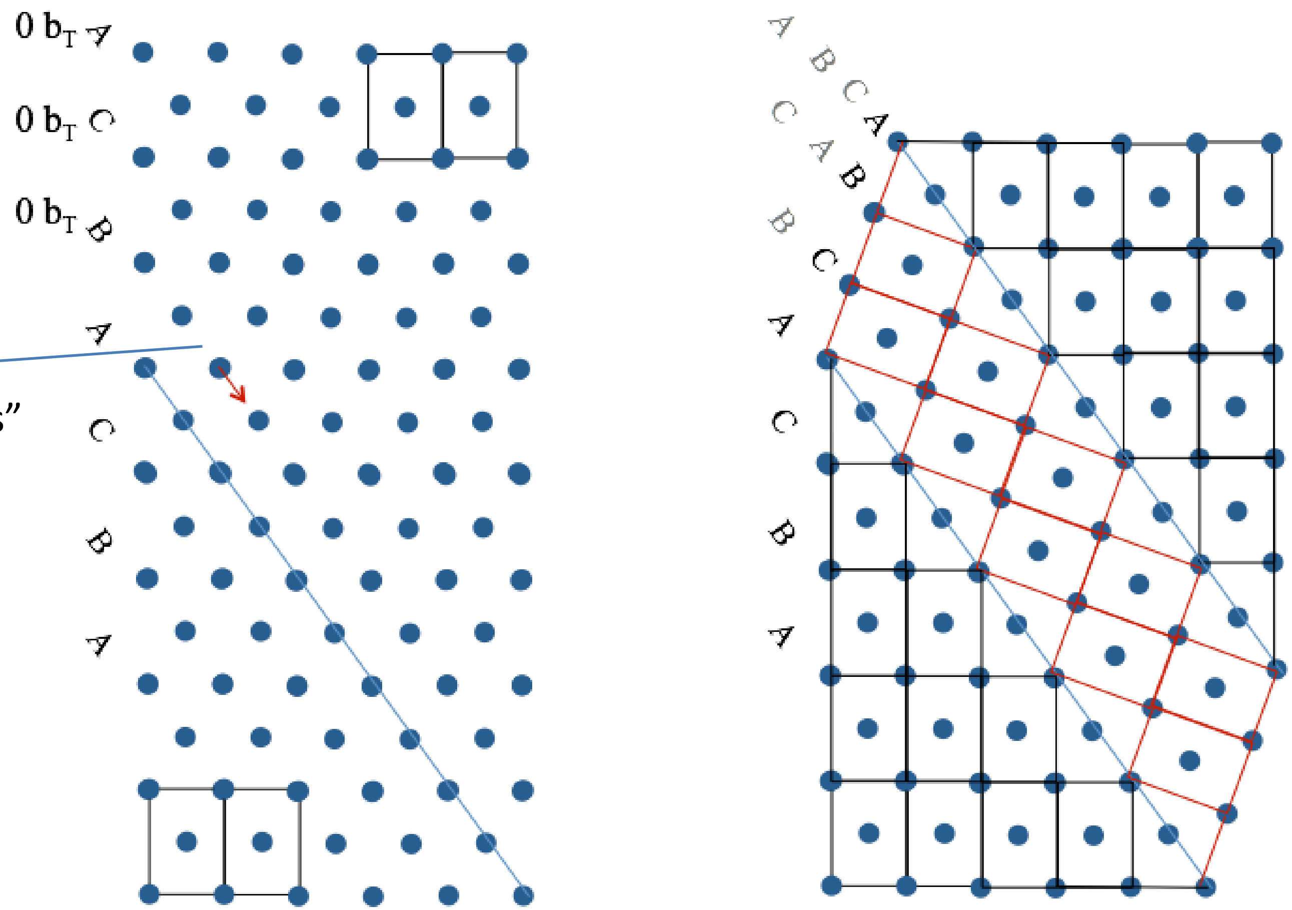
What about strain in the *c* direction ?

Reorientation of the crystal to accommodate/produce plastic strain



A common way of doing this is **deformation twinning**

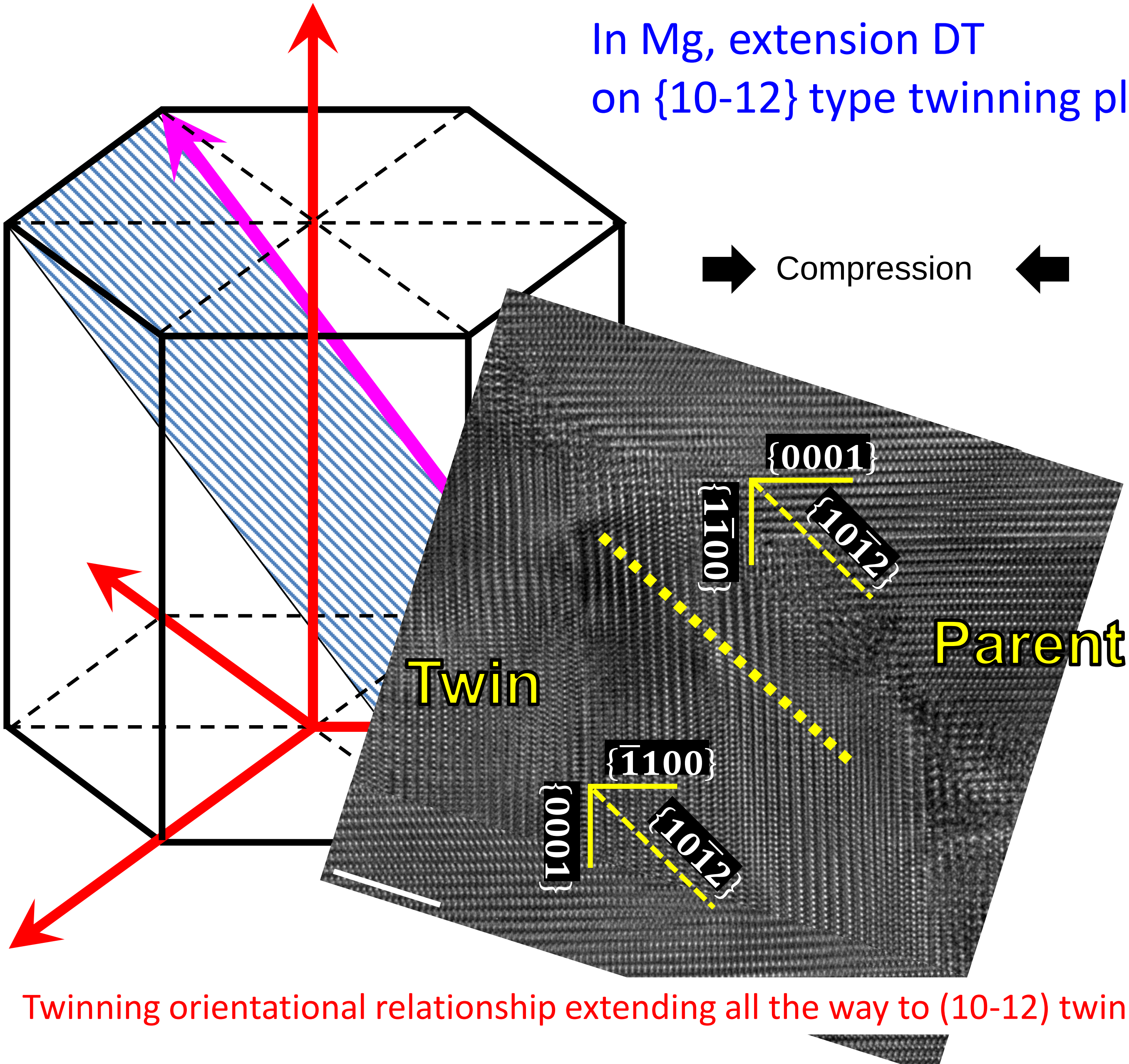
Deformation twinning (DT) reorients the crystal lattice



"Twining partials"
shear,
layer-by-layer

During plastic deformation, **stress reorients** part of the crystal to a new orientation in which the lattice structure is **identical** to that in matrix, and atoms in the two parts keep a mirror relationship through an invariant **low-index crystal plane**.

In Mg, extension DT
on {10-12} type twinning plane



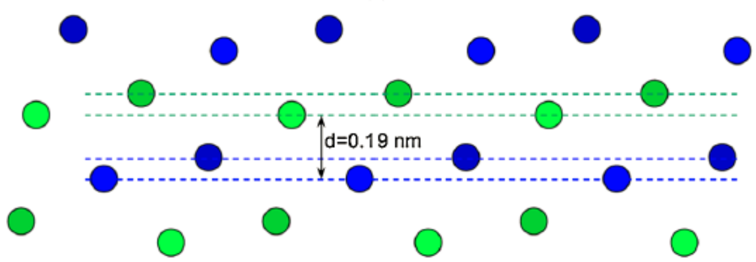
Twinning orientational relationship extending all the way to (10-12) twin boundary

But, the DT mechanism in Mg is quite involved:

a twin shear (twinning dislocation)

on a specific

twinning plane (invariant, mirror) ?



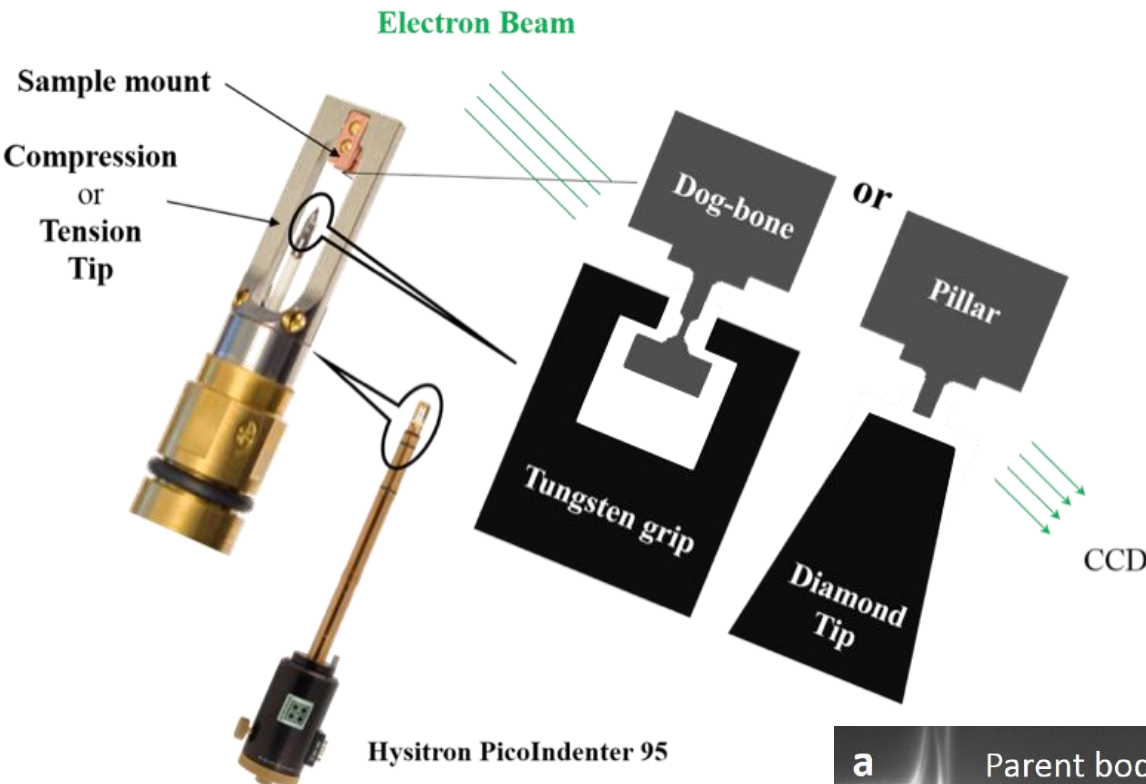
(10-12) is not a flat plane, but double layered (corrugated), w/ small spacing

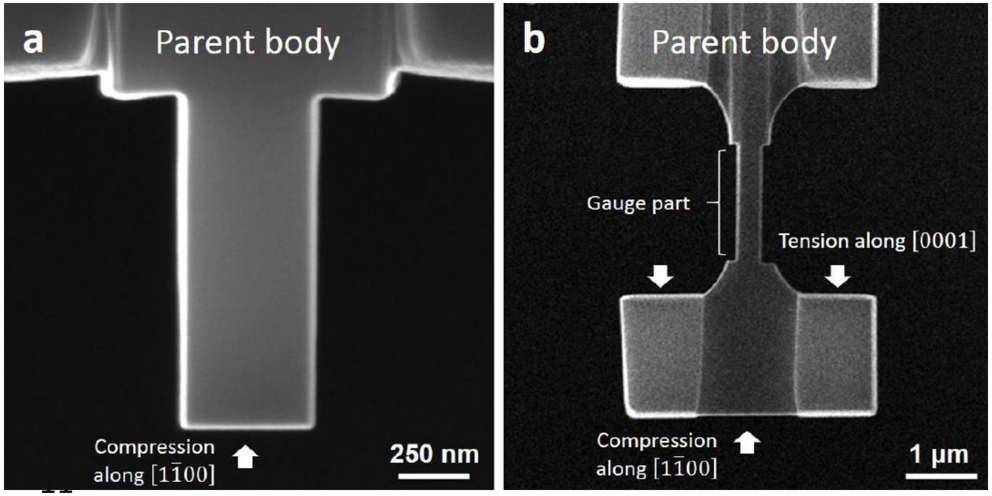
For (10-12) DT, the twin shear via a disconnection can only move ¼ of the atoms to the correct locations

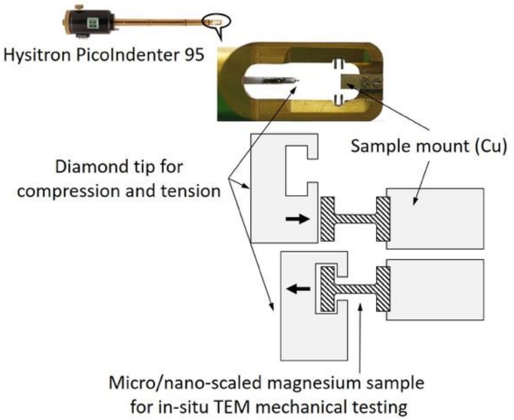
Q#2: Something else could also be happening ?

TEM suggests that something unusual is happening with this DT mode in Mg

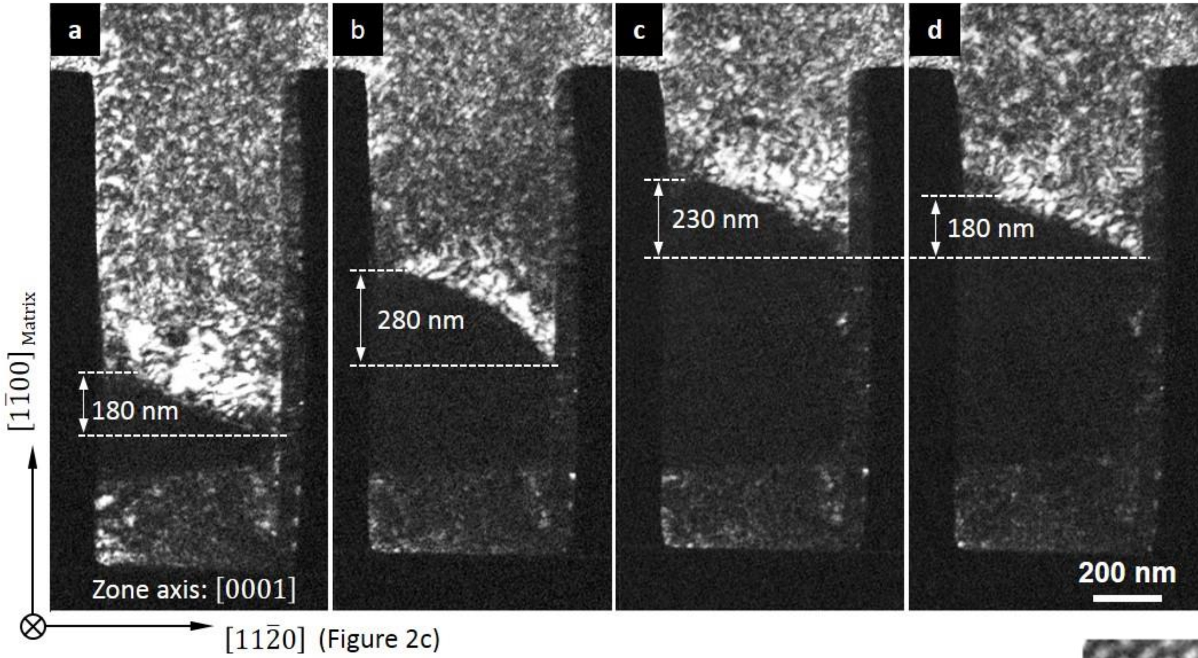
We used TEM to look at the deforming Mg





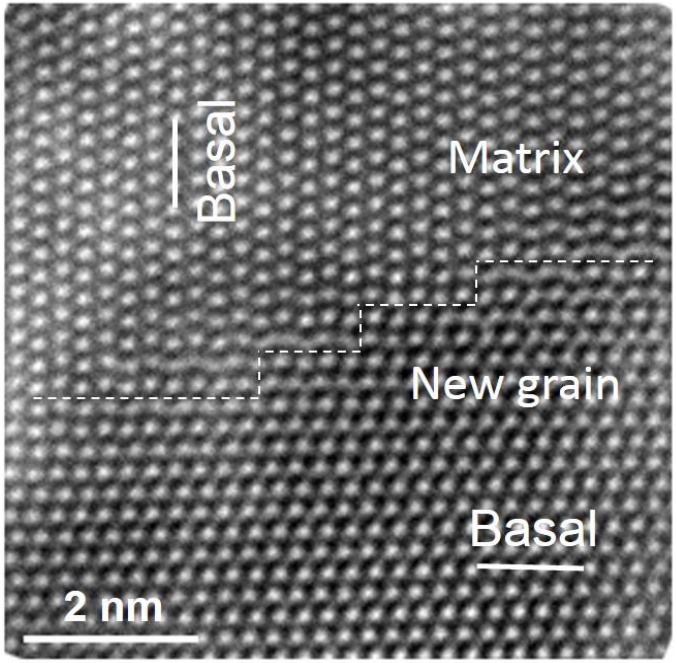


Migrating (twin) boundary, producing strains (in axial and transverse directions)



Cs-corrected STEM image of
a Nano-milled (<90 nm) sample

Terrace-like interface



(10-12) DT could involve,

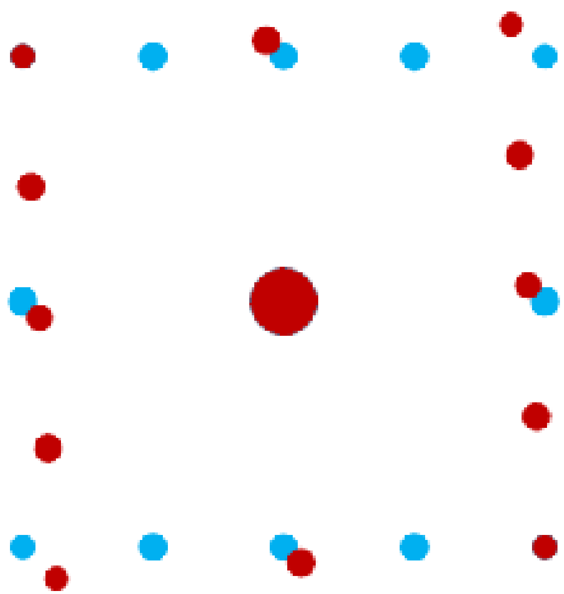
or proceed side-by-side with,

“another” mechanism during boundary migration?

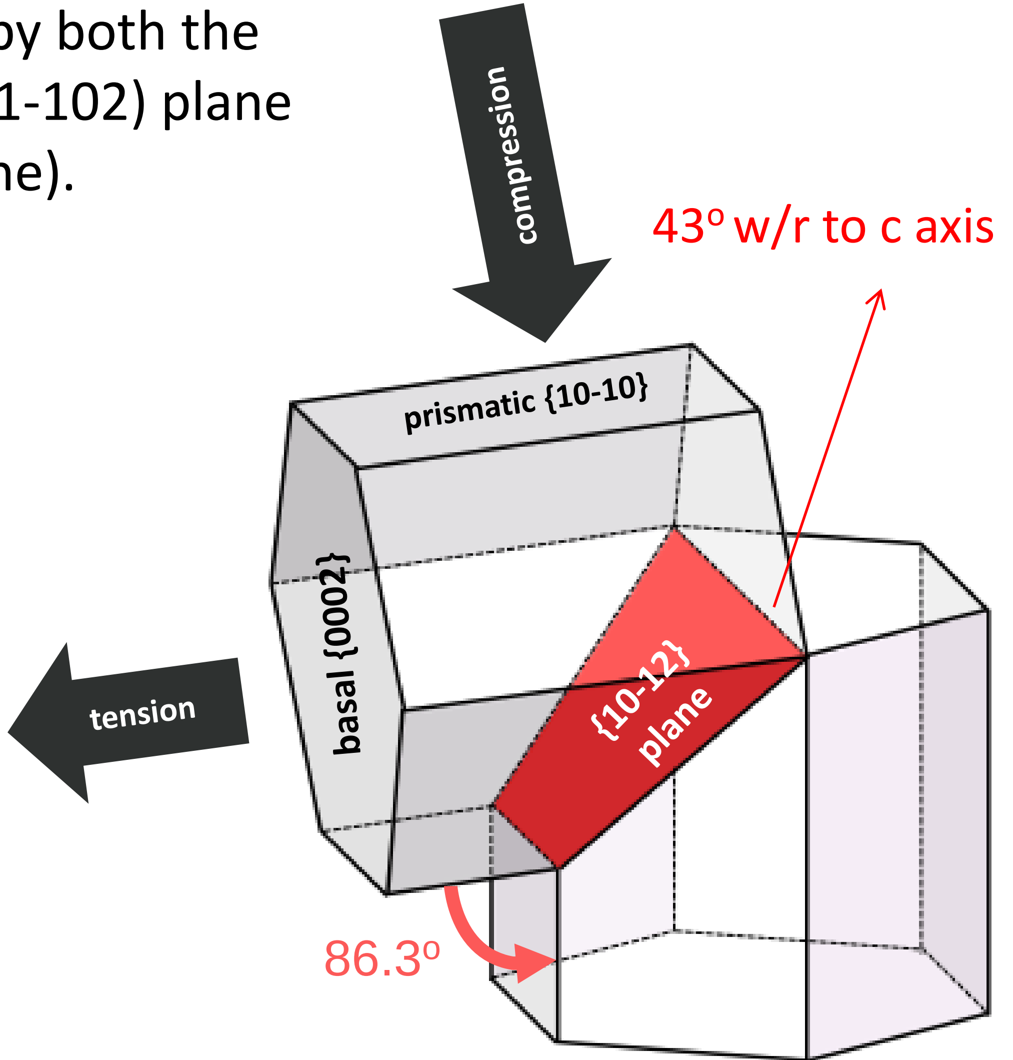
Q#3: Detailed features unexpected from deformation twinning ?

Let's compare the details w/ DT, under TEM, post mortem

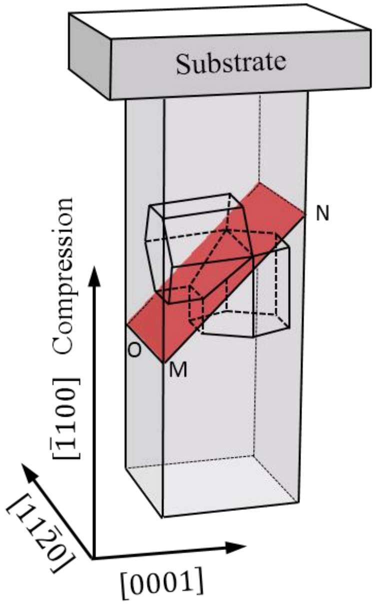
If it is pure {10-12} twinning, the lattice will have a mirror symmetry, by 86.3° across the twinning plane.
In diffraction pattern, {10-12} spots overlap with the original ones, as the twin boundary {10-12} is shared by both the matrix and the twin (the parent (1-102) plane is parallel to the twin (-1102) plane).

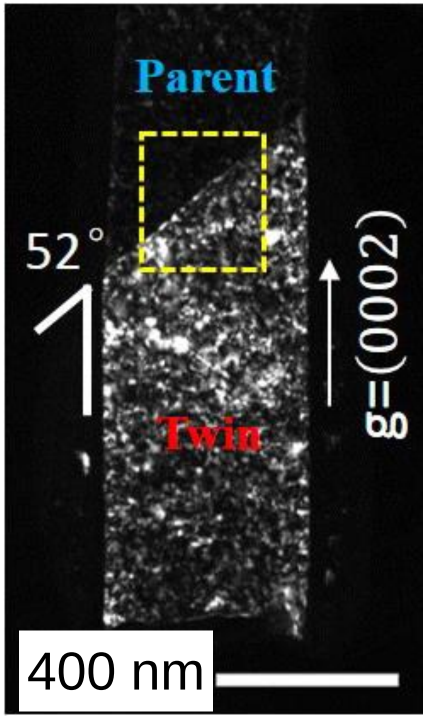


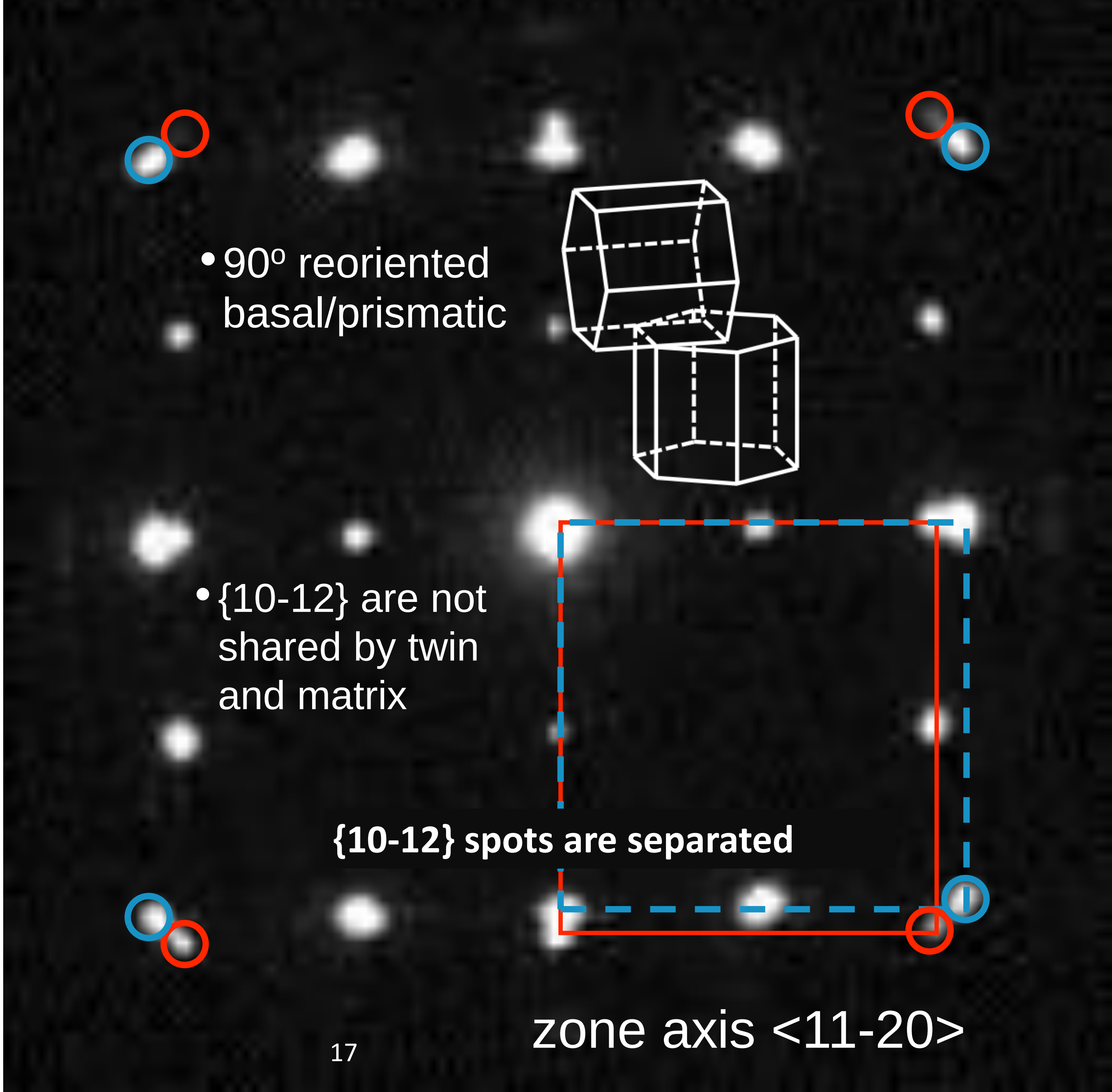
zone axis <2-1-10>

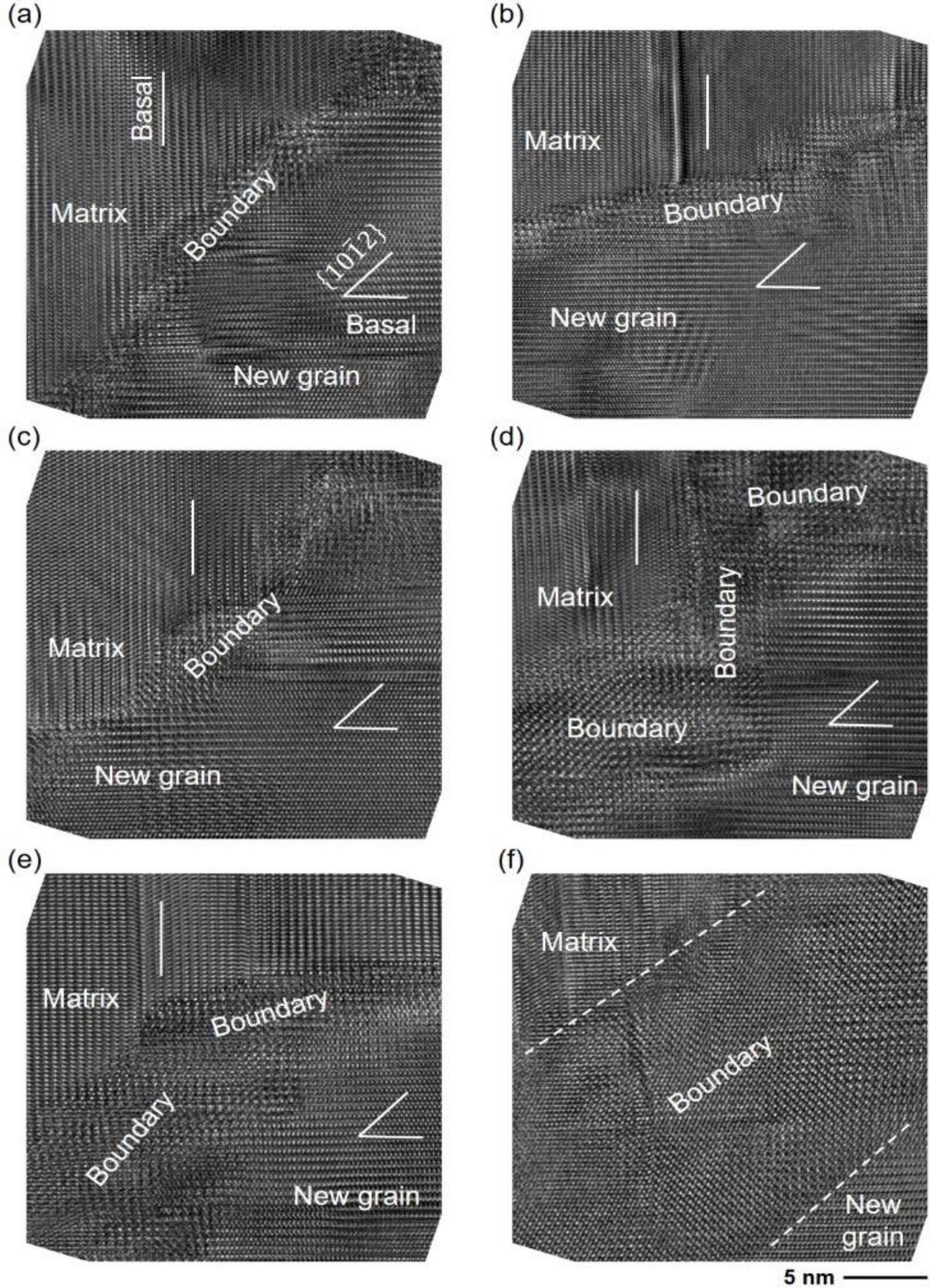


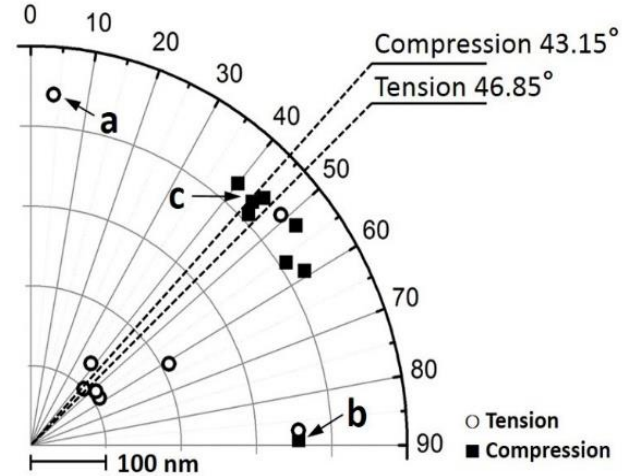
Angle can be 52º, not the expected 43º

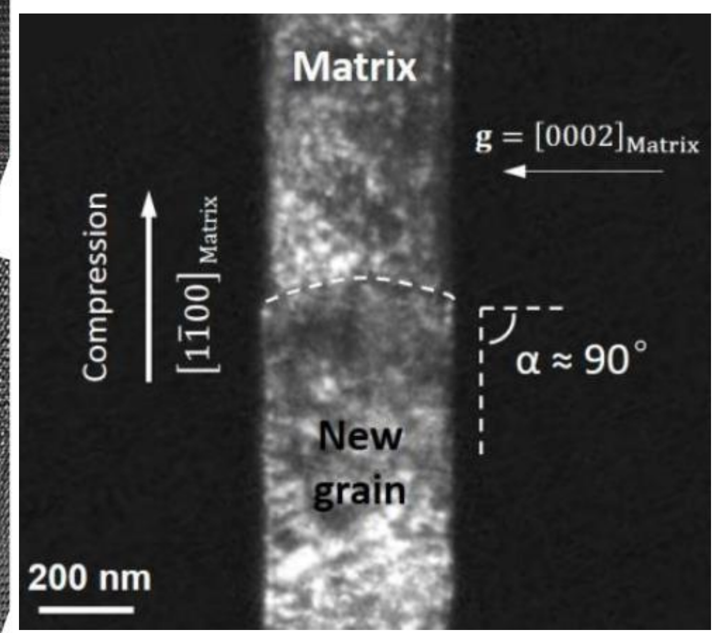


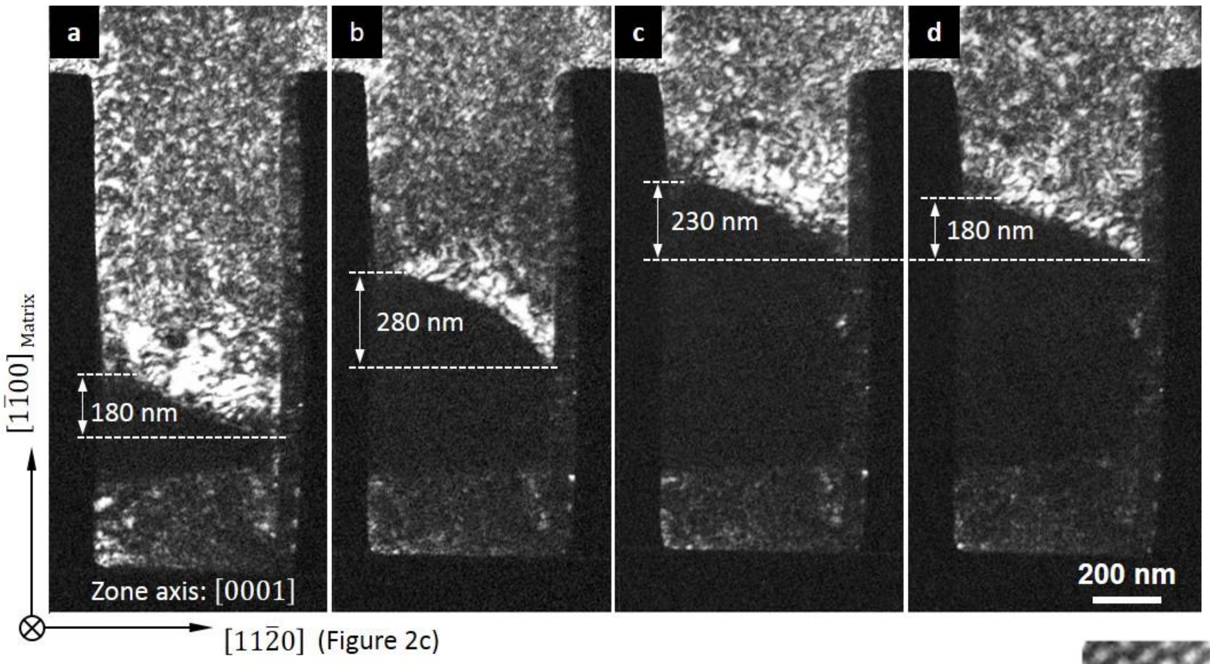





(a)
Basal
Matrix
Boundary
{10$\bar{1}$2}
Basal
New grain
(b)
Matrix
Boundary
New grain
(c)
Matrix
Boundary
New grain
(d)
Boundary
Matrix
Boundary
Boundary
New grain
(e)
Matrix
Boundary
Boundary
New grain
(f)
Matrix
Boundary
New grain
5 nm

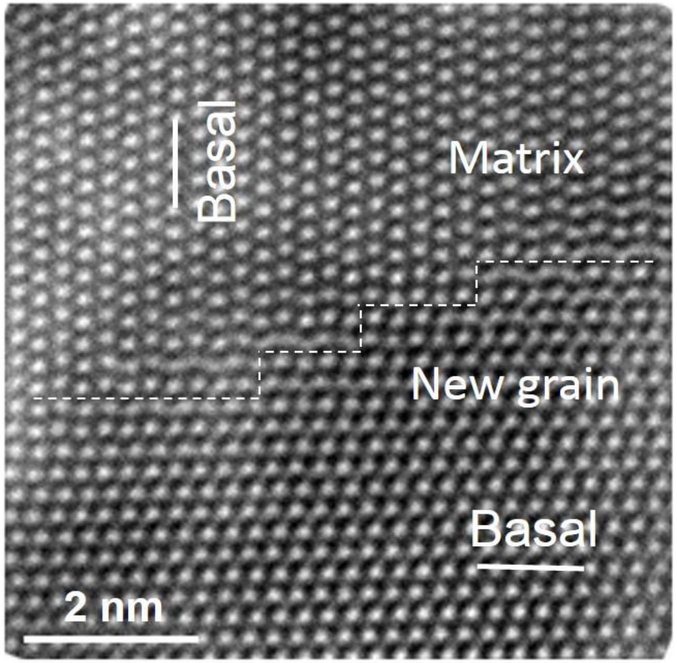

0
10
20
30
40
50
60
70
80
90
Compression 43.15°
Tension 46.85°
a
b
c
100 nm
○ Tension
■ Compression


Matrix
g = [0002]$_{Matrix}$
Compression
[1$\bar{1}$00]$_{Matrix}$
α ≈ 90°
New grain
200 nm



Cs-corrected STEM image of
a Nano-milled <90 nm sample

Terrace-like interface

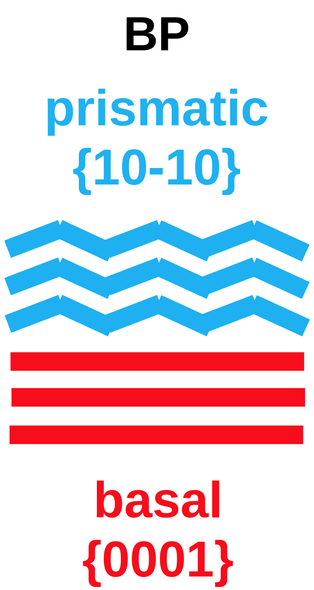


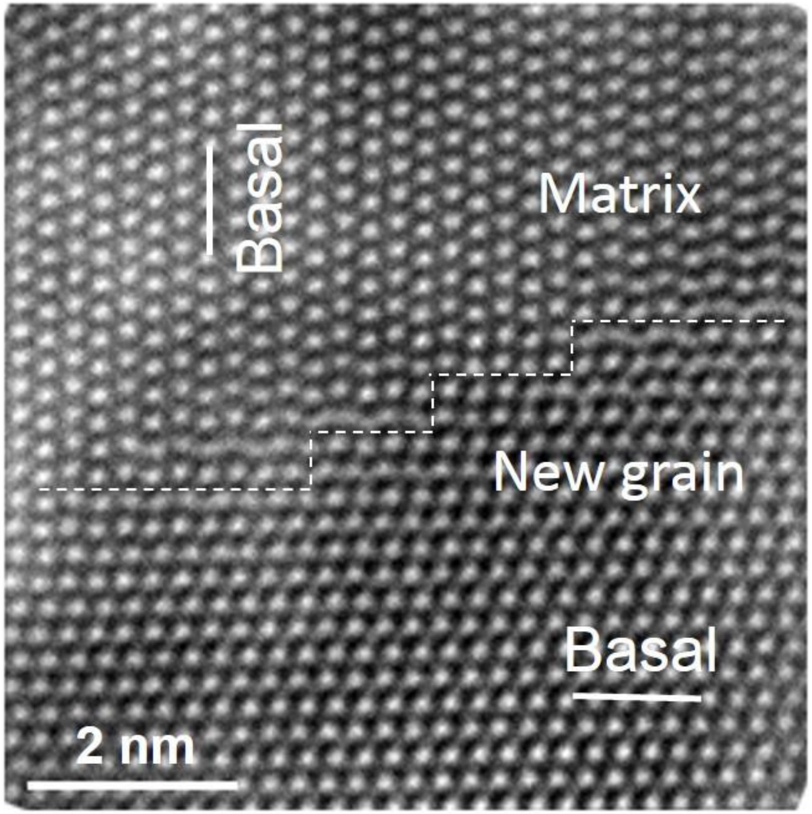
At atomic resolution: STEM image of the boundary

(Twin)basal/prismatic(Matrix) interface:

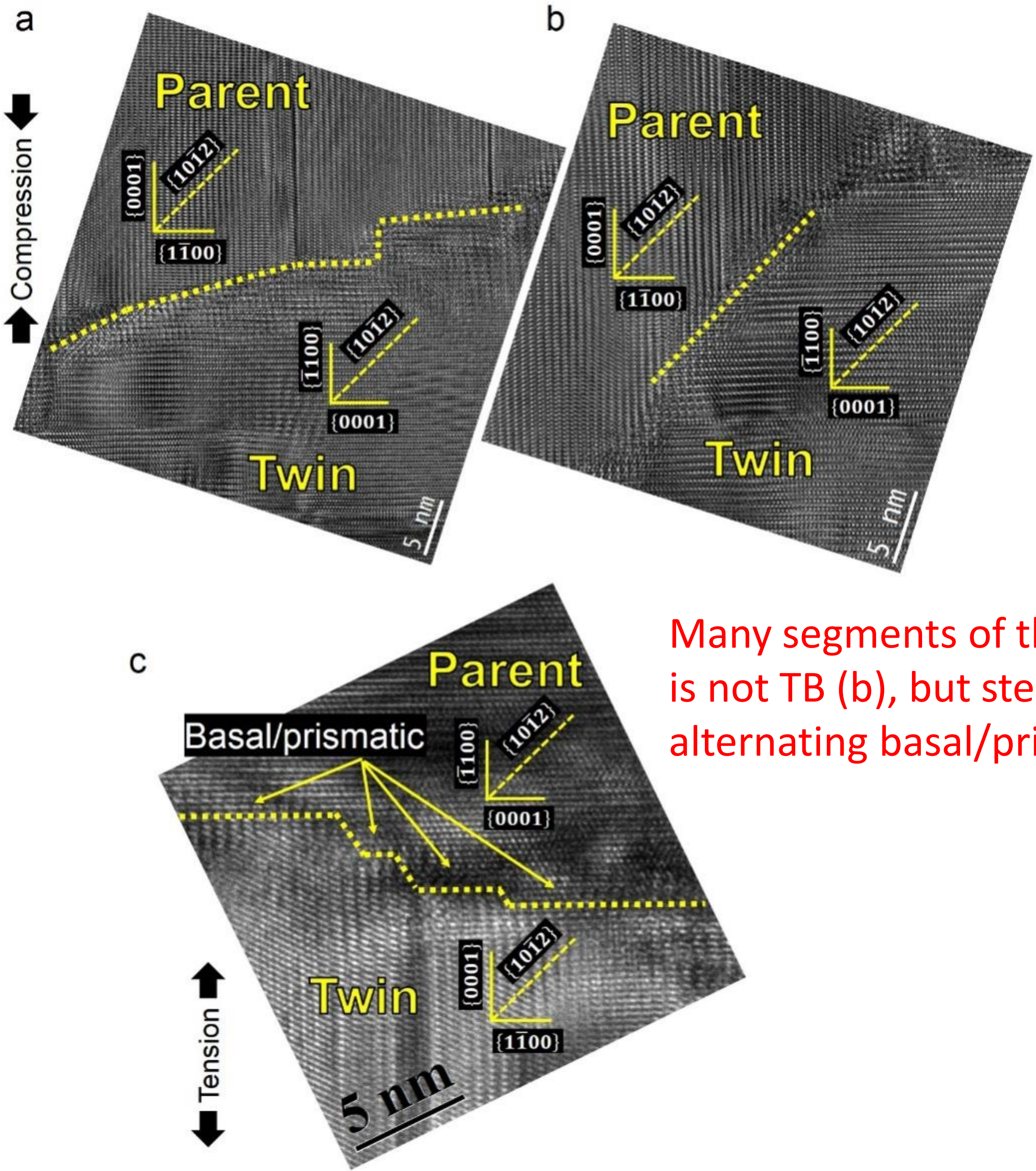
BP interface

Local interfaces
are often not {10-12},
but basal/prismatic



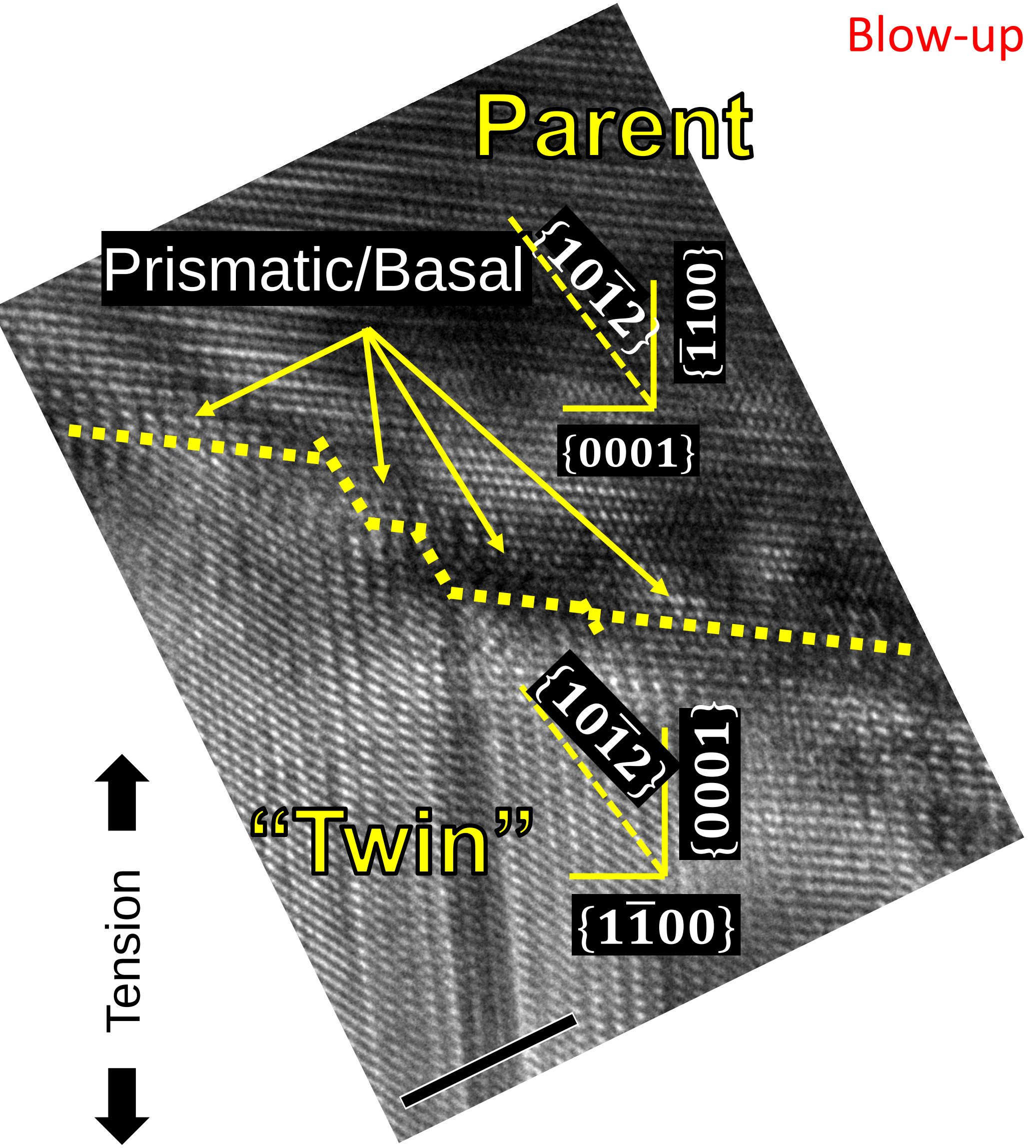


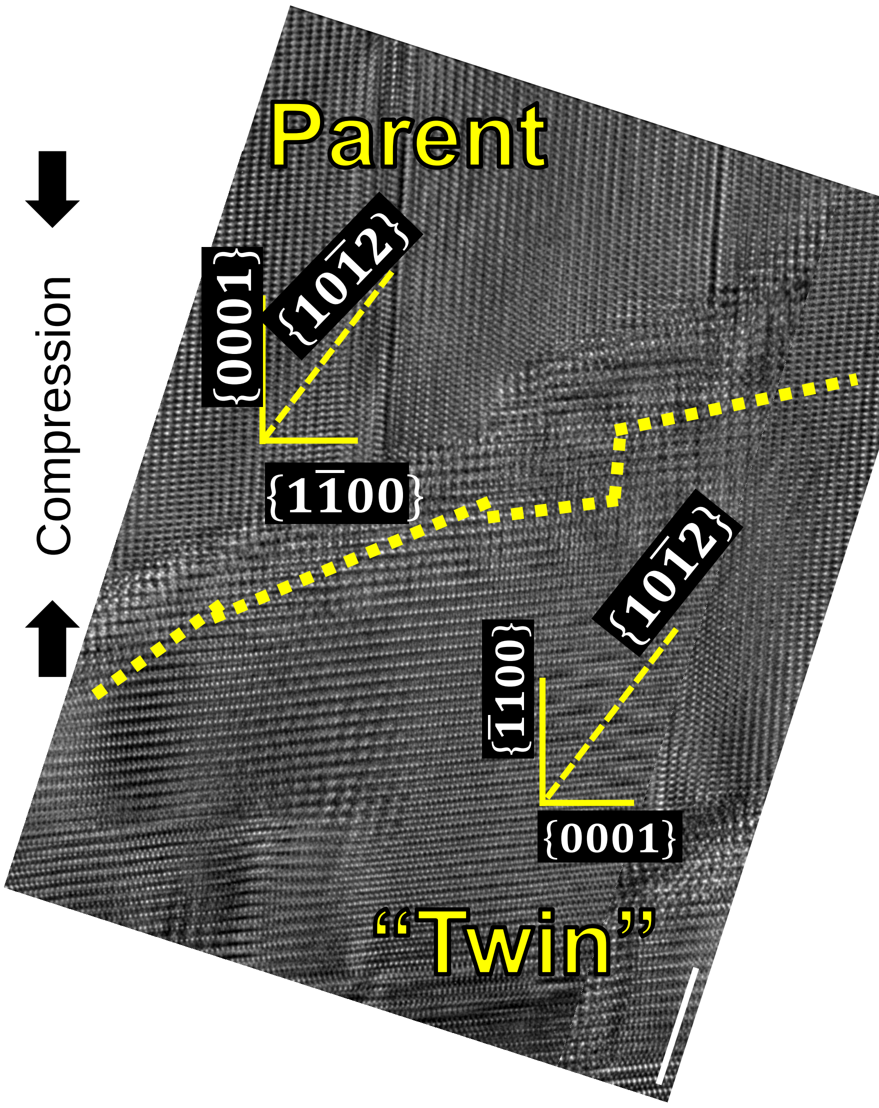
Bo-Yu Liu *et al.*, Nature Communications (2014)



Many segments of the boundary
is not TB (b), but steps composed of
alternating basal/prismatic interfaces

Blow-up of the previous 2 images:

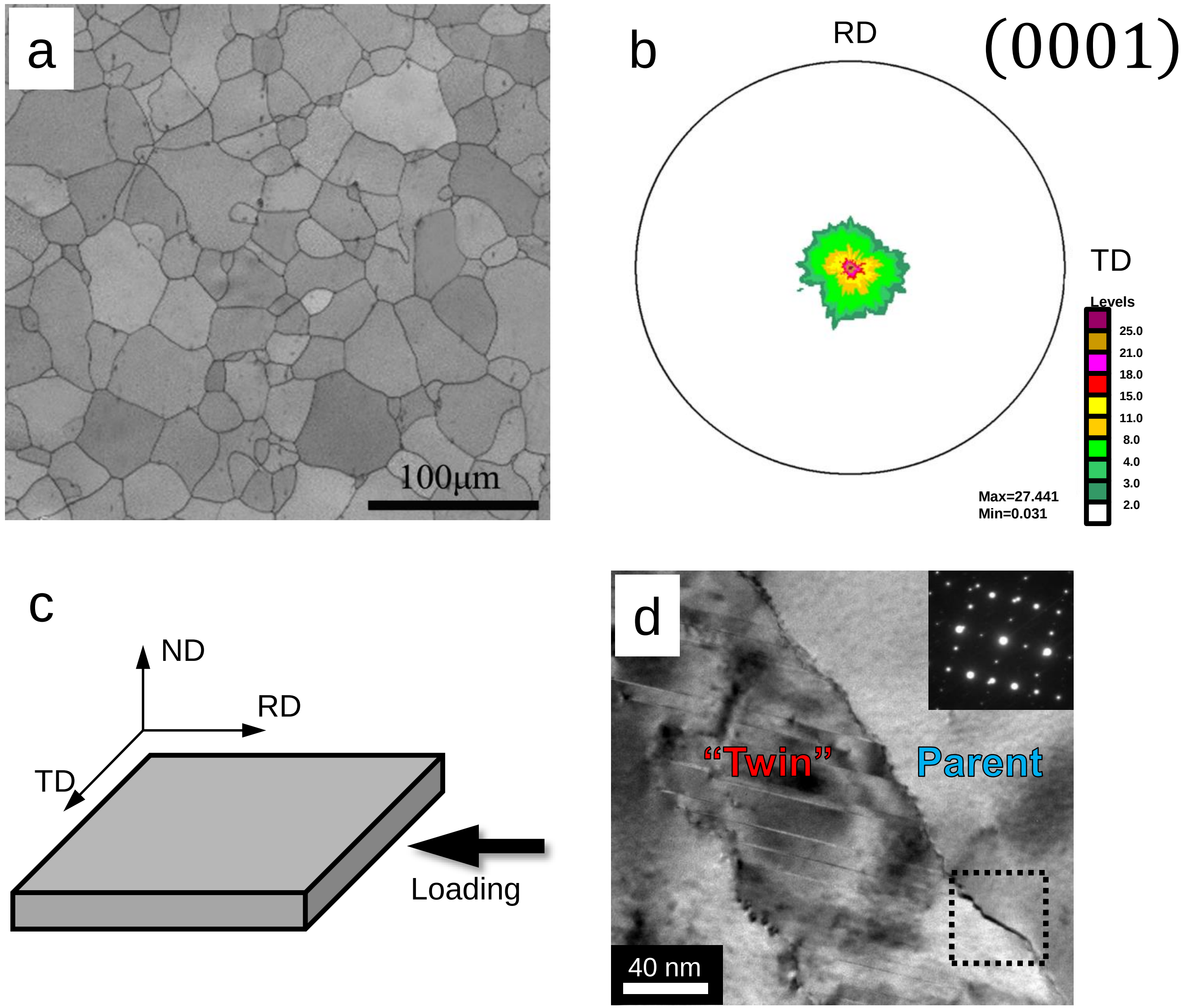




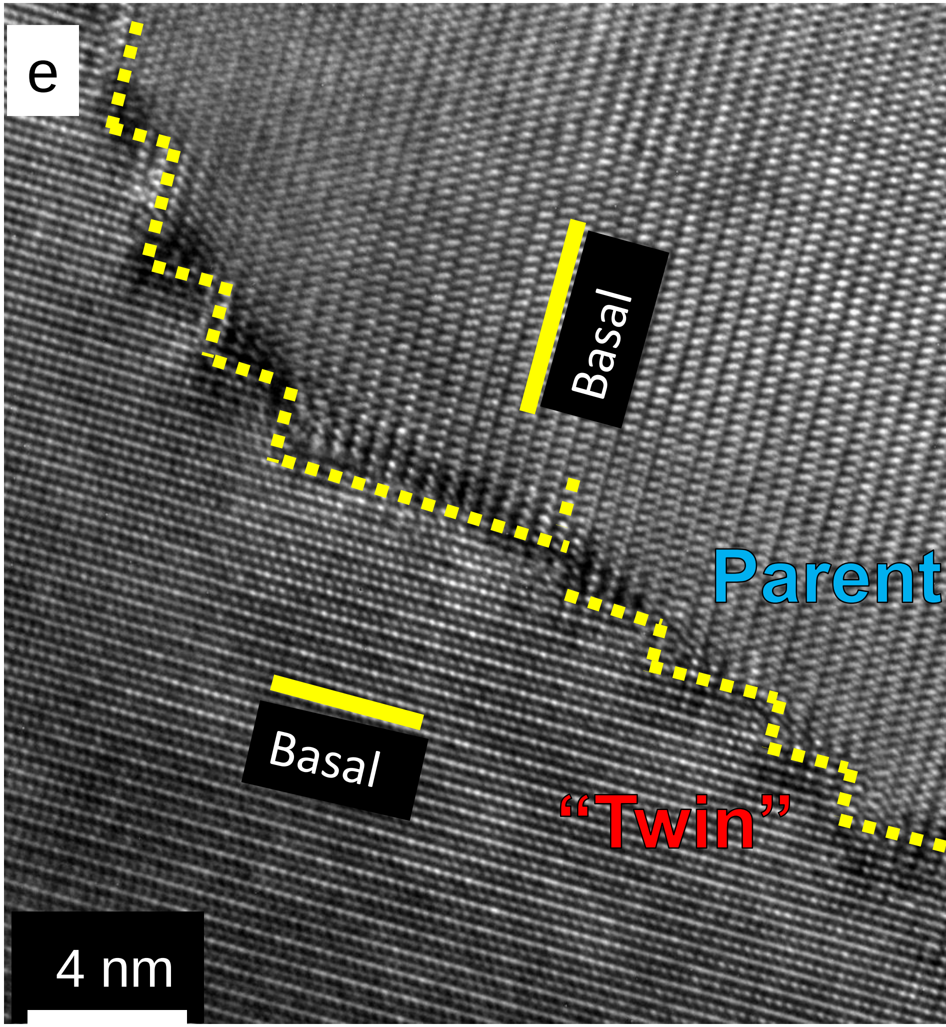
So, accompanying (10-12) DT, there are many interface regions undergoing the ~90^o reorientation; there the interface is not (10-12), nor a mirror invariant twinning plane!

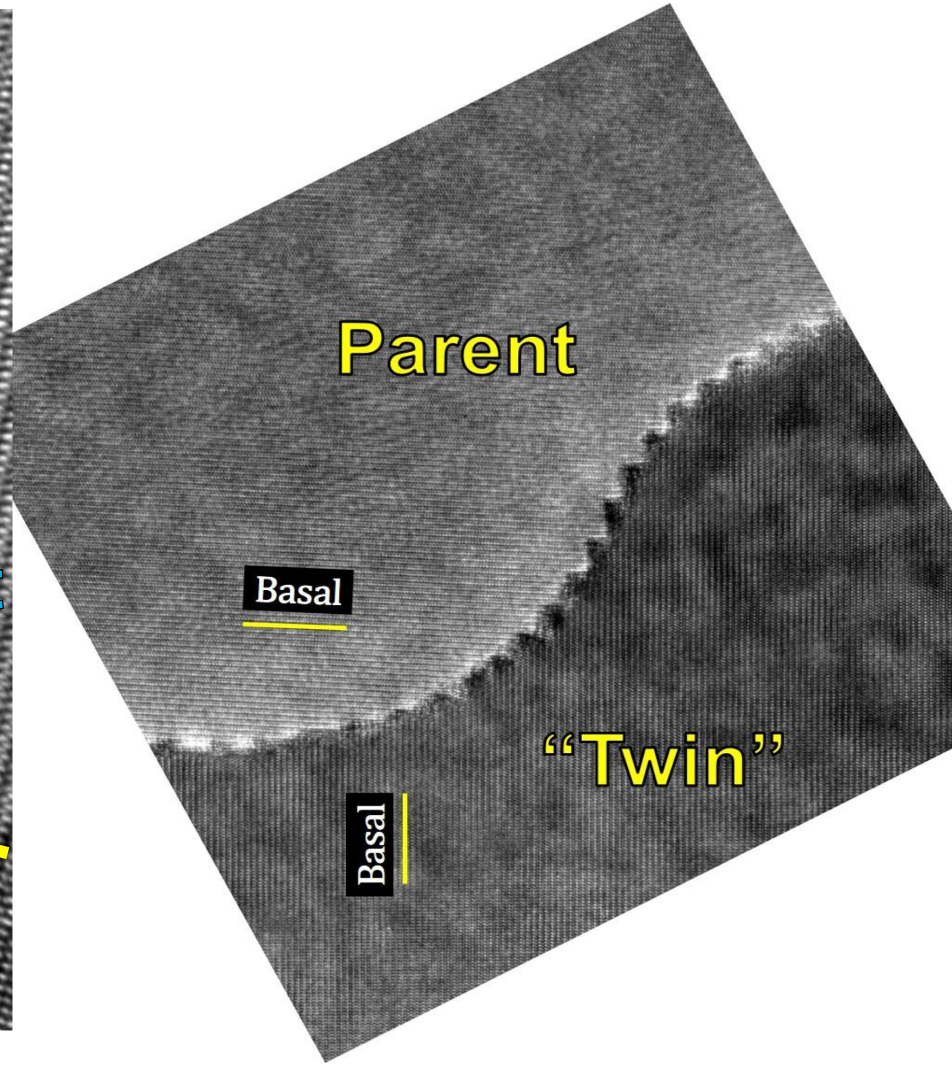
Q#4: Could also happen in larger samples ?

Seen also in large grains of conventional Mg alloys …



Larger grains in AZ31 Mg alloy sheet (30 mm × 30 mm × 22 mm) w/ equi-axed and strongly textured grains (average grain size ~34 μm). The compression loading was applied perpendicular to [0001] at a strain rate of $10^{3}s^{-1}$ and a total strain of ~7%.





AZ31 Mg alloy sheet (30 mm × 30 mm × 22 mm) w/ equi-axed and strongly textured grains (average grain size ~34 µm). The compression loading was applied perpendicular to [0001] at a strain rate of $10^3 s^{-1}$ and a total strain of ~7%. Note the orthogonal steps. This morphology is more obvious near twin tips.

Q#5: Why so many basal-prismatic boundaries?

Just twin boundary relaxed into steps ?

Or,

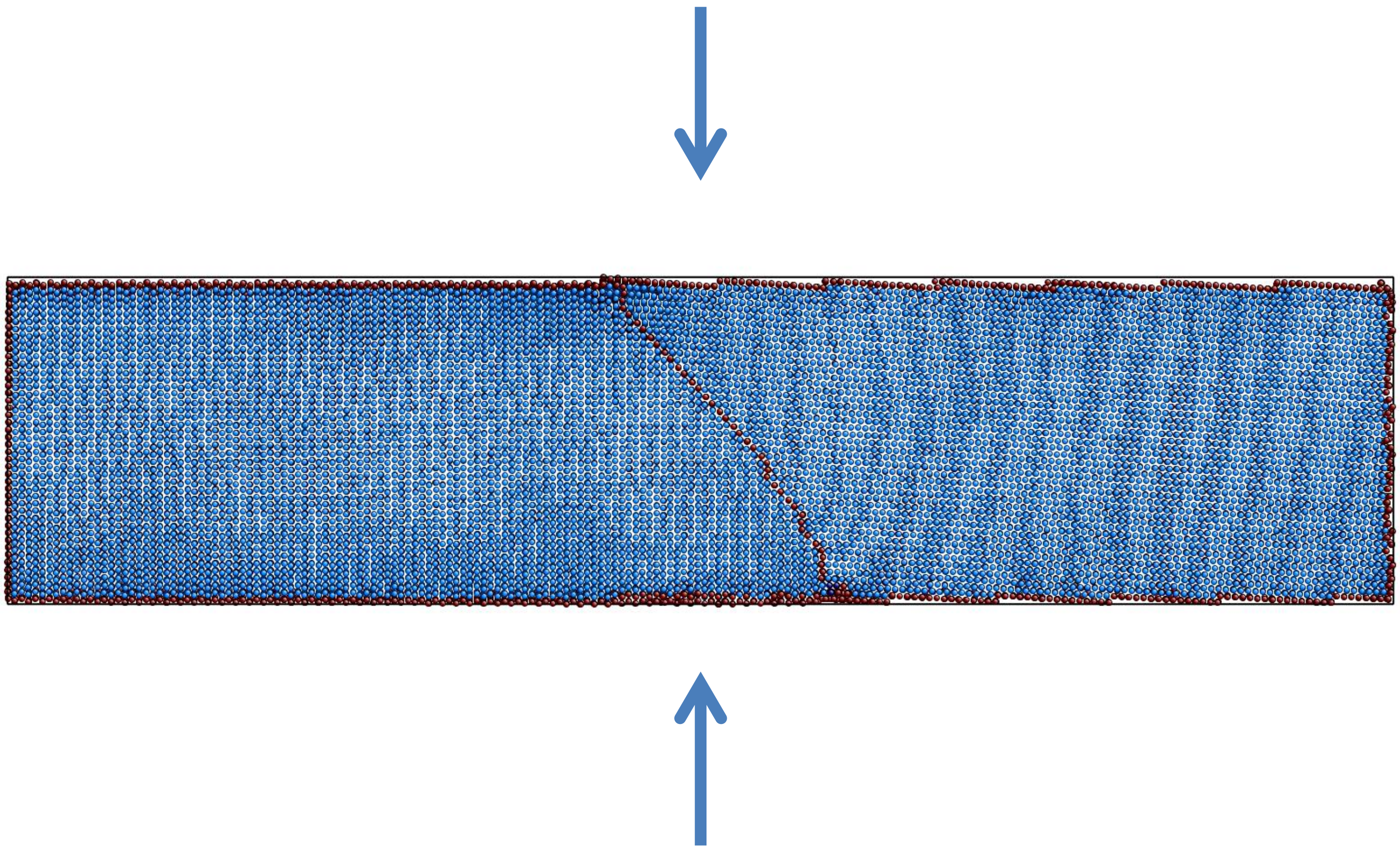
action not on (10-12) plane in the first place?

no twinning plane (invariant, mirror)?

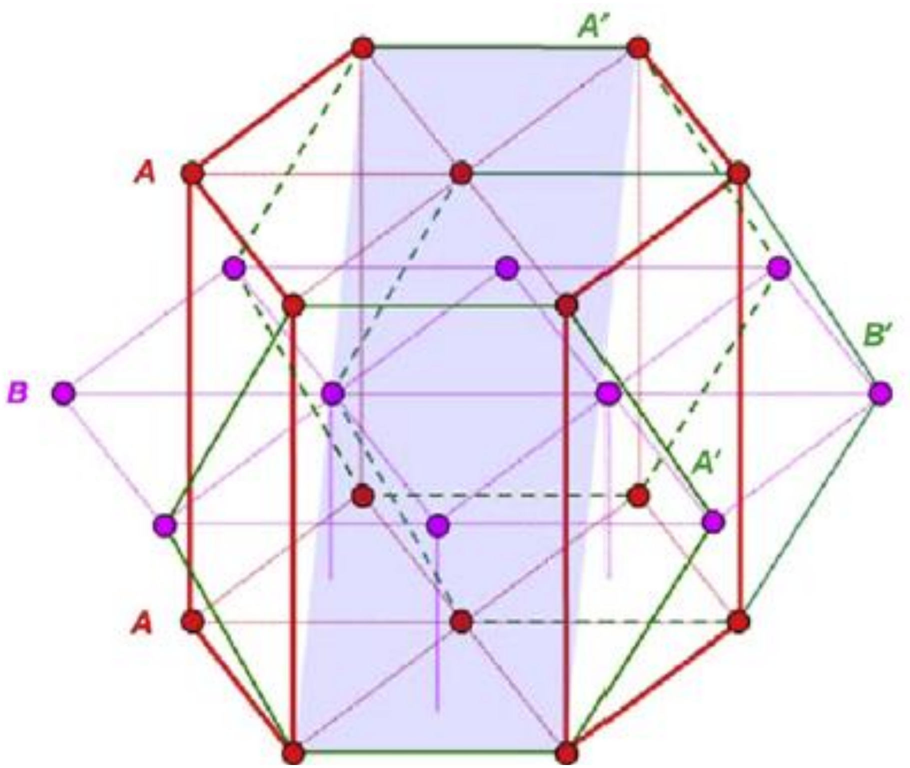
no well-defined twin shear (twinning dislocations)?

involving **other processes** ……

MD simulation shows basal-prismatic conversion at the B-P interface



Proposal: basal-prismatic transformation



red (standing-up) => green (lying-down)

shaded, inclined plane); hence, they satisfy the twin relationship. Shuffling is required to correct the distortion in the new hcp lattice such that the correct stacking sequence and the c/a ratio can be established. Note that the shaded twinning plane has to be distorted when the atoms of the twin lattice shuffle to the correct positions, i.e. the invariant plane strain condition for deformation twinning breaks

We notice that across the (10-12) plane (purple), the original bottom basal plane and the front prismatic plane form a 90^{o} angle.

If the front (prismatic) plane can be re-configured into a flat basal plane (of the twin lattice), it approaches a mirror relationship across (10-12) with the bottom basal plane.

In other words, such a 90^{o} "lattice reconstruction" is close to what the twinning action produces!

If we achieve this prismatic-basal conversion, not via action on (10-12), the net result can still be close to that of (10-12) twinning.

Like DT, the resulting strain along <*c*> is 6.7% for Mg

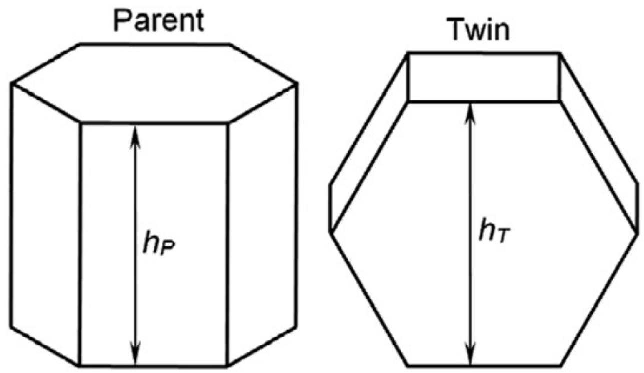
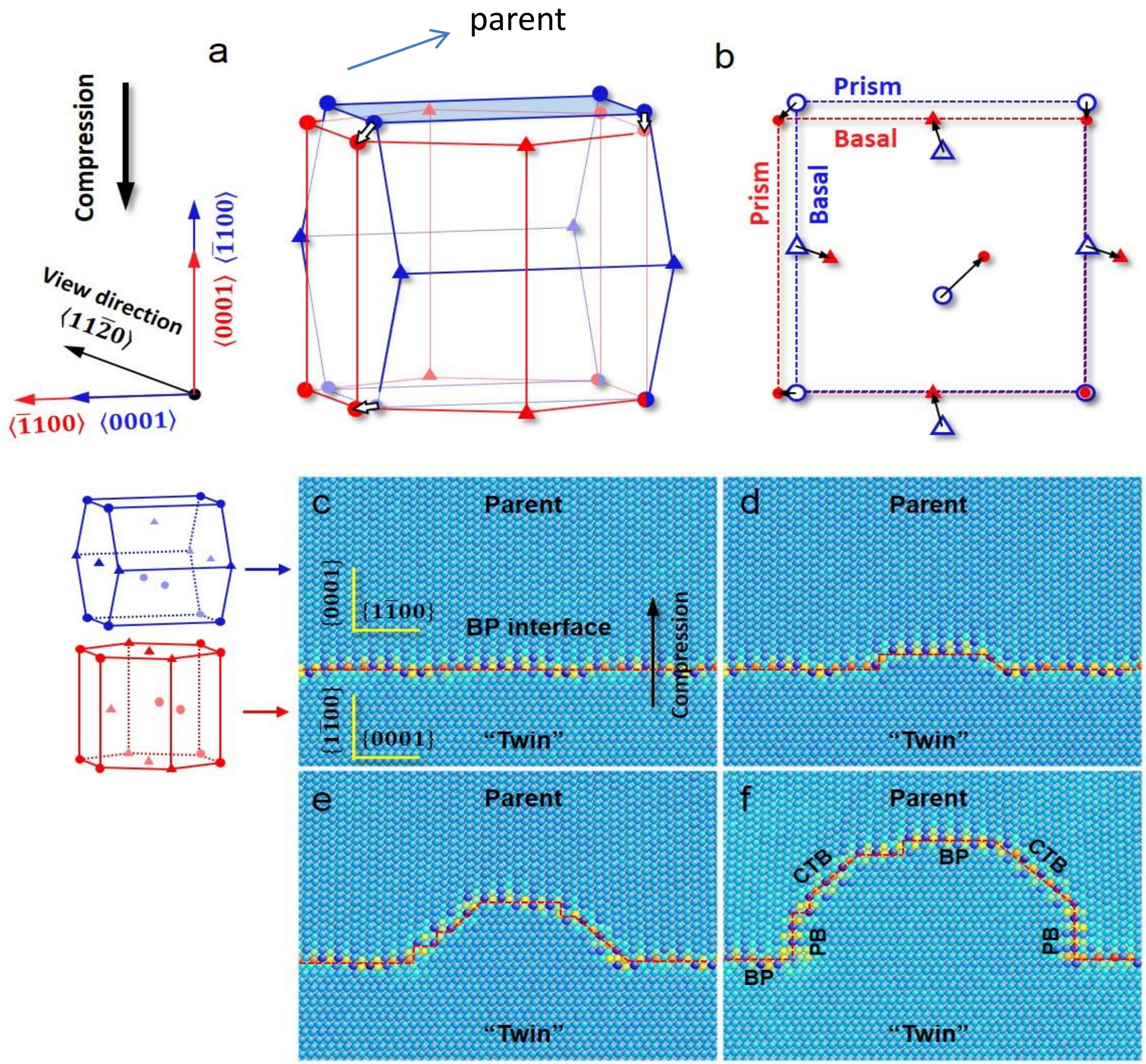


Figure 3. Separation of the parent and the twin lattice in Figure 2. After $\{10\bar{1}2\} < 10\bar{1}\bar{1} >$ twinning, the parent lattice is reoriented by $\sim 90°$ around $< 1\bar{2}10 >$, which generates a misfit strain between the parent and the twin lattice along the c-axis of the parent: $\varepsilon \approx (h_T - h_P)/h_P = (\sqrt{3} - \gamma)/\gamma$ (γ is the c/a ratio). Thus, for hcp metals with $\gamma < \sqrt{3}$, a positive tensile strain is generated, i.e. tension twinning occurs; for hcp metals with Mg $\gamma > \sqrt{3}$, a negative strain is generated, i.e. compression twinning occurs.

For Mg, γ =c/a=1.633, very close to "ideal" (Co is similar, but γ=1.58 for Ti)

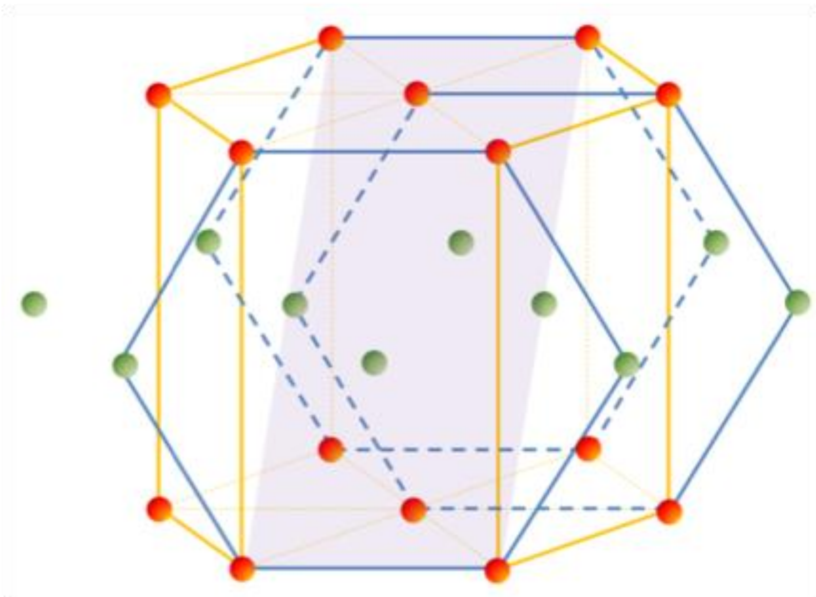
In MD simulation, conversion can be accomplished via atomic shuffling

The far-field parent and “twin” lattices still mimic the (10-12) DT orientational relationship, approaching ~90^o ; So it is a “(10-12) twinning-like lattice reorientation, but the action is not on the crystallographic (10-12) plane !



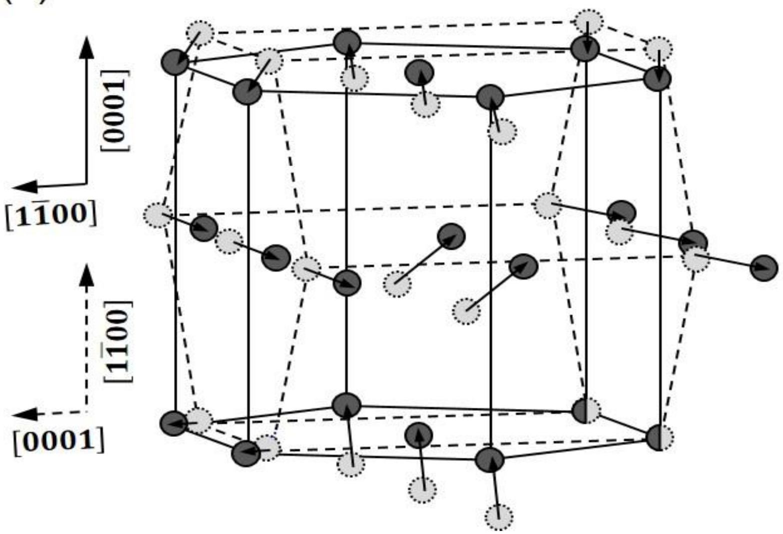
This is not just deformation twinning, although it accompanies the latter: there is no mirror relationship at the moving boundary, nor uniform twinning shear

Q#6: Why is the basal-prismatic conversion "easy" ?



For Mg, a lateral HCP embryo is already “waiting” to take shape in the stand-up HCP

(b)

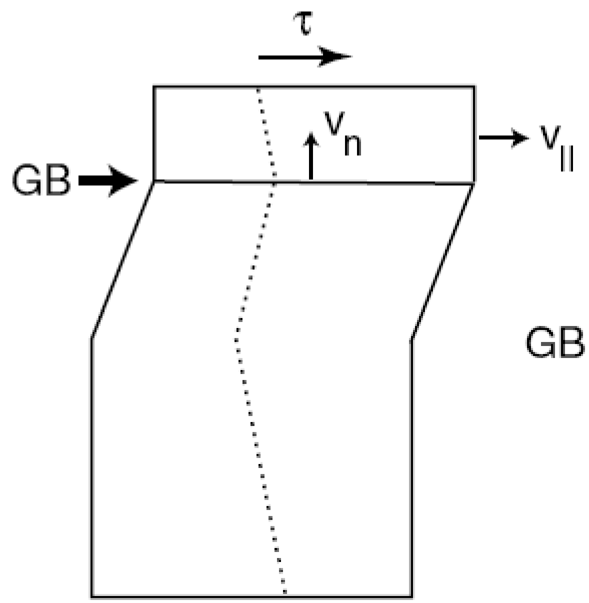


This B-P conversion only requires short-distance collective atomic rearrangements: shuffle distances are relatively small (0.02 to 0.09 nm);

Maybe, atomic shuffling for the most part, + minor/no help from pre-existing interfacial defects (dislocations) ?

Q#7: Different from "stress coupling with GB"?

Not just shear strain

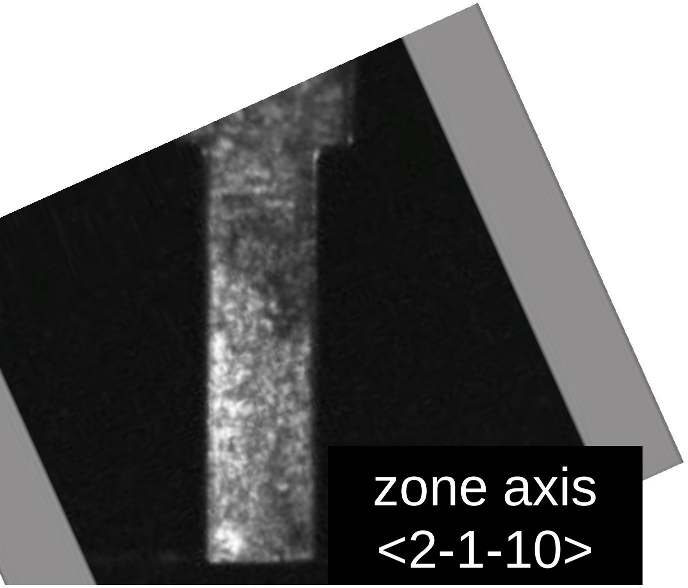


Acta Materialia 54 (2006) 4953–4975

"Shear stresses coupled to a GB can induce its normal motion"

Coupling grain boundary motion to shear deformation

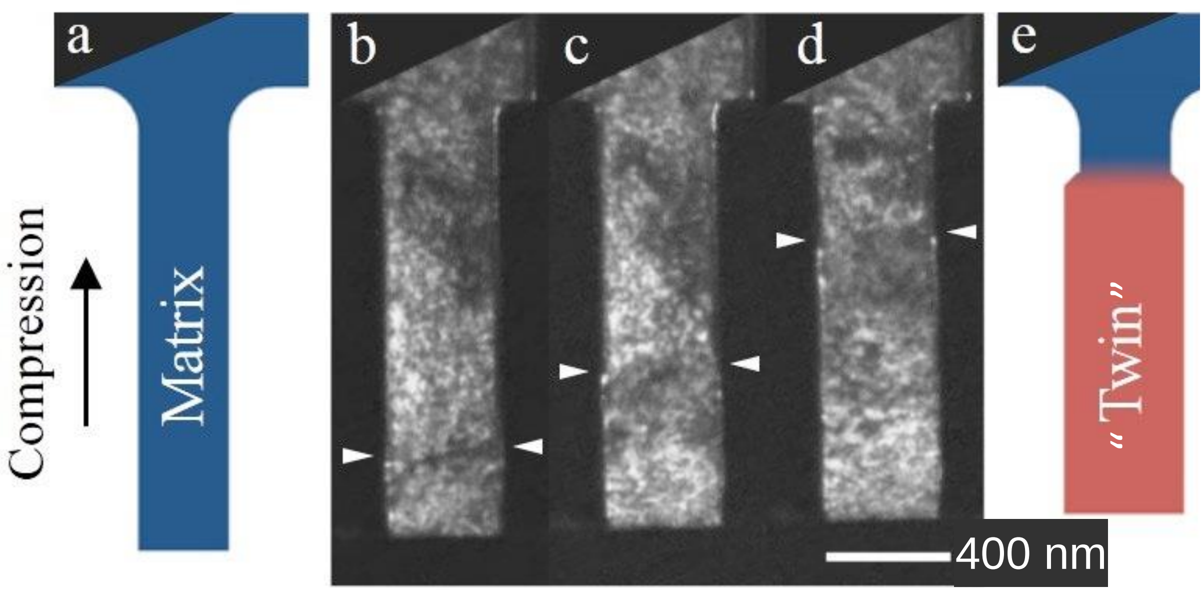
John W. Cahn [a], Yuri Mishin [b,*], Akira Suzuki [b]

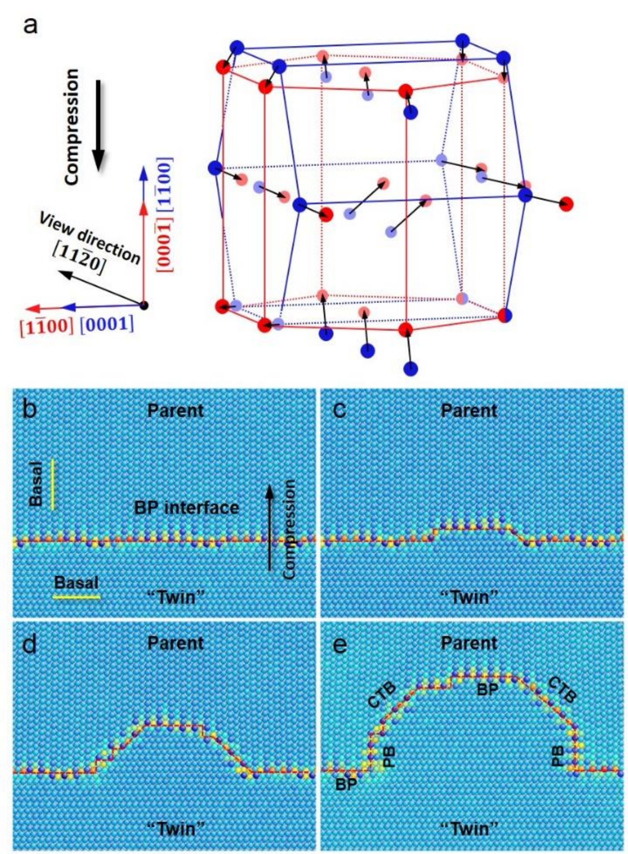


Not shear (twinning dislocation creating shear step on one side),

but shortening in *z* direction and swelling sideways on both sides

Bo-Yu Liu *et al.*,
Nature Communications (2014)





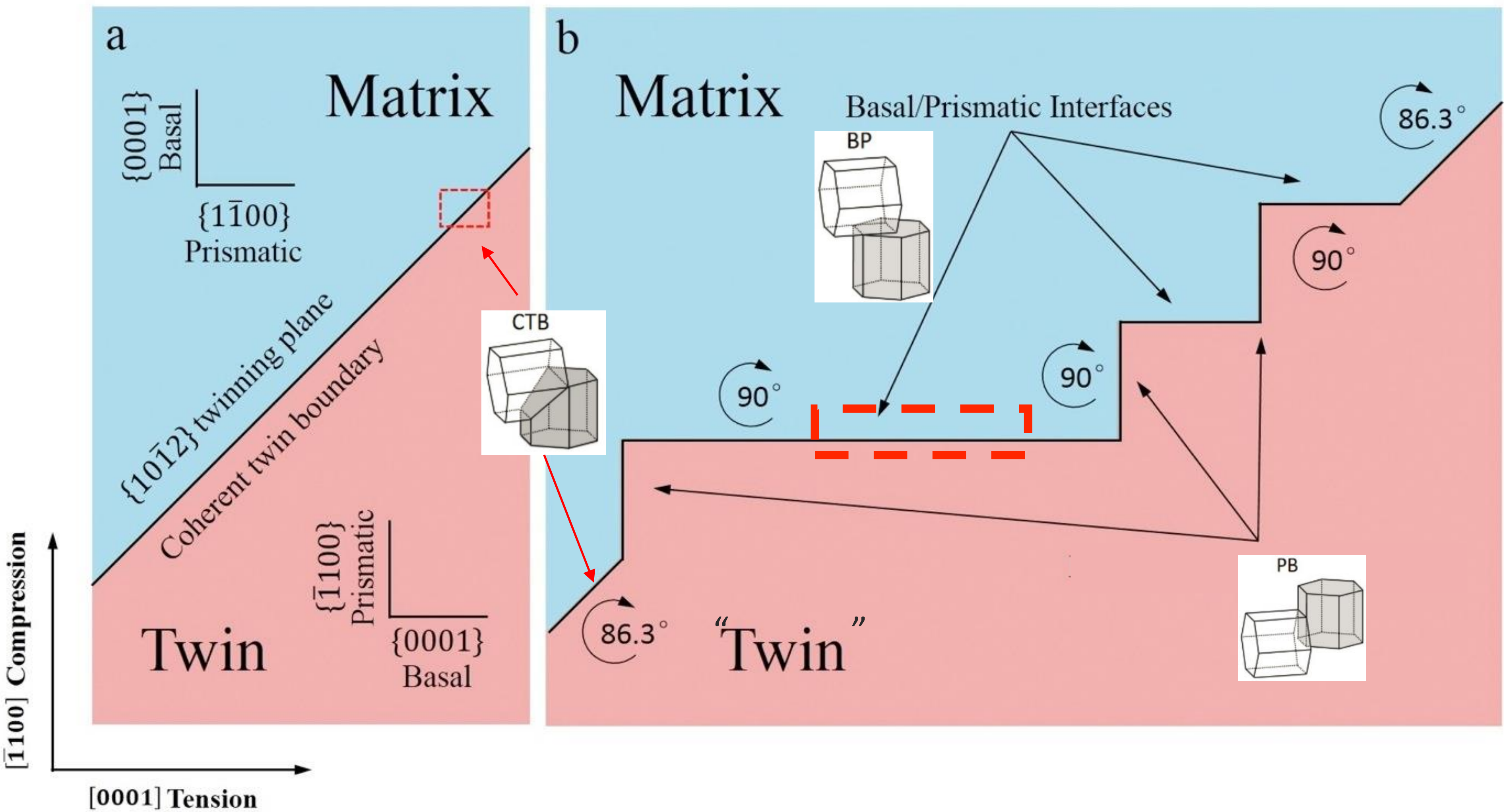
Q#8: Can we explain the 52^o (or any other) inclination angle ?

Why would the boundary look straight (from a distance),

but can have an unexpected angle (when zoomed in)?

The angle seen at lower mag is due to a combination of alternating BP and PB interfaces

The “mixed” boundary can be of any angle; if BP-PB is 50-50, => ~45°, close to {10-12}

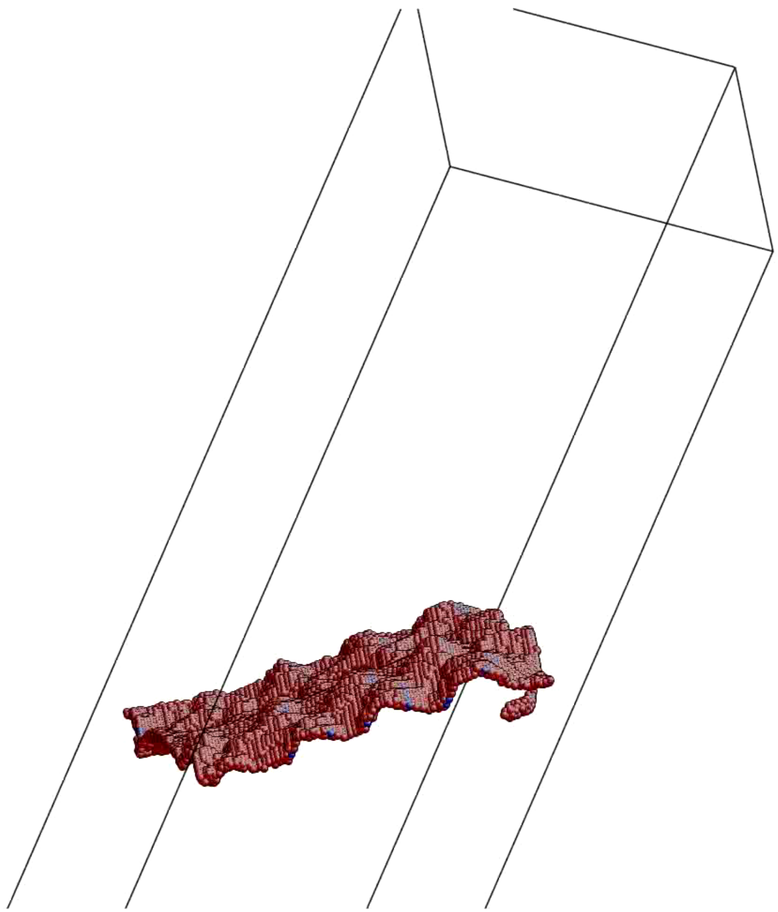


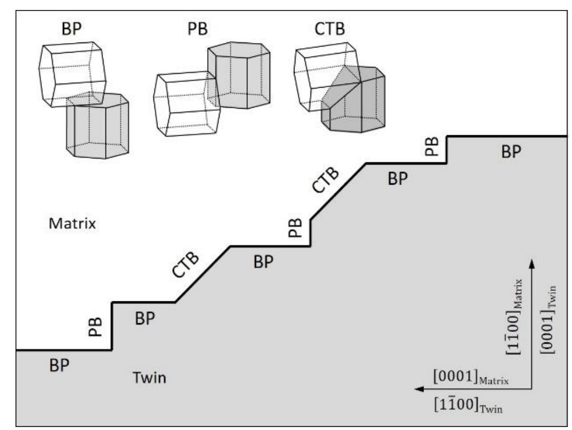
Q#9: Why would this B-P conversion accompany (10-12) twinning?

The B-P action (under high stresses) appears to be an alternative route to quickly produce strain, especially when TB motion becomes sluggish.

“Flexible”: BP interfaces intermixed w/ {10-12} twin boundary

- Only slightly less favorable interface energy (~150 mJ/m^2, < those of other interfaces)
- Kinetically favorable (helps boundary mobility) and alternative pathway in energy landscape





- Only slightly less favorable interface energy (~150 mJ/m^2)
- Kinetically more favorable to switch to B-P action

  (flexible kinetic pathways in energy landscape)

- The stress for {10-12} twinning increases with decreasing sample size due to limited mobility or availability of twinning dislocations (disconnections)

Vol 463 | 21 January 2010 | doi:10.1038/nature08692 nature

LETTERS

Strong crystal size effect on deformation twinning

Qian Yu[1], Zhi-Wei Shan[1,2], Ju Li[3], Xiaoxu Huang[4], Lin Xiao[1], Jun Sun[1] & Evan Ma[1,5]

Deformation twinning[1–6] in crystals is a highly coherent inelastic shearing process that controls the mechanical behaviour of many materials, but its origin and spatio-temporal features are shrouded in mystery. Using micro-compression and *in situ* nano-compression experiments, here we find that the stress required for deformation twinning increases drastically with decreasing sample size of a titanium alloy single crystal[7,8], until the sample size is reduced to one micrometre, below which the deformation twinning is entirely replaced by less correlated, ordinary dislocation plasticity. Accompanying the transition in deformation mechanism, the maximum flow stress of the submicrometre-sized pillars was observed to saturate at a value close to titanium's ideal strength[9,10]. We develop a 'stimulated slip' model to explain the strong size dependence of deformation twinning. The sample size in transition is relatively large and easily accessible in experiments, making our understanding of size dependence[11–17] relevant for applications.

micrometres[7,8,21–24]. It is then interesting to see what will happen when the sample dimensions are reduced to the same scale or even smaller.

We used a bulk square Ti–5 at.% Al single crystal as the starting material, from which all the samples in this study were cut. The experimental details are described in the Methods and in the Supplementary Information. Supplementary Fig. 2 shows the behaviour of the bulk single crystal under [0001] compression. Profuse deformation twinning is seen, in agreement with the literature[24]. In micro-compression tests of pillars with $d \geq 1.0\,\mu m$, almost all the deformed samples showed obvious shearing traces on the surfaces. Examples are shown in Fig. 1a and b. A trace analysis of the $d = 1.0\,\mu m$ micro-pillar showed that the shearing occurred on the $\{11\bar{2}2\}$ plane, which is a common twinning plane in hexagonal-close-packed Ti and its alloys. Electron backscatter diffraction (EBSD) analysis of these deformed pillars provides evidence that deformation

Q#10: What are the take-home messages ?

Take-home messages:

Akin to normal (10-12) DT, basal-prismatic conversion reorients the lattice, migrates the boundary interface and produces the same plastic strain. But it is not straight DT *per se*, providing an alternative and sometimes accompanying pathway for plastic deformation in Mg (especially when DT on that plane encounters difficulties).

A mixture of this local twinning-like lattice reconstruction together with DT is a reason why the “twin boundary” observed in previous experiments can deviate significantly from 43^{o}, while the global orientational relationship is always consistent with (10-12) twinning.

The “reconstruction at BP interface” mechanism may become more active when stresses are high (high strain rate, small sample, …); a high stress (or strain rate) forces faster “twin” boundary movement, which may be enabled by BP transformation.