

# ***Bicrystallography Applications***

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1. Plane grain boundaries / bicrystals possess no less than **nine** independent parameters
2. **Bicrystallography to the rescue** (provides an idealized description at the atomic level, extension of CSL concept to structures, - **grain boundaries are actually not defects in the classical sense**, "special" CSL bicrystals are 2D periodic crystals in 3D – general grain boundaries can be approximated as very large  $\Sigma$  CSLs, similar to quasicrystals)
3. Effective representation in CIF with 2D periodic layer groups and asymmetric unit (for CSL boundaries only)
4. 2D version of simple bicrystallography for didactic purposes (as typical comparisons are with 2D images from Z-STEM, ADF-STEM or HRTEM)
5. Comparisons between related materials - Bärnighausen trees
6. Work in rather slow progress, 3D printed models, open access databases, ...
7. **Comparisons to experimental probe-corrected Z-STEM results**
8. General grain boundaries are quasicrystalline, CSLs with arbitrary large  $\Sigma$  are their approximants
9. Summary and Conclusions

*planar*

**Table 1.1** The nine geometrical degrees of freedom of a grain boundary: six for the interface operation and three for the grain boundary plane orientation and position

	Macroscopic parameters		Microscopic parameters	
	Number	Type	Number	Type
Interface operation	2	$[uvw]$ Rotation axis	2	$\tau_1$ and $\tau_2$ Translation in the grain boundary plane
	1	$\theta$ Rotation angle	1	$\tau_3$ Expansion
Grain boundary plane	2	$n$ Orientation of the grain boundary plane	1	$d < n$ Position of the grain boundary plane

Five are macroscopic parameters. The dimension of each of the four microscopic parameters is less than the grain boundary period

There are five macroscopic degrees of freedom:

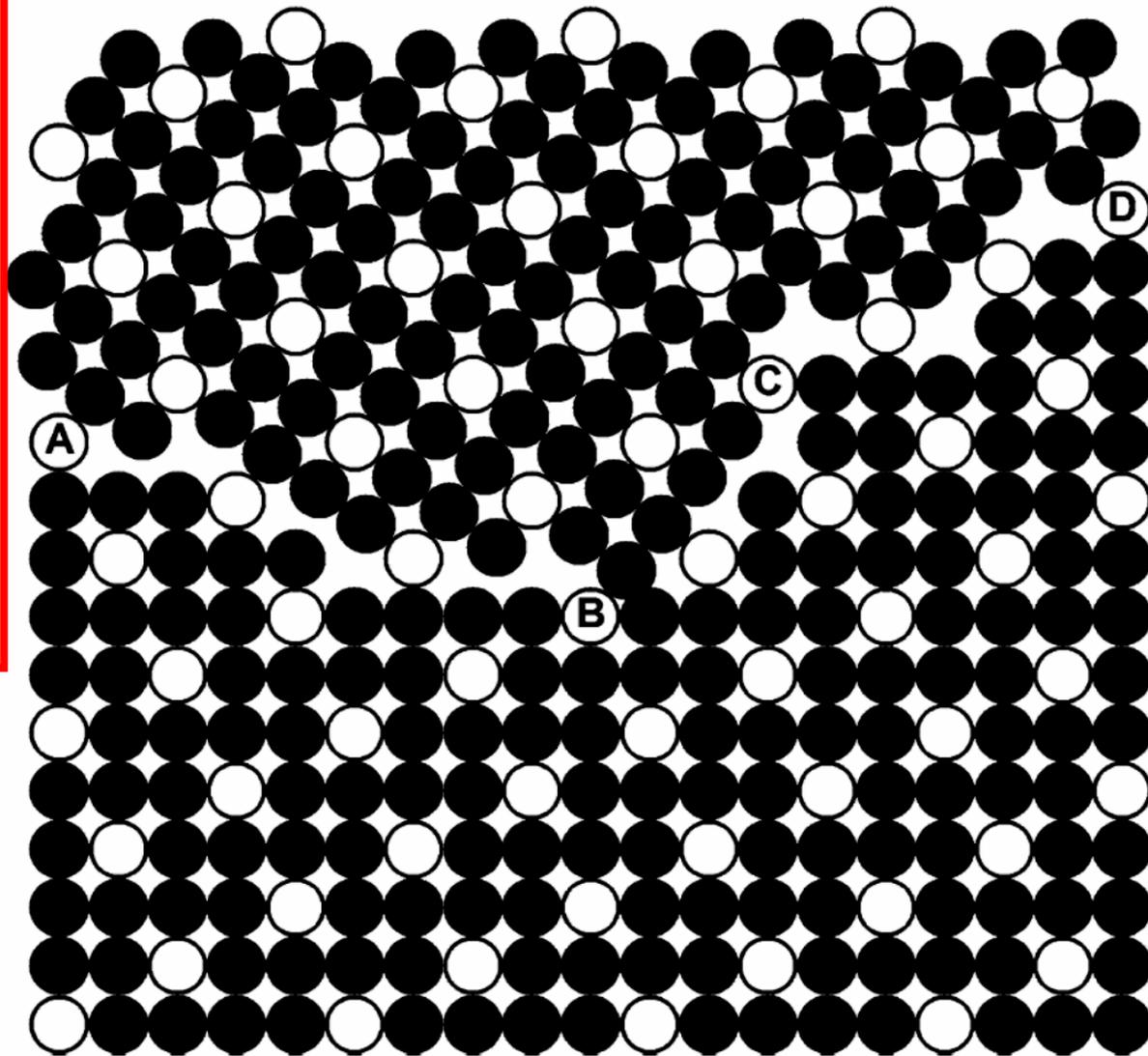
- One for the rotation angle  $\theta$  between the two crystals
- Two for the rotation axis  $[uvw]$  defined by its direction cosines
- Two for the orientation of the grain boundary plane defined by its normal  $n$ .

There are four microscopic degrees of freedom:

- Three for the translation of one crystal with respect to the other: the rigid body translation vector  $\tau$
- One for the vector  $d$  normal to the gain boundary plane that indicates the position of the plane along its normal; the magnitude of  $d$  is necessarily less than the unit vector  $n$ .

With so many free parameters, there is quite a potential for confusion and different notations in the literature.

When more than one atom per lattice point is considered, i.e. essentially all the time, an extra degree of freedom for GB position!



$Pm\bar{3}m$

P. Lejcek,  
Grain  
Boundary  
Segregation  
in Metals,  
Springer,  
2010

**Fig. 2.6** Geometric model of the  $36.87^\circ$  [100] tilt bicrystal with simple cubic lattice. The *circles* represent the positions of individual atoms in misoriented crystals, the *empty circles* denote the coincidence sites. The orientation of the grain boundary varies from  $\{013\}$  symmetrical (A–B), through (001)/(034) asymmetrical (B–C) to  $\{012\}$  symmetrical (C–D) [20]

Probe corrected STEM Z-contrast image courtesy of Nigel D. Browning, PNNL

2 nm  
↔

↔  
2 nm

2 nm  
↔

**SrTiO<sub>3</sub>, cubic primitive lattice but five atoms per lattice points**

Probe corrected Z-STEM image of SrTiO<sub>3</sub>  $\Sigma$  13a (510), tilt boundary 22.62° around [001], bicystallography in 2D predicts both structures, and the “heights” of the possible steps between them as  $n \cdot \frac{1}{4} [510] \cong n \cdot 0.498 \text{ nm}$ , with n integer

$Pm\bar{3}m$

<http://reference.iucr.org/dictionary/Crystal>

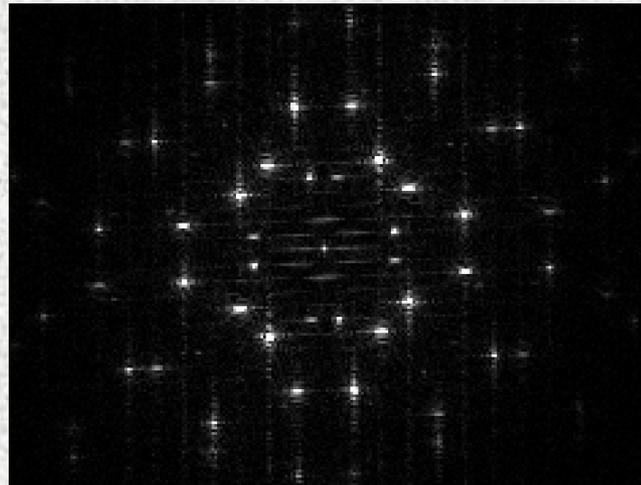
A material is a crystal if it has **essentially** a sharp diffraction pattern. The word **essentially** means that most of the intensity of the diffraction is concentrated in relatively sharp **Bragg peaks**, besides the always present diffuse scattering. In all cases, the positions of the diffraction peaks can be expressed by  $\mathbf{H} = \sum_{i=1}^n h_i \mathbf{a}_i^*$  ( $n \geq 3$ )

Here  $\mathbf{a}_i^*$  and  $h_i$  are the basis vectors of the reciprocal lattice and integer coefficients respectively and the number  $n$  is the minimum for which the positions of the peaks can be described with integer coefficient  $h_i$ . The conventional crystals are a special class, though very large, for which  $n = 3$ . Since 1991

Courtesy  
Nigel D.  
Browning,  
PNNL

$\text{SrTiO}_3$

$\Sigma 13a (510)$



bicrystals are also crystals and so are quasicrystals, a general planar grain boundary is quasicrystalline,  $n = 6$

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doi: 10.1107/97809553602060000112



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# bilbao crystallographic server



<http://www.cryst.ehu.es/>

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**GENPOS** Generators and General Positions of Space Groups

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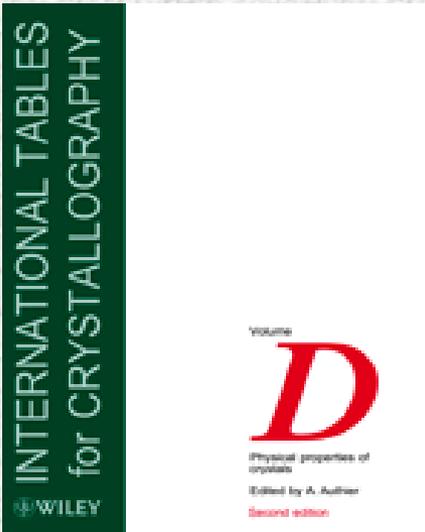


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(iii) *Bicrystals*: This term is mainly used in metallurgy. It refers to the (usually synthetic) intergrowth of two single crystals with a well defined orientation relation. A bicrystal contains a *grain boundary*, which in general is also well defined. Usually, homophase bicrystals are synthesized in order to study the structure and properties of grain boundaries. An important tool for the theoretical treatment of bicrystals and their interfaces is the *coincidence-site lattice* (CSL). A brief survey of bicrystals is given in Section 3.2.2; a comparison with twins and domain structures is provided by Hahn *et al.* (1999). <http://it.iucr.org/Db/itdb.pdf>

**bicrystallography** and the related theory of domain twins are described in less than 10 pages spread over volumes D and E, (quasicrystals are not described at all)

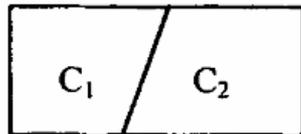
**bicrystallography** and **bicrystal** are mentioned at a total of 27 pages in these two volumes and nowhere else in the whole series, which has currently 5,973 pages

To cite this article: Theo Hahn , Vaclav Janovec & Helmut Klapper (1999)  
 Bicrystals, twins and domain structures - a comparison, *Ferroelectrics*, 222:1,  
 11-21, DOI: [10.1080/00150199908014793](https://doi.org/10.1080/00150199908014793)

To link to this article: <http://dx.doi.org/10.1080/00150199908014793>

TABLE I Bicrystals, twins, domain structures

Given an edifice:

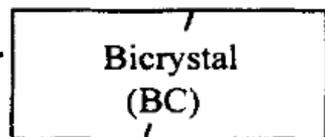


B

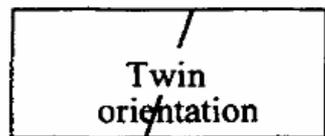
$C_1, C_2$ : Two perfect component crystals with *oriented* structures  $S_1, S_2$  and interface (boundary) B

Three cases:

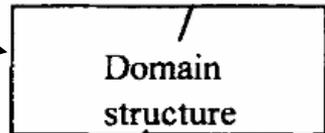
**domain twin**



- $|S_1| \neq |S_2|$ : Heterophase BC
- $|S_1| = |S_2|$ : Homophase BC;
- $|S_1|, |S_2|$ : *non-oriented* structures of  $C_1, C_2$
- No specific relation between  $S_1$  and  $S_2$



- $|S_1| = |S_2|$ : Same non-oriented structures
- "Well-defined" crystallographic relation between  $S_1$  and  $S_2$



- $S_1, S_2$  related by an operation suppressed during the group-subgroup phase transition

from 1988 onwards **D. Gratias** and A. Thalal, connection of general grain boundaries to quasicrystalline state revealed (*Hidden symmetries in general grain boundaries*, *Phil. Mag. Lett.* 57 (1988) 63-68)

Crystal physics theory 1972-85

**Pond**, Vlachavas, Kalonji, Cahn, Gratias, Portier, Janovec, Zikmund, Bollmann

1783 by Romé de l'Isle and countless others

Weiss 1896 Valashek 1921

Klassen-Neklyudova *et al.* 1948

**multiferroics**, Schmid 1994 and countless others

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Volume E  
SUBPERIODIC GROUPS

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### 5.2.5.2. Interfaces in crystalline materials

The scanning for the sectional layer groups is a procedure which finds applications in the theory of *bicrystals* and their *interfaces*. The first of these two terms was introduced in the study of grain boundaries (Pond & Bollmann, 1979; Pond & Vlachavas, 1983; Vlachavas, 1985; Kalonji, 1985). An *ideal bicrystal* is understood to be an aggregate of two semi-infinite crystals of identical structure, meeting at a common planar boundary called the *interface*, where one of the structures, occupying half-space on one side of the interface, is misoriented and/or displaced relative to the other structure occupying the other half-space. The word *interface* is a synonym for a boundary and interfaces considered here are *homophase interfaces*, in contrast with *heterophase interfaces*, where the two structures are different (Sutton & Balluffi, 1995).

An independent study of domain and twin boundaries (Janovec, 1981; Zikmund, 1984) resulted in a terminology parallel to that of the *bicrystallography*. The basic concept here is the *domain twin*, which is technically a particular case of a bicrystal. In this section, we use the terminology of bicrystals, giving the terminology of domain twins, used in the next section, parenthetically.

<http://it.iucr.org/Eb/iteb.pdf>

Layer group **c2'mm'** multiplicity 8, **(x,y,z) (x,-y,z) (x,y,-z) (x,-y,-z), (0,0,0)+ (1/2,1/2,0)+**,  
 (modern standard notation cm2m, L35), **asymmetric GB unit just 6 atoms for W**

```

data_123
_chemical_name_systematic 'Tungsten  $\Sigma$  5 (310) [001] with mirror '
_cell_length_a          10.008
_cell_length_b          3.165
_cell_length_c          5.004
# no periodicity along c, specified length 1/2 of unit vector due to z, -z pairs
_cell_angle_alpha      90
_cell_angle_beta       90
_cell_angle_gamma     90
_symmetry_space_group_name_H-M 'c2'mm', monochrome L35, cm2m'
loop_
  _symmetry_equiv_pos_as_xyz
  
```

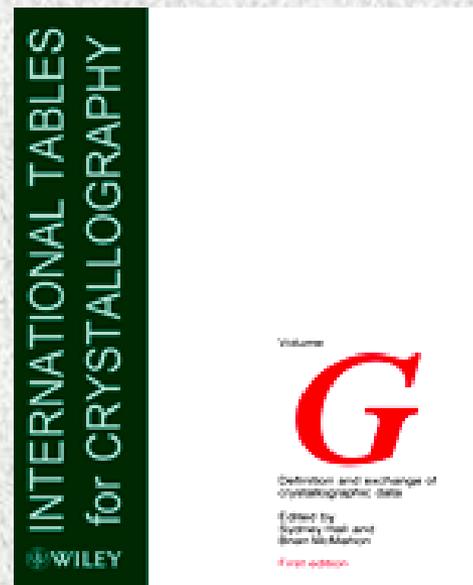
```

...
loop_
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
  
```

**W 2 a 1/2 0 0**

**W 4 c 0 0 1**

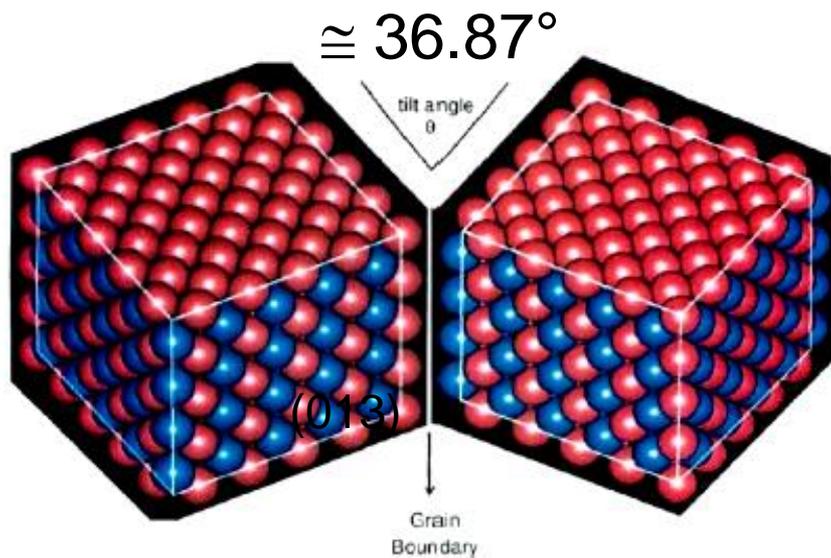
**+ only four more atoms in order to fill up one GB unit cell (with  $c_{GB} = \sqrt{0.5 \cdot \Sigma} \cdot a_W$  width on both sides of the interface, ... in any case only a small number of atoms in this loop for complete description of one unit cell of 2D periodic grain boundary layer in 3D**



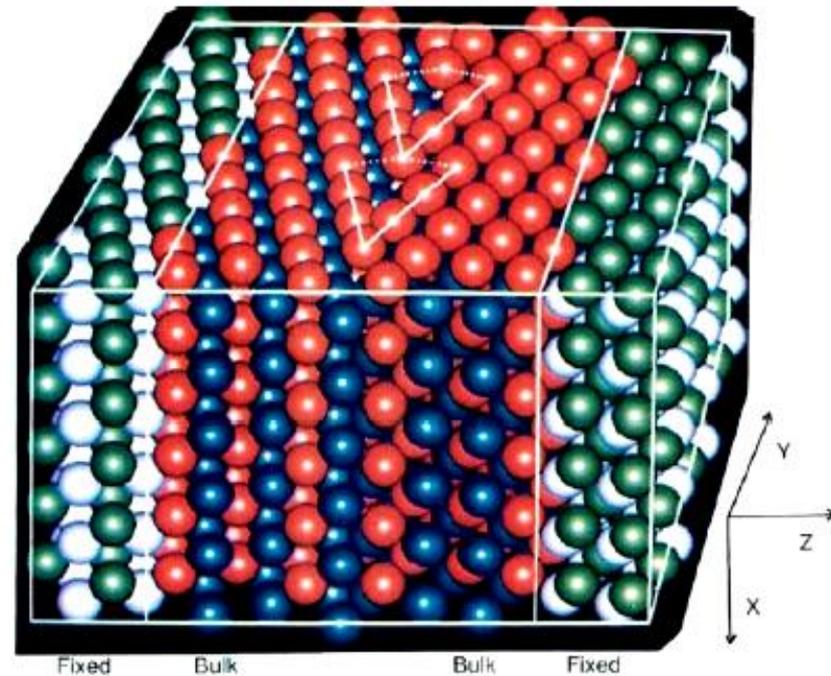
**1080 W atoms in 5 x 4 x 3 unit cells (approx. 19.3 nm<sup>3</sup>) of this grain boundary by specification of ± 10 extra planes with atoms parallel to interface in CIF**

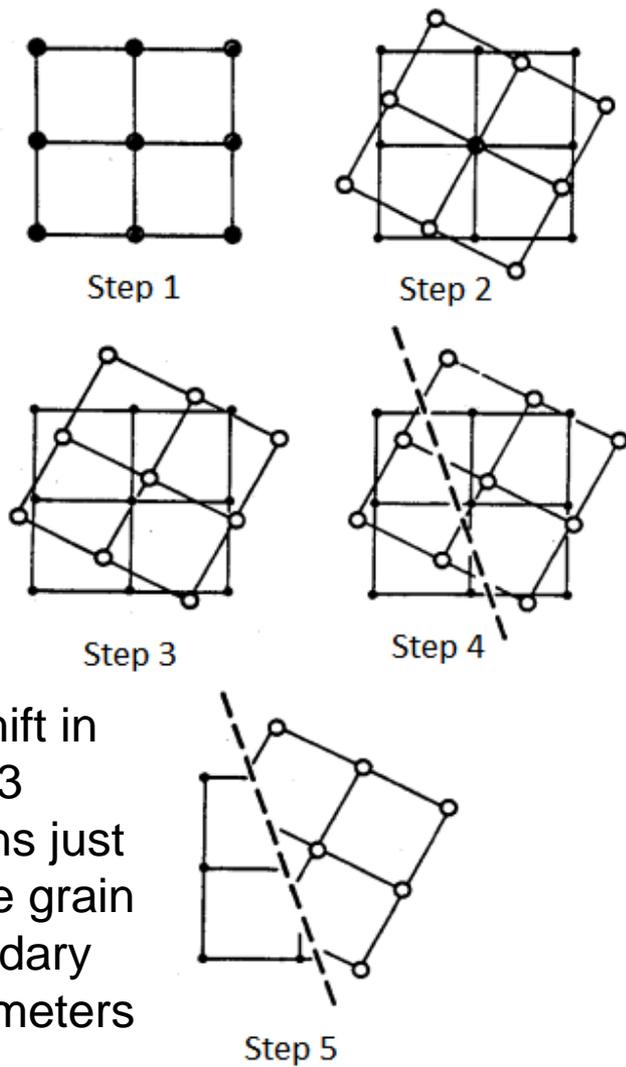
That sure is progress for people who want to run large simulations ...

$\sim 1000$  atoms  $\Sigma 5$  (031) [100]

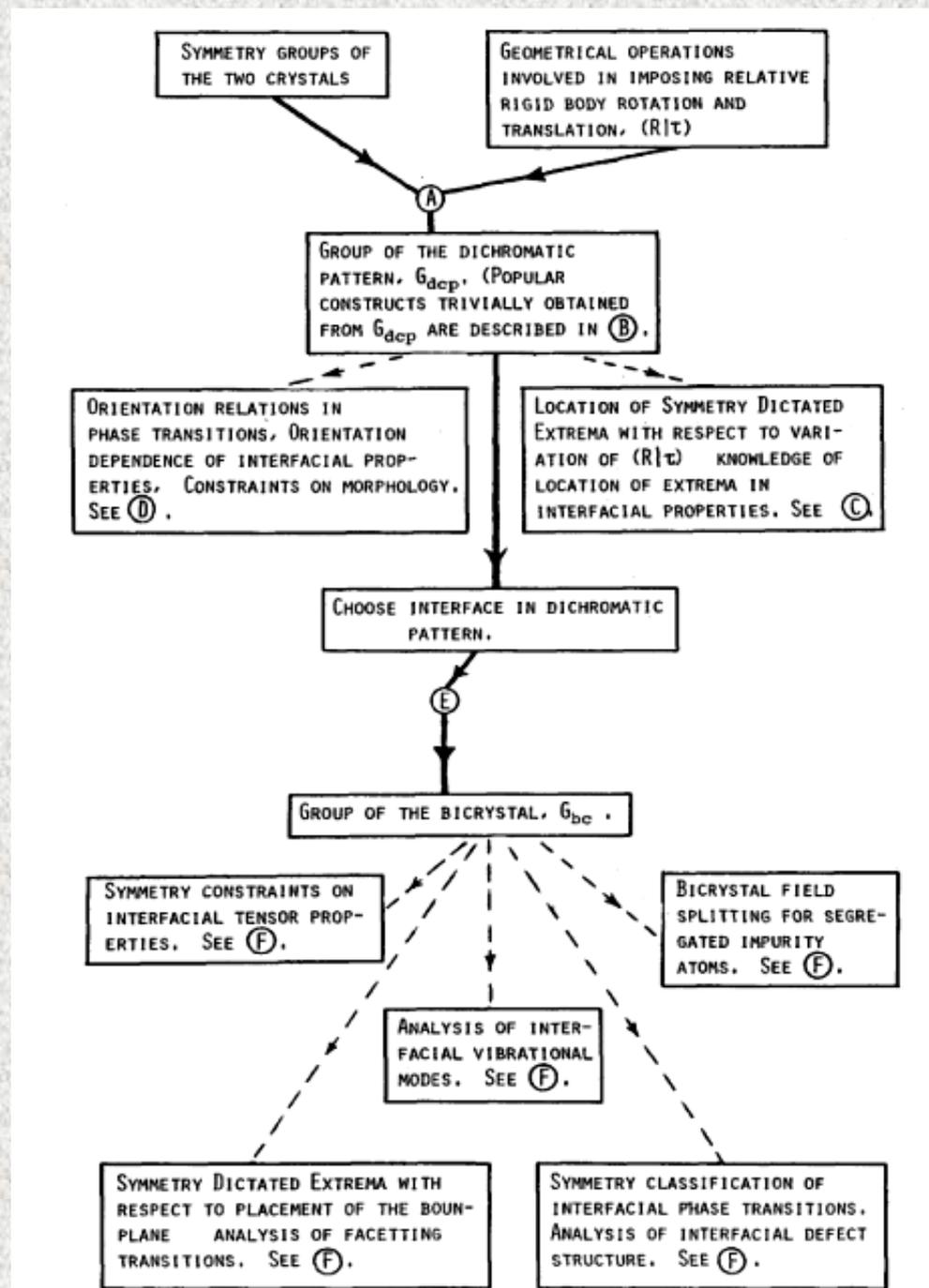


fcc structure, e.g. Cu



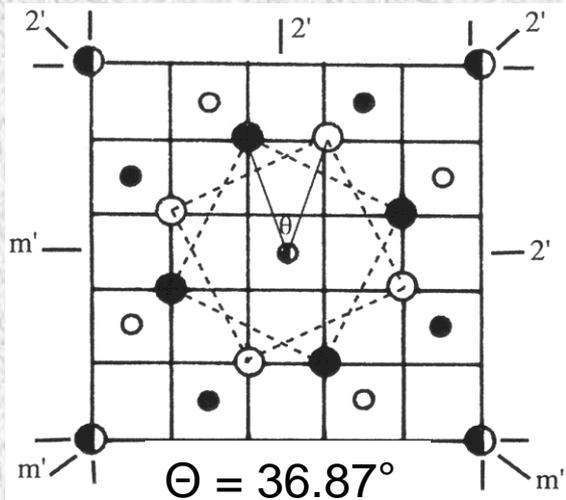


no shift in step 3 means just 6 free grain boundary parameters

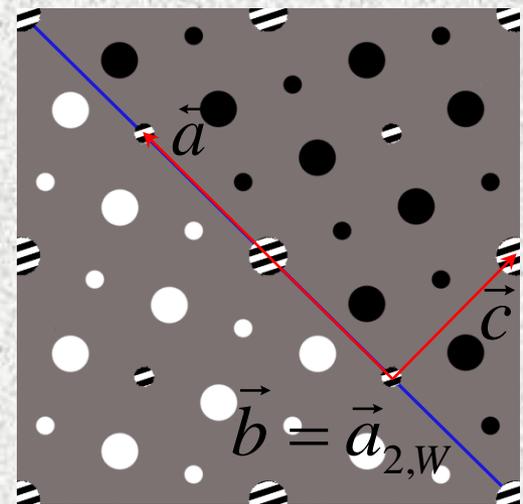
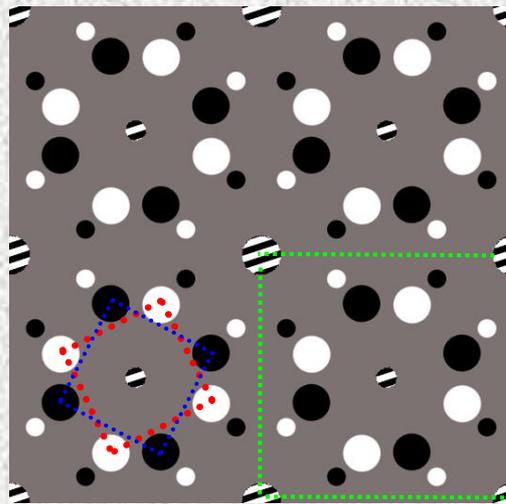


G. Kalonji, J. Phys. Colloq. **46** (1985) C4-249, bicrystallography procedure, Shubnikov-Curie Principle relates bicrystallography to physical properties

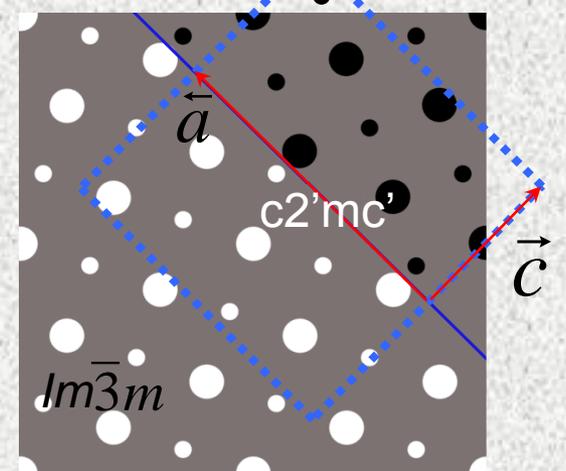
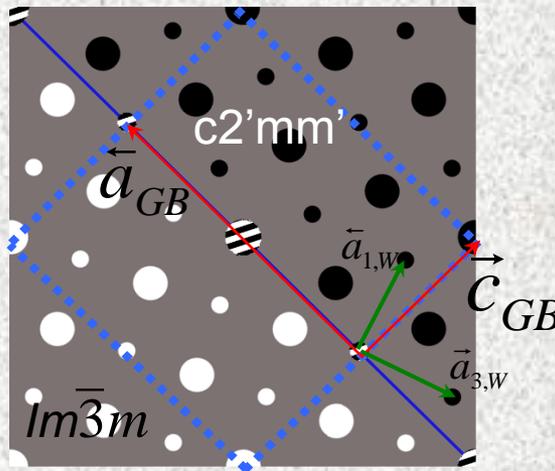
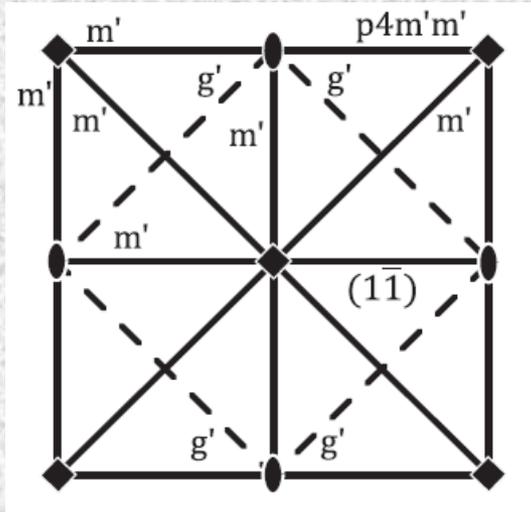
14/mm'm for an bcc metal, e.g. W, dichromatic pattern / complex



$\Theta = 2 \arctan(1/3)$



$\Sigma$  5 tilt boundary with (310) planes can have two types of “symmetric” structures, 18 atoms 2D periodic (incl. centering)



2D version of bicystallography:  
P. Moeck et al., *Crystal Res. Technol.* **49** (2014) 708

layer group  $c2'mm'$   
projects to  $\mu 11m'$

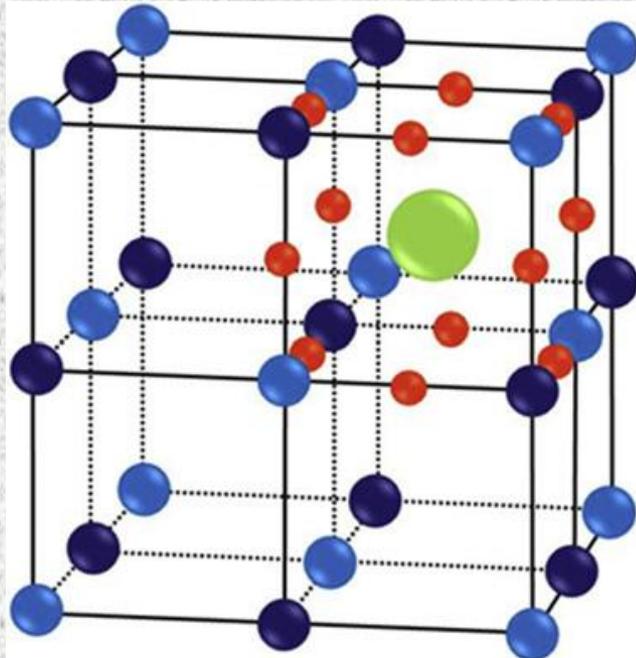
layer group  $c2'mc'$   
projects to  $\mu 11g'$

# Symmetries of migration-related segments of all [001] coincidence site lattice tilt boundaries in (001) projection for all holohedral cubic materials

Peter Moeck<sup>1,\*</sup>, Bryant W. York<sup>2</sup>, and Nigel D. Browning<sup>3</sup>

Table 1 Symmetry reductions due to the two-step sectioning procedure as function of the position of the sectioning line in figure 4.

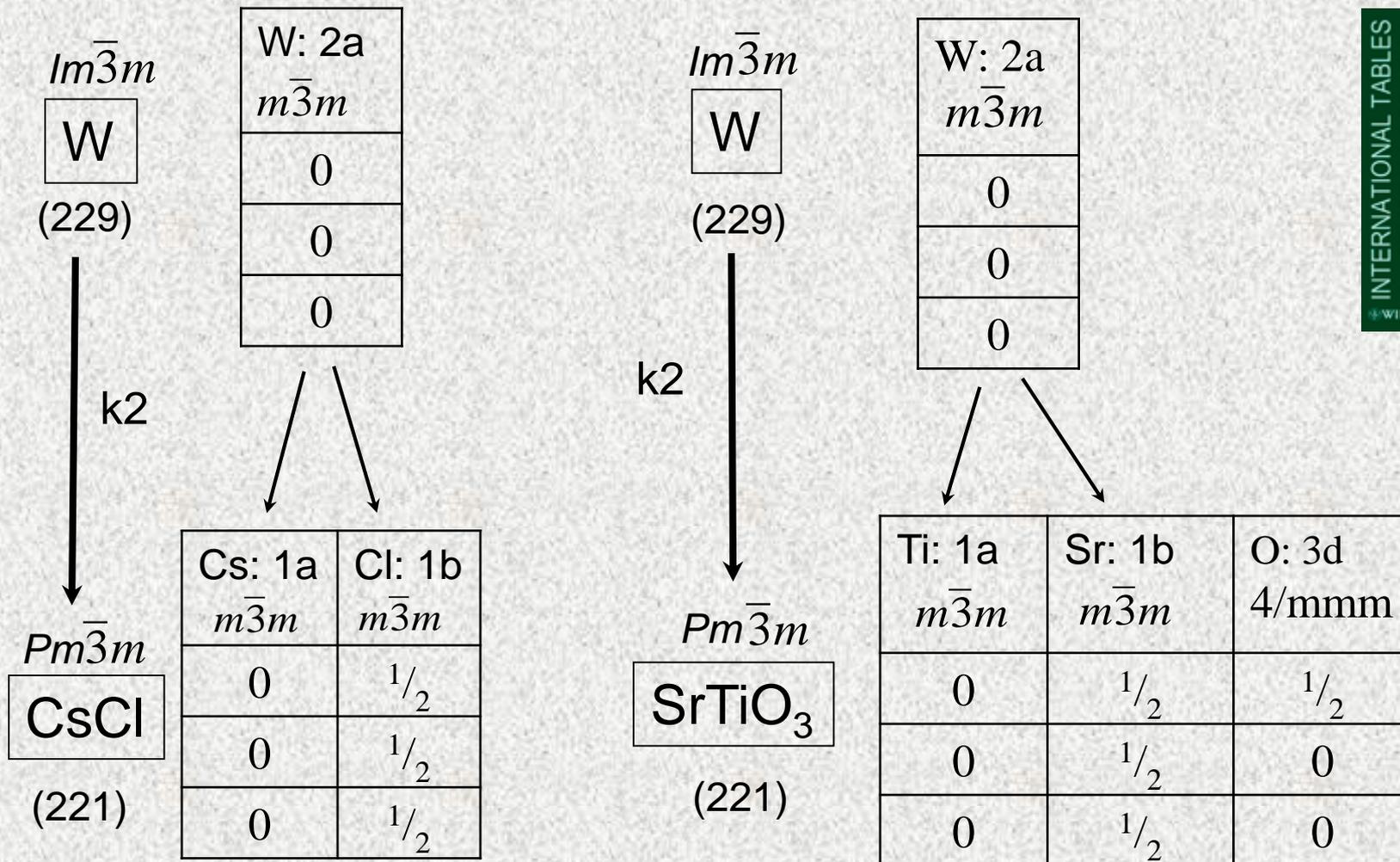
Type 1	Type 2	Type 3
$p4m'm'$	$p4m'm'$	$p4m'm'$
$/i2m'm'$	$/i2m'g'$	$/i1m'1$
$/i11m'$	$/i11g'$	$/i1$



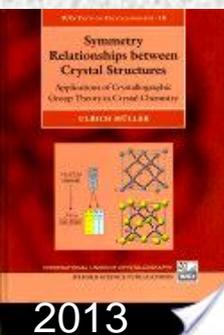
Materials	Space Group				
SrTiO <sub>3</sub>	$Pm\bar{3}m$	Sr	O	Ti	Ti
ReO <sub>3</sub>	$Pm\bar{3}m$	□	O	Re	Re
CeO <sub>2</sub>	$Fm\bar{3}m$	O	□	Ce	□
Mg <sub>2</sub> Sn	$Fm\bar{3}m$	Mg	□	Sn	□
MgO	$Fm\bar{3}m$	□	□	Mg	O
FCC	$Fm\bar{3}m$	□	□	metal	□

***all related by Bärnighausen trees***

all [001] tilt boundaries in all of these materials will be related - “*look similar*”, there will always be two types of [001] tilt GB (one with mirror- and one with glide-symmetry), experimental confirmation: W. Tong et al., *Acta Materialia* **61** (2013) 3392–3398



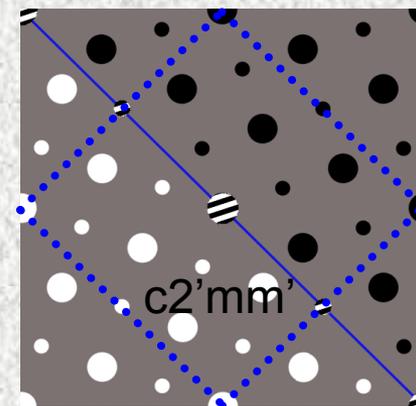
*Bärnighausen trees for structurally related monocystals, standard in modern crystal chemistry, greatly facilitated by the International Tables of Crystallography vol. A, vol. A1, <http://www.cryst.ehu.es/>, IUCr's on-line Symmetry Database, and <http://nanocrystallography.net>*



$\Sigma 5$  (310) [001] and layer symmetry  $p2'mm'$

$c2'mm'$   
 $W_{GB}$   
 (L35)

<b>W: 2a</b> $2'mm'$	<b>W: 4c</b> .m.				
$1/2$	$1/5$	$2/5$	$1/10$	$3/10$	0
0	0	$1/2$	$1/2$	0	0
0	$1/5$	$2/5$	$3/5$	$4/5$	1



$\Sigma 5$  (310) [001]

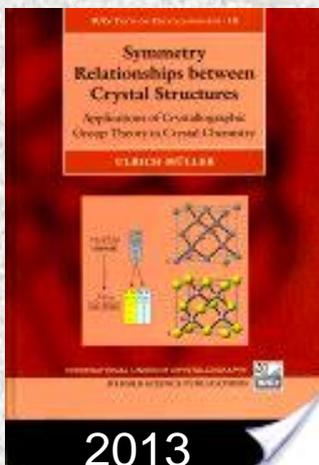
k2

<b>Cs: 1a</b> $2'mm'$	<b>Cl: 1c</b> $2'mm'$	<b>Cs: 2g</b> .m.	<b>Cl: 2g</b> .m.	<b>Cl: 2g</b> .m.	<b>Cs: 2g</b> .m.	<b>Cl: 2g</b> .m.	<b>Cs: 2g</b> .m.	<b>Cs: 2g</b> .m.	<b>Cl: 2g</b> .m.	<b>Cs: 2g</b> .m.	<b>Cl: 2g</b> .m.
$1/2$	0	$1/5$	$7/10$	$2/5$	$9/10$	$1/10$	$6/10$	$3/10$	$4/5$	0	$1/2$
0	$1/2$	0	$1/2$	$1/2$	0	$1/2$	0	0	$1/2$	0	$1/2$
0	0	$1/5$	$1/5$	$2/5$	$2/5$	$3/5$	$3/5$	$4/5$	$4/5$	1	1

$p2'mm'$

$CsCl_{GB}$

(L23)



*Bärnighausen trees for **structurally related bicrystals**, just a straightforward extension of common practice from crystallography of monocrystals, greatly facilitated by the International Tables of Crystallography Vol. E, <http://www.cryst.ehu.es/>, and <http://nanocrystallography.net>*



Structure of the equivalent boundary, derived from the symmetry decent  $W$  to  $\text{SrTiO}_3$  according to the rules of the Bärnighausen tree

Ti: 1a 2'mm'	Sr: 1c 2'mm'	Ti: 2g .m.	Sr: 2g .m.	O: 1a and 2g <b>continued</b>								
1/2	0	2/10	7/10	4/10	9/10	1/10	6/10	3/10	8/10	0	1/2	<b>below</b>
0	1/2	0	1/2	0	1/2	0	1/2	0	1/2	0	1/2	<b>total of</b>
0	0	1/5	1/5	2/5	2/5	3/5	3/5	4/5	4/5	1	1	<b>16</b>

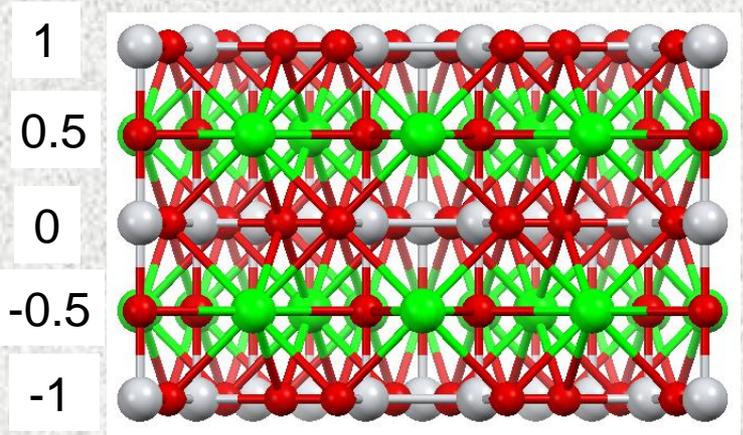
O: 1a .m.	O: 2g .m.														
1/2	1/20	2/10	3/20	5/20	7/20	4/10	9/20	1/10	11/20	13/20	3/10	15/20	0	17/20	19/20
1/2	0	1/2	0	0	0	1/2	0	1/2	0	0	1/2	0	1/2	1/2	0
0	3/10	1/5	9/10	5/10	1/10	2/5	7/10	3/5	3/10	9/10	4/5	1/2	1	1/10	7/10

28 positions need to be specified for one asymmetric unit in grain boundary unit cell with  $\sum 5 (310) [001]$  and layer symmetry  $p2'mm'$

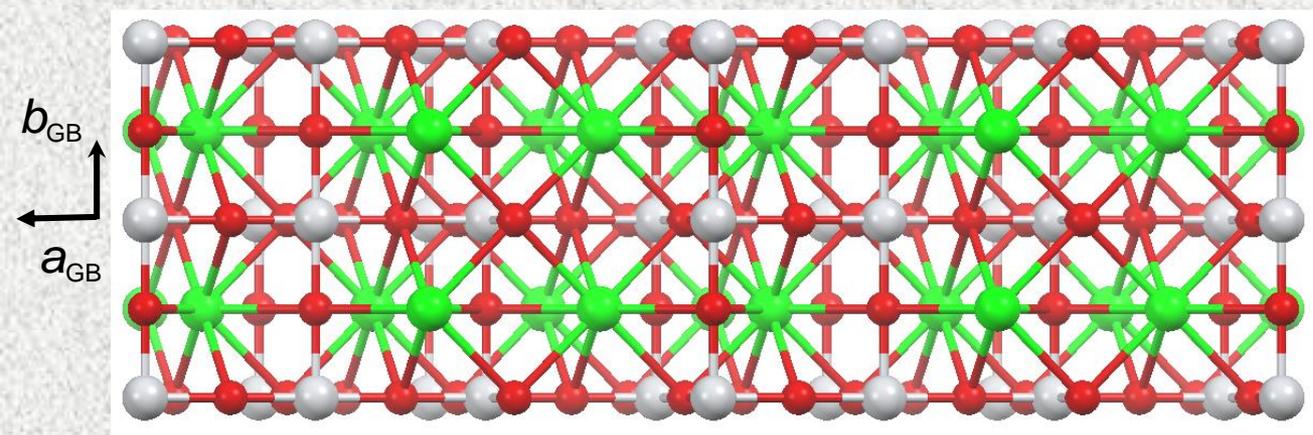
$\Sigma 5 (310)$   
 $[001]$  tilt  
 boundary in  
 $\text{SrTiO}_3$

*gray*: Ti at height -1, 0 and 1  
*red*: O at height -1, -0.5, 0, 0.5 and 1  
*green*: Sr at height -0.5 and +0.5

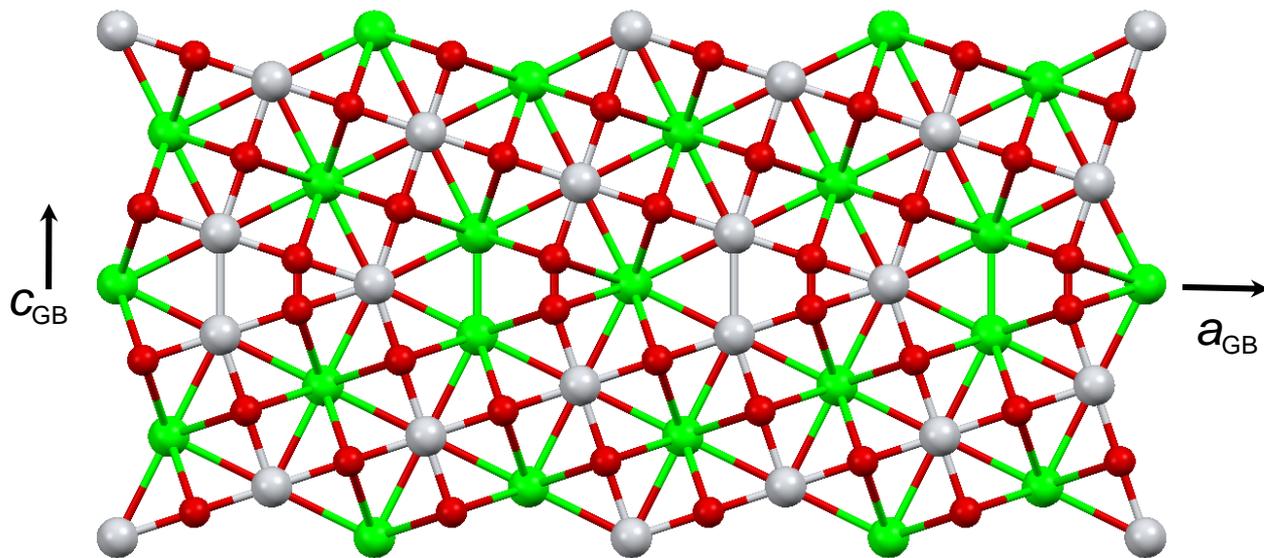
*with "depth clues", i.e. balls with more intense colors are supposed to be closer to the observer*



projection along GB  $a$ -direction, i.e. the grain boundary periodicity, mirrors in both the grain boundary plane (vertical line in the middle of the sketch) and the  $\{001\}$  and  $\{002\}$  planes of  $\text{SrTiO}_3$  (perpendicular to that line) are visible, two-fold axis along GB- $a$  is viewed edge on



projection along GB  $c$ -direction, mirror in  $\{001\}$  and  $\{002\}$  planes of  $\text{SrTiO}_3$  are visible (horizontal lines)



Projection along [010]

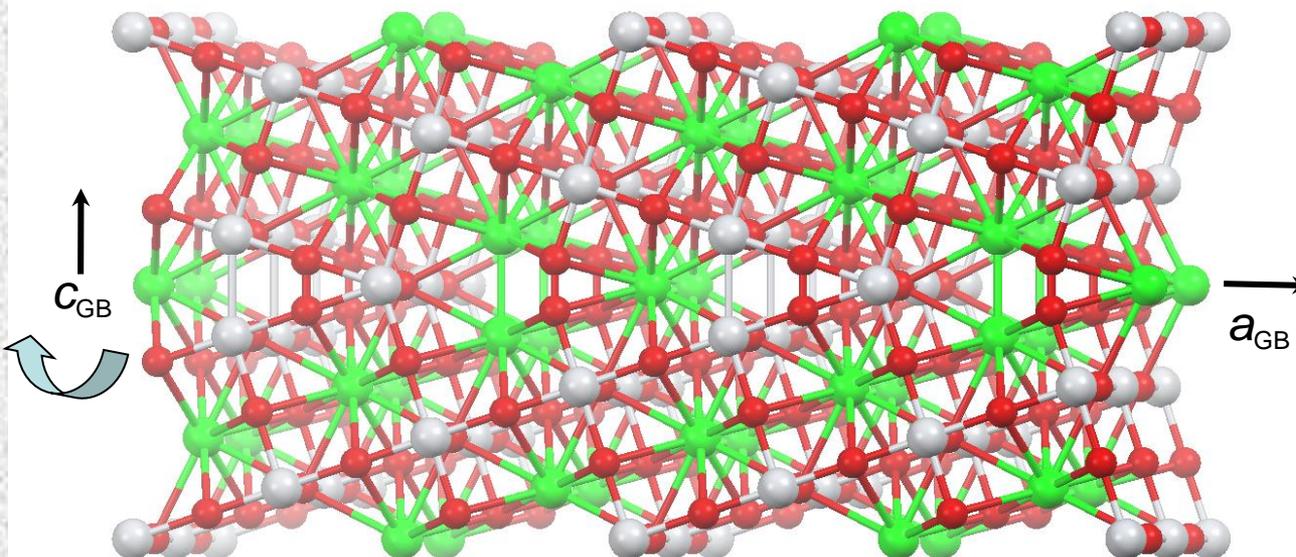
*gray*: Ti at height 0 and 1

*red*: O at height 0 and 1  
(at height 0.5 obscured by Ti)

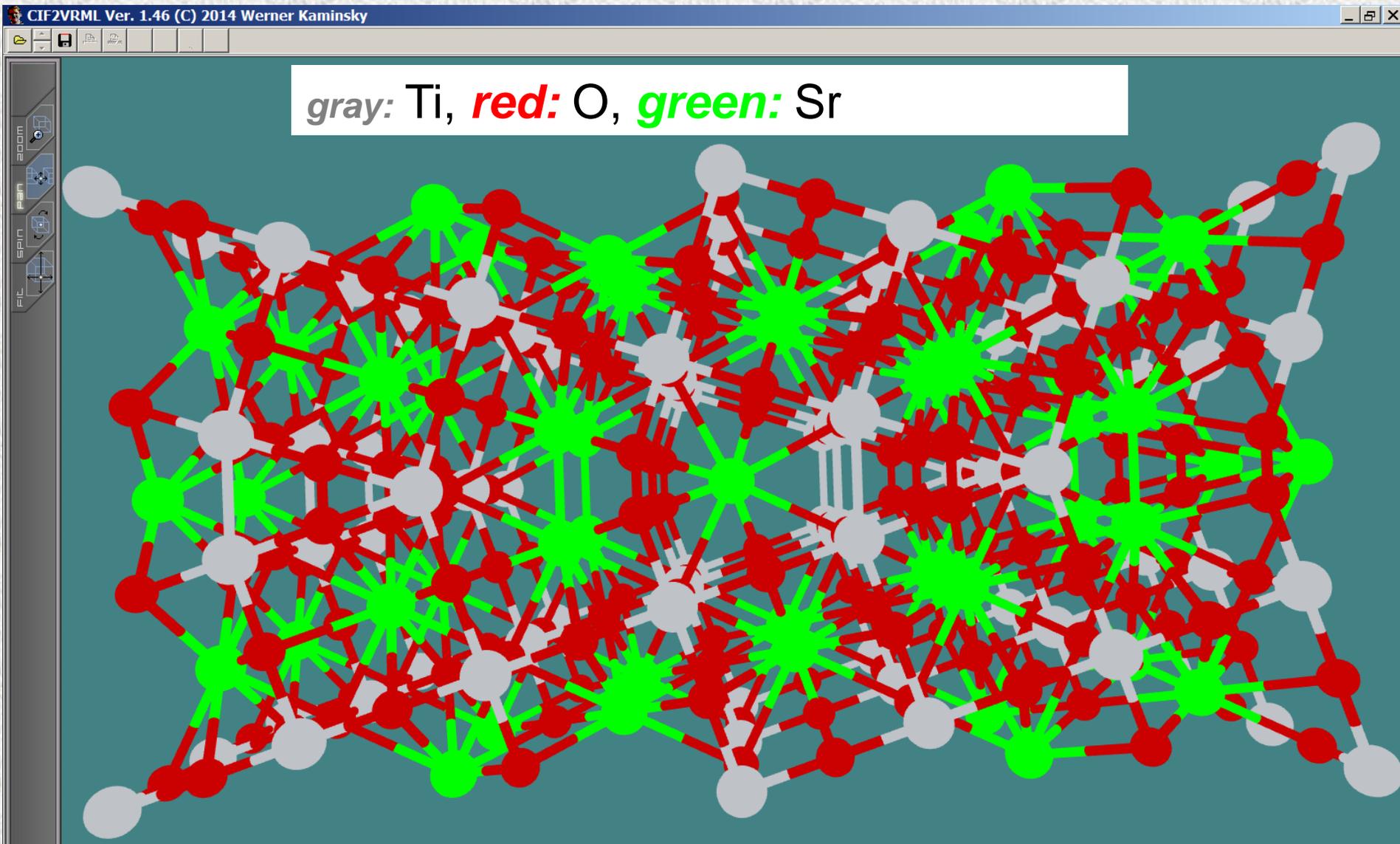
*green*: Sr at height 0.5

projected along GB *b*-direction, total of 364 atoms (2 x 2 x 2 GB unit cells). If display program would understand layer symmetries, only 28 atom positions would need to be specified

$\Sigma 5 (310)$   
[001] tilt  
boundary  
in  $\text{SrTiO}_3$

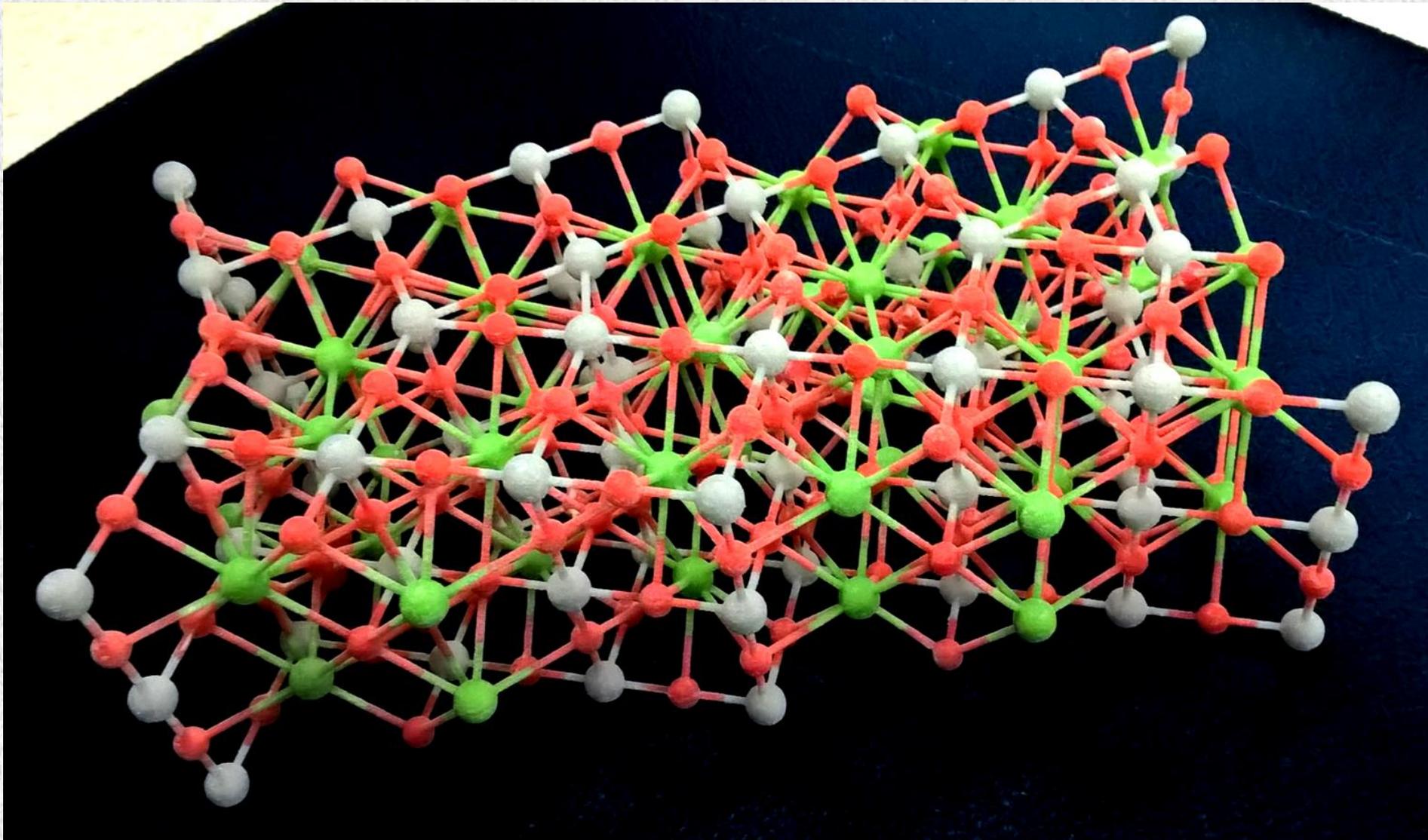


Viewing direction  $15^\circ$  off [010]<sub>GB</sub>, rotated around [001]<sub>GB</sub> anticlockwise with “depth clues”, i.e. “balls” with more intense colors are supposed to be closer to the observer



\*.wrl file of  $\Sigma 5$  (310) [001] in SrTiO<sub>3</sub> ready to be send to 3D color printer

364 plastic balls, 2 x 2 x 2 GB unit cells



out of an approx. \$70k color printer:  $\Sigma 5$  (310) [001] in SrTiO<sub>3</sub>



# Interactive Databases

Open Access Crystallography

3D Print Files

Interactive Databases

COD Mirror

EDU-COD

Crystal Morphology Database

Nano-Crystallography Database

Wiki Crystallography Database

Nano-Crystallography Group

Tools

IYCr 2014

Crystallography in the World

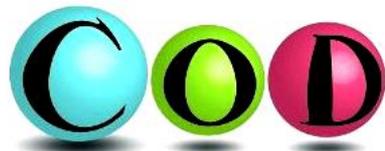
Facets of Electron  
Crystallography 2010

MRS Tutorial and Seminars  
2009

Links

Login

Upload



**Crystallography Open Database** [Mirror, modified search interface and JSmol/Jmol displays] [Search and view](#)



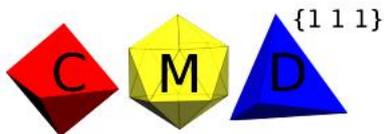
**Wiki Crystallography Database**  
[Search and view](#)



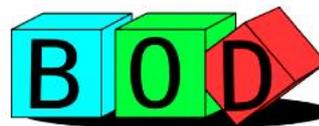
**Educational COD offshoot** [Search and view](#)



**Nano-Crystallography Database**  
[Search and view](#)



**Crystal Morphology Database**  
[Search and view](#)



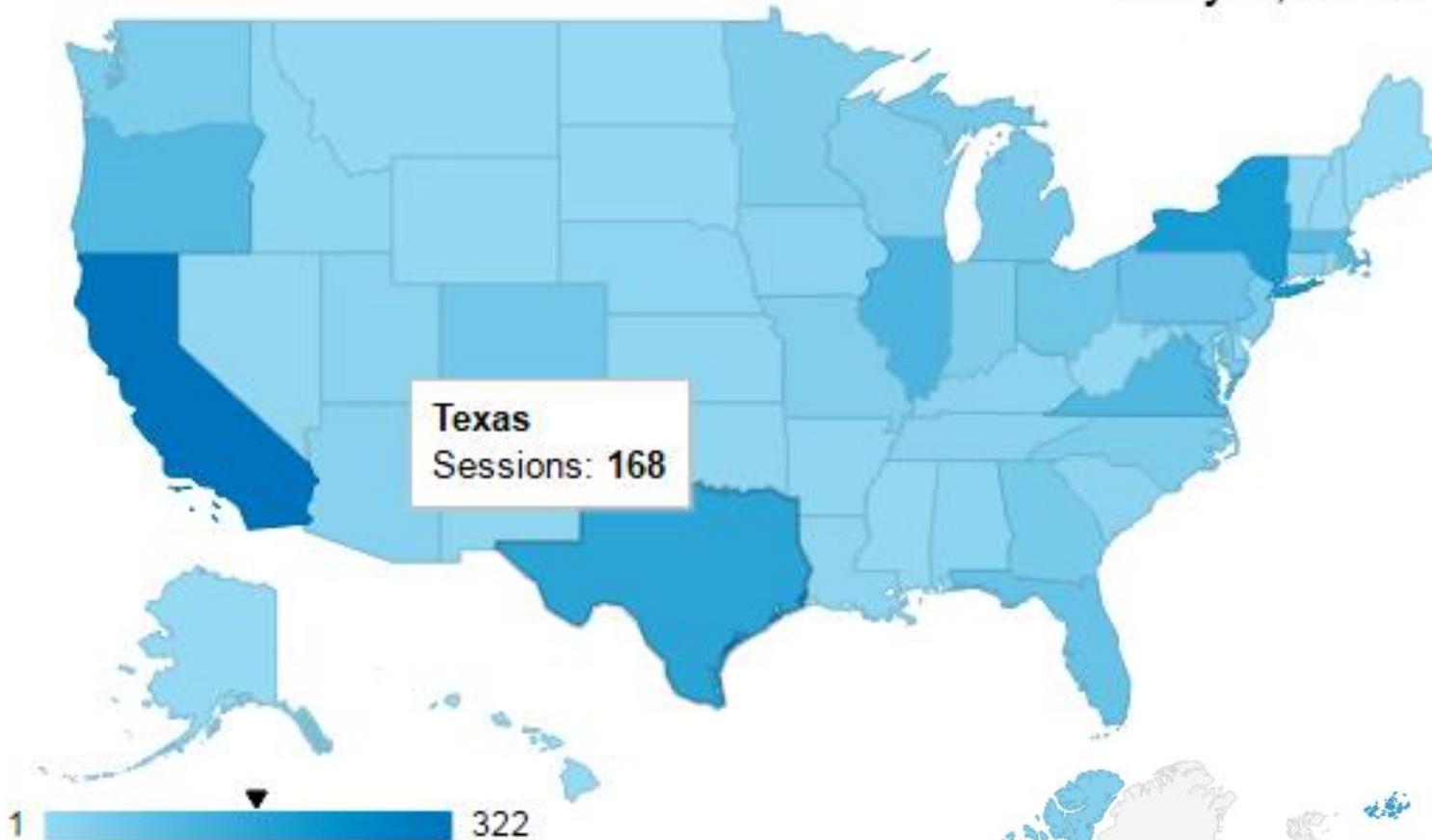
**Bicrystallography Open Database** coming soon

Several crystallography databases are offered for browsing. You can search the databases, download and display the contained [Crystallographic Information Files](#) (CIFs),

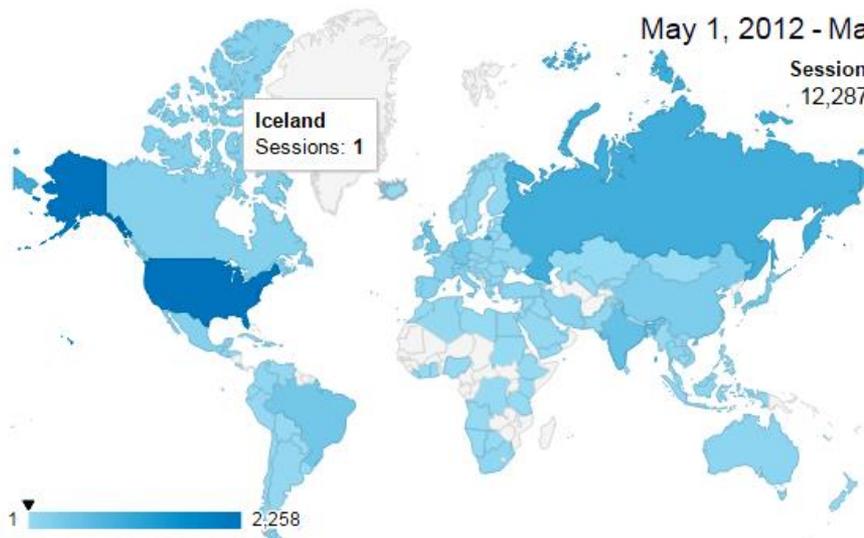
nanocrystallography.research.pdx.edu/search/ncd

ncoded crystal structures and morphologies.

Sessions  
2,258



May 1, 2012 - May 1, 2016  
Sessions  
12,287



Country	Sessions	% New Sessions	New Users
	<b>9,980</b>	<b>93.45%</b>	<b>9,326</b>
	<small>% of Total 100.00% (9,980)</small>	<small>Avg for View 93.42% (0.03%)</small>	<small>% of Total 100.03% (9,323)</small>
1.  United States	<b>2,258</b> (22.63%)	93.58%	2,113 (22.66%)
2.  Russia	<b>951</b> (9.53%)	88.33%	840 (9.01%)
3.  (not set)	<b>886</b> (8.88%)	99.55%	882 (9.46%)
4.  India	<b>545</b> (5.46%)	93.21%	508 (5.45%)
5.  Brazil	<b>395</b> (3.96%)	94.43%	373 (4.00%)
6.  United Kingdom	<b>382</b> (3.83%)	95.55%	365 (3.91%)
7.  Germany	<b>380</b> (3.81%)	92.11%	350 (3.75%)
8.  Japan	<b>312</b> (3.13%)	91.67%	286 (3.07%)
9.  China	<b>269</b> (2.70%)	94.80%	255 (2.73%)
10.  Italy	<b>215</b> (2.15%)	94.42%	203 (2.18%)

Probe corrected STEM Z-contrast image courtesy of Nigel D. Browning, PNNL

$p2'mm'$  a gray group

$\mu 11m'$

2 nm



$\mu 11m'$

2 nm



2 nm

$\mu 11g'$

$p2'm'b'$

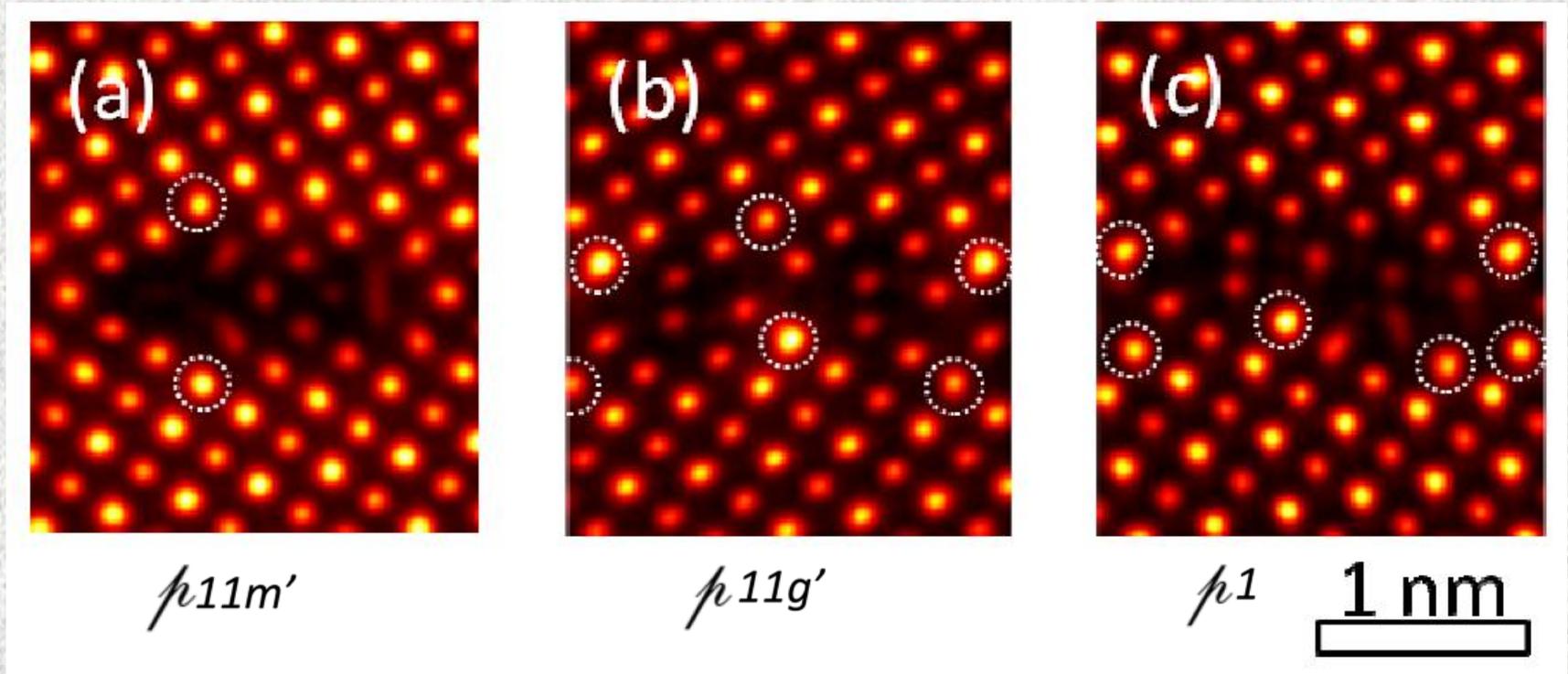
a genuine black white (polar) group, polar properties can exist across the interface

$SrTiO_3$ , cubic primitive lattice but five atoms per lattice points, **Eu/W doped**

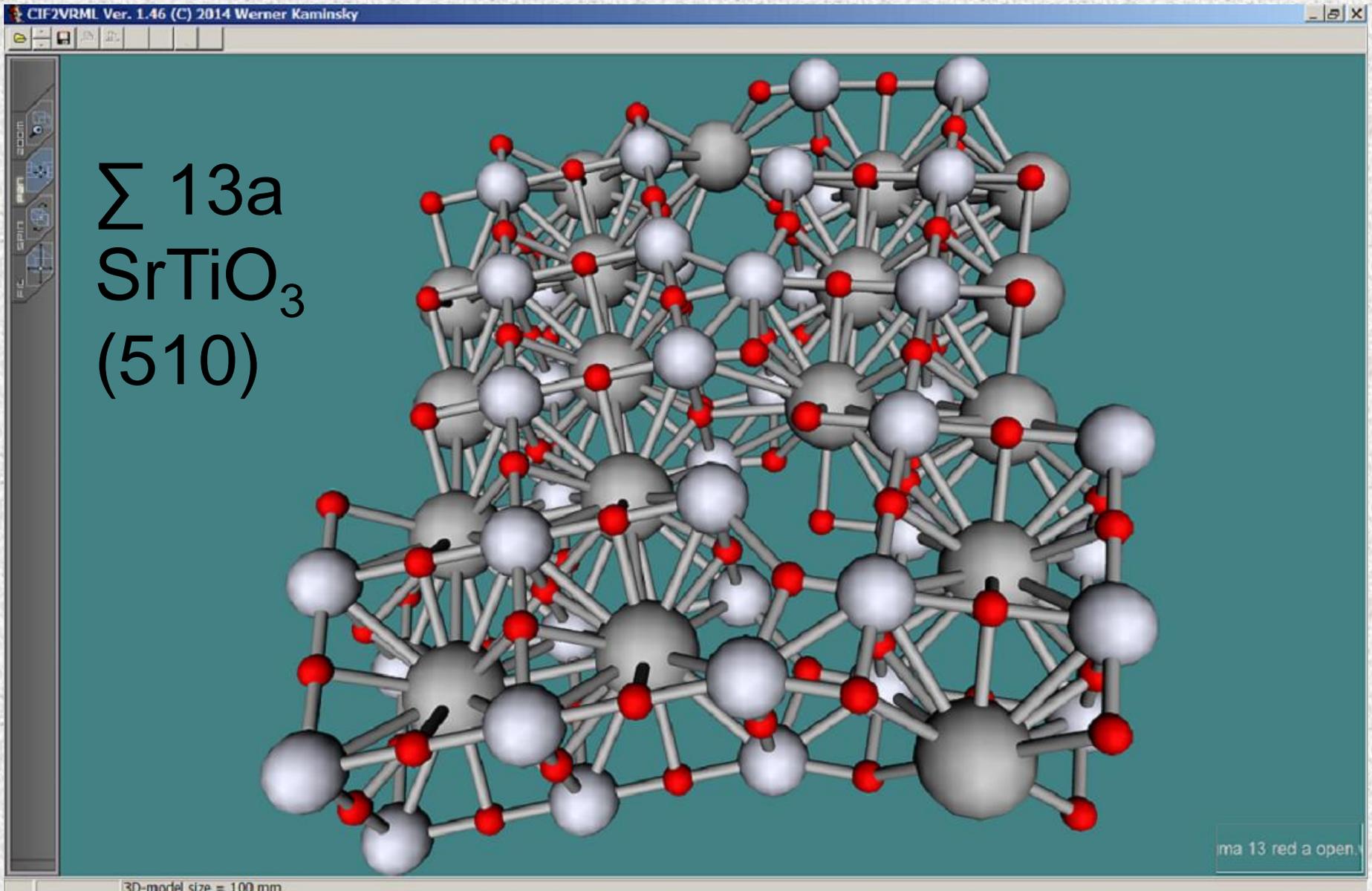
probe-corrected Z-STEM image of  $SrTiO_3 \Sigma 13a (510)$ , tilt boundary  $22.62^\circ$  around  $[001]$ , bicystallography in 2D predicts both structures, and the “heights” of the possible steps between them as  $n \cdot 1/4 [510] \cong n \cdot 0.498 \text{ nm}$ , with n integer

$Pm\bar{3}m$

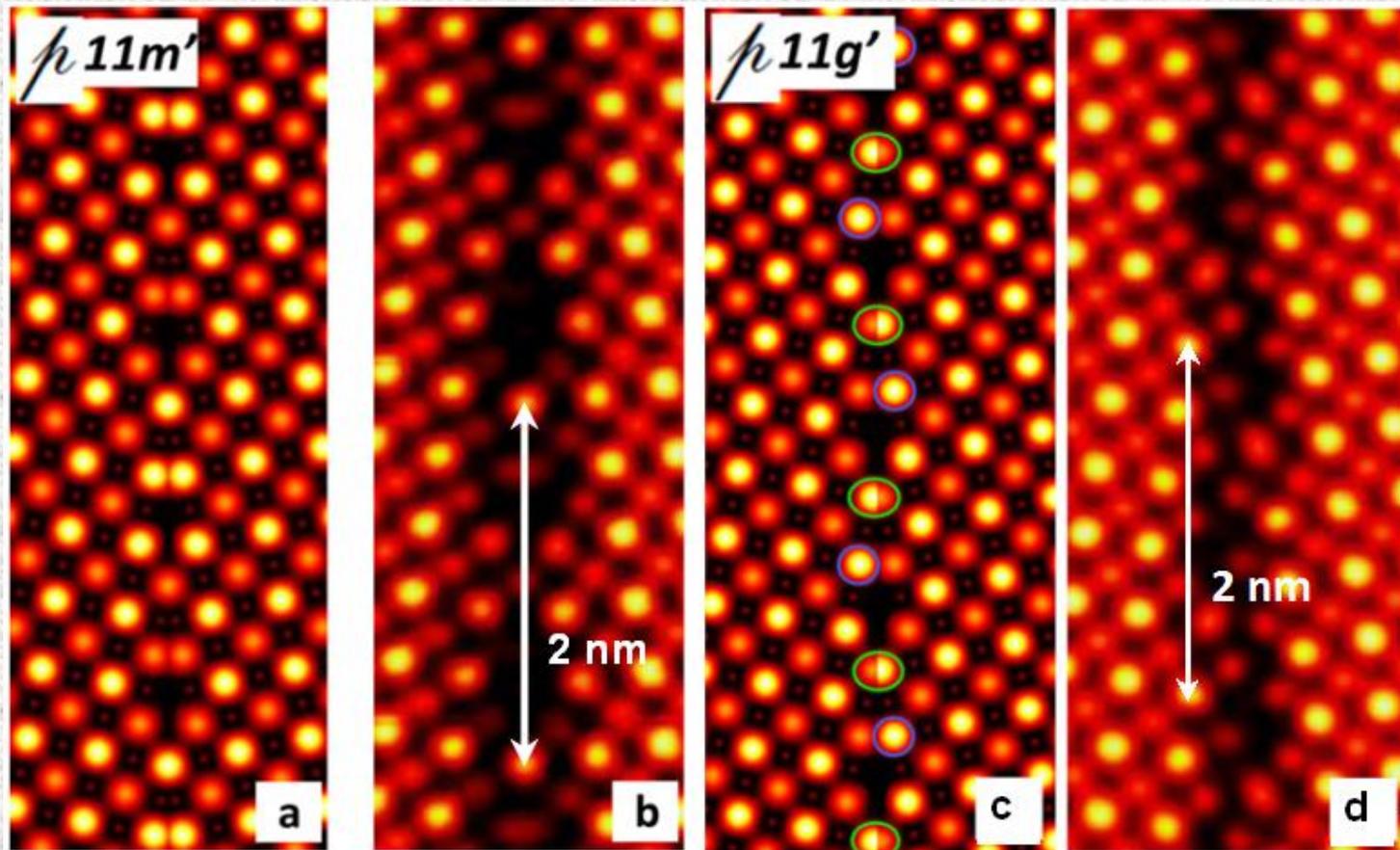
In case of doping of this tilt boundary with Eu and W, segments of the grain boundary with different frieze symmetries feature different amounts of dopants, mixed Ti/O columns are substituted, the relative abundance of the segments changes with doping



$\text{SrTiO}_3 \Sigma 13a$	undoped	Eu,W doped	Pr doped
$p11m'$	35 %	43 %	81 %
$p11g'$	65 %	26 %	19 %
$p1$	negligible	31 %	negligible

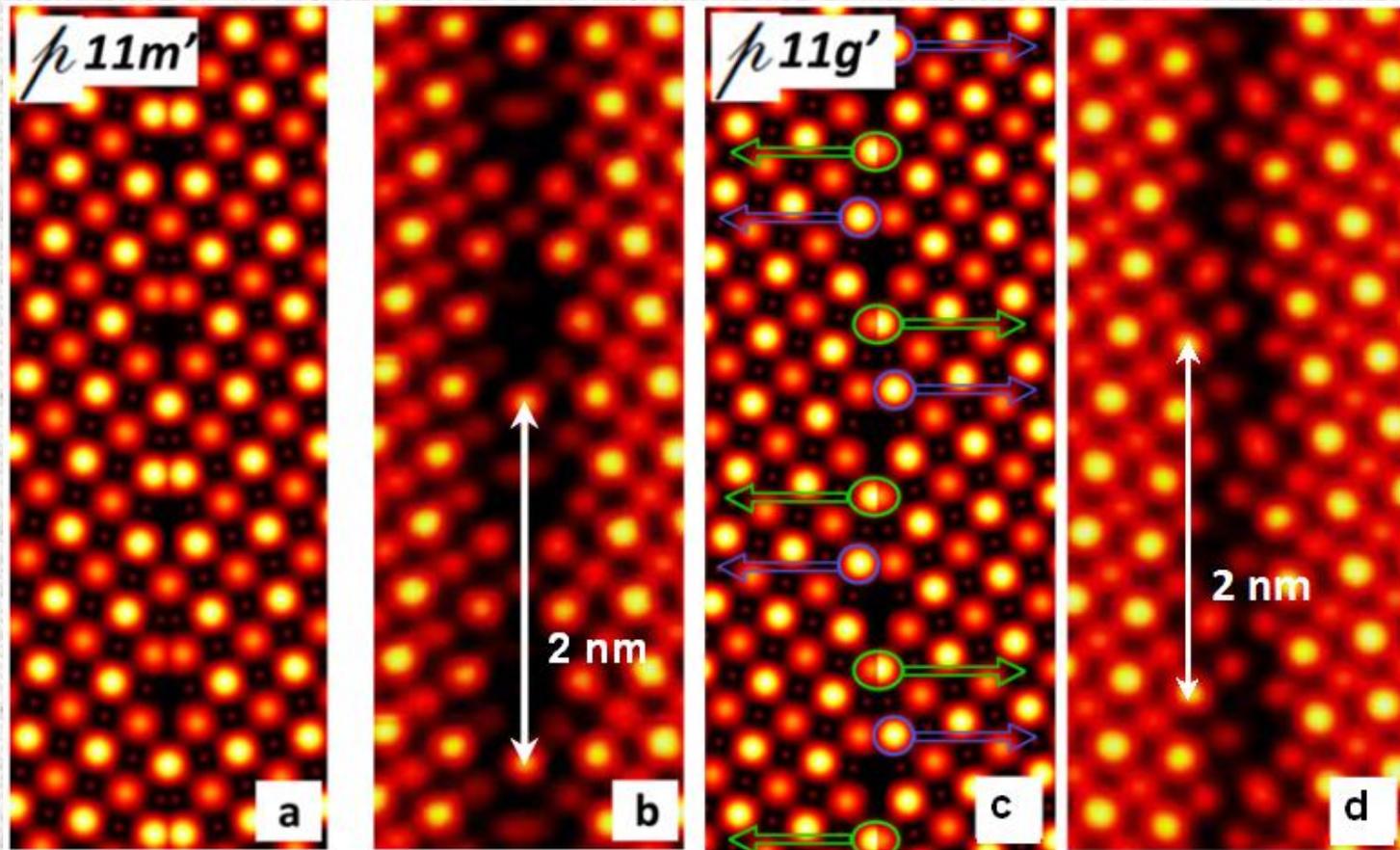


experimental confirmation for  $\Sigma$  13a SrTiO<sub>3</sub> (510): H. Yang et al.  
Phil Mag. **93** (2013) 1219-1229



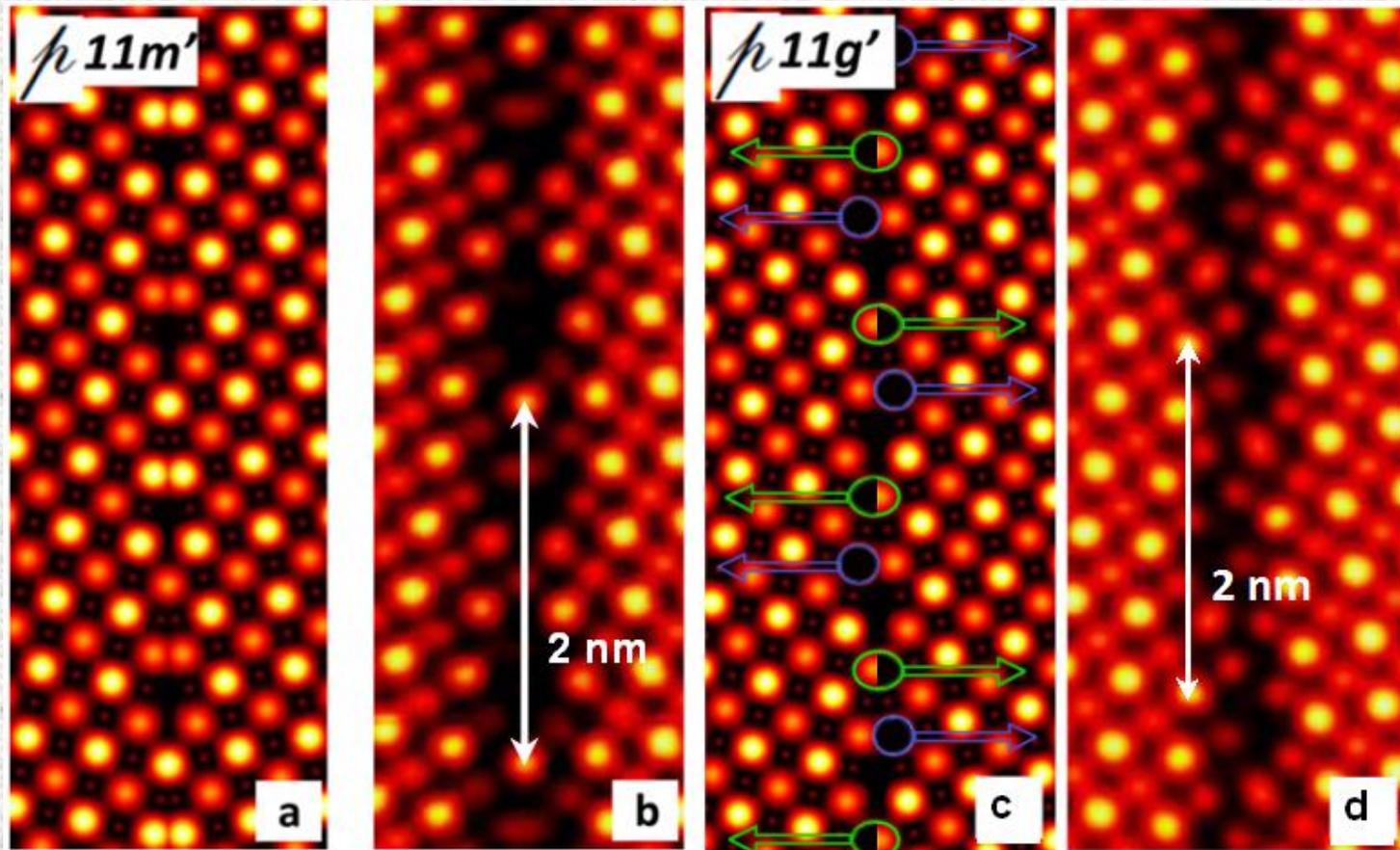
Figures a, c are predicted structures, Figures b, d are probe corrected Z-contrast STEM images

experimental confirmation for  $\Sigma$  13a SrTiO<sub>3</sub> (510): H. Yang et al.  
Phil Mag. **93** (2013) 1219-1229



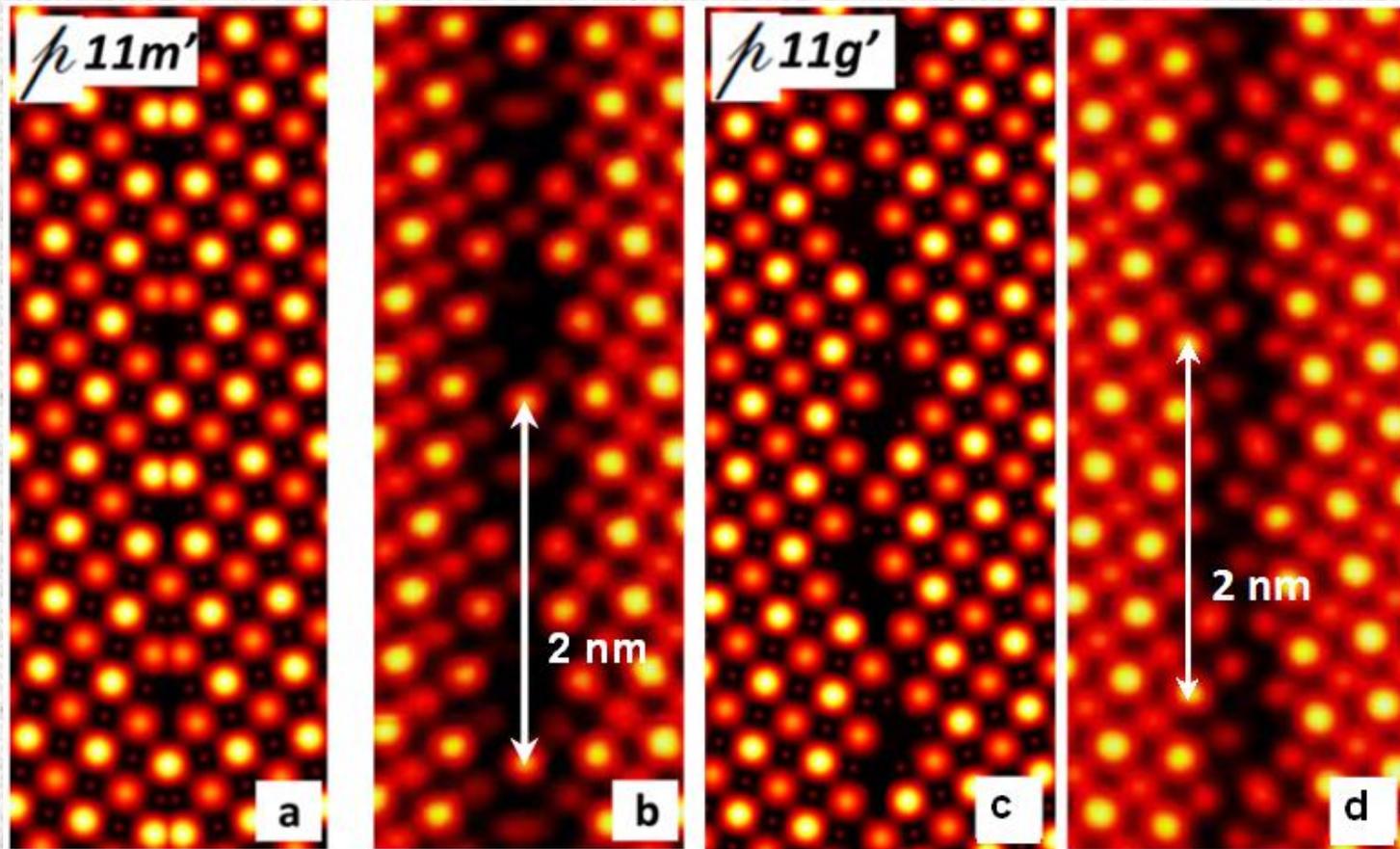
Figures a, c are predicted structures, Figures b, d are probe corrected Z-contrast STEM images

experimental confirmation for  $\Sigma$  13a SrTiO<sub>3</sub> (510): H. Yang et al.  
Phil Mag. **93** (2013) 1219-1229



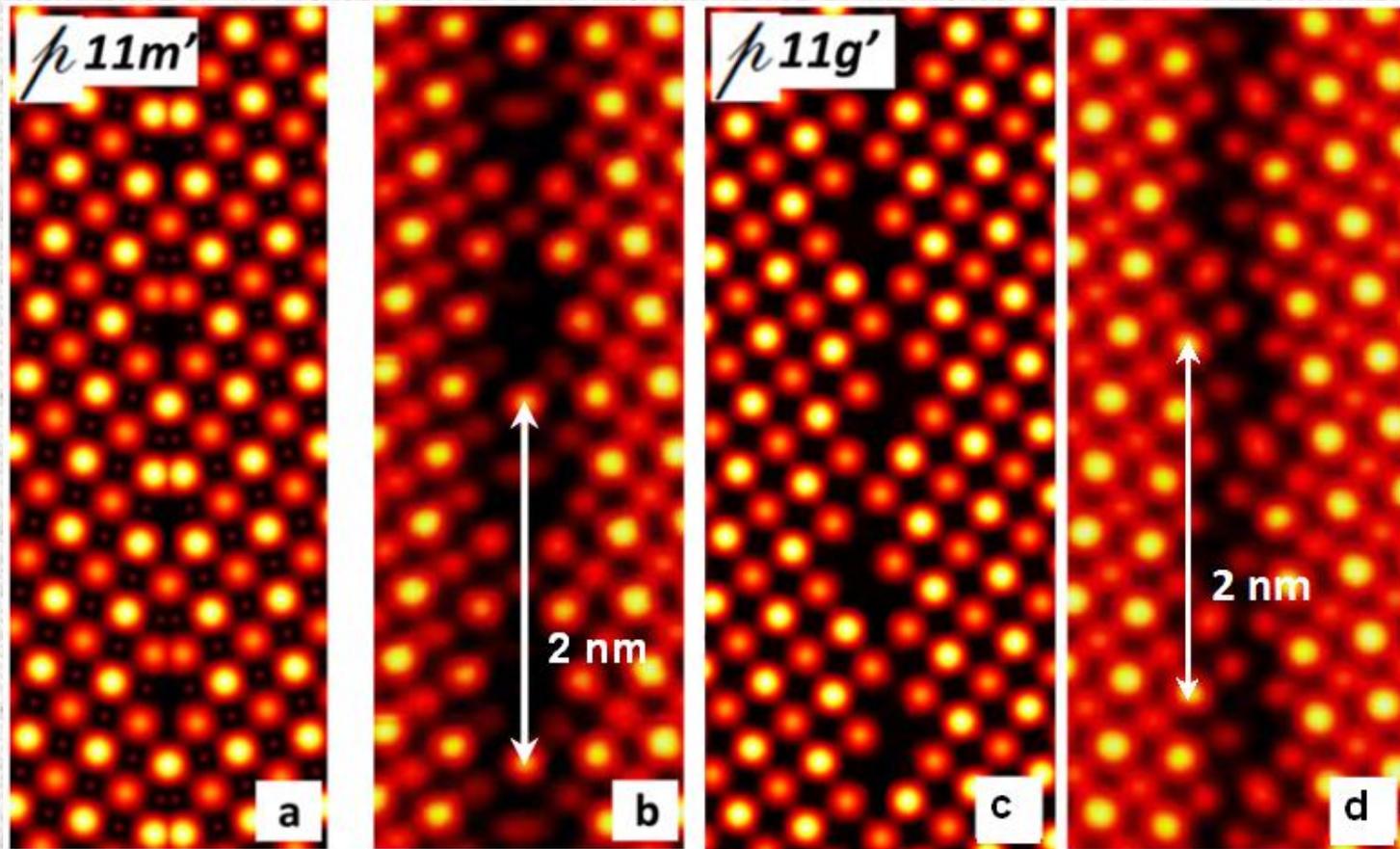
Figures a, c are predicted structures, Figures b, d are probe corrected Z-contrast STEM images

experimental confirmation for  $\Sigma$  13a SrTiO<sub>3</sub> (510): H. Yang et al.  
Phil Mag. **93** (2013) 1219-1229



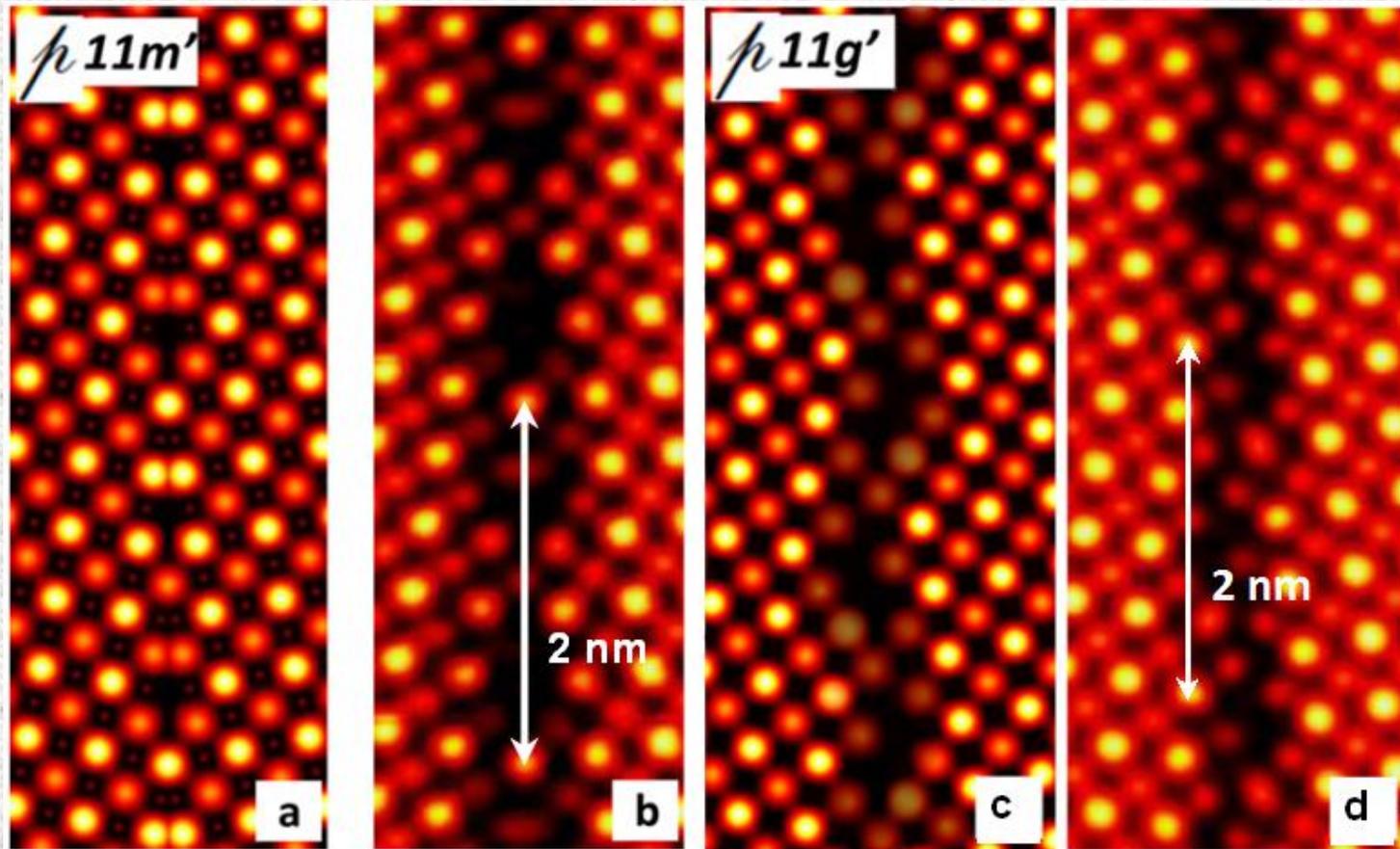
Figures a, c are predicted structures, Figures b, d are probe corrected Z-contrast STEM images

experimental confirmation for  $\Sigma$  13a SrTiO<sub>3</sub> (510): H. Yang et al.  
Phil Mag. **93** (2013) 1219-1229



Figures a, c are predicted structures, Figures b, d are probe corrected Z-contrast STEM images

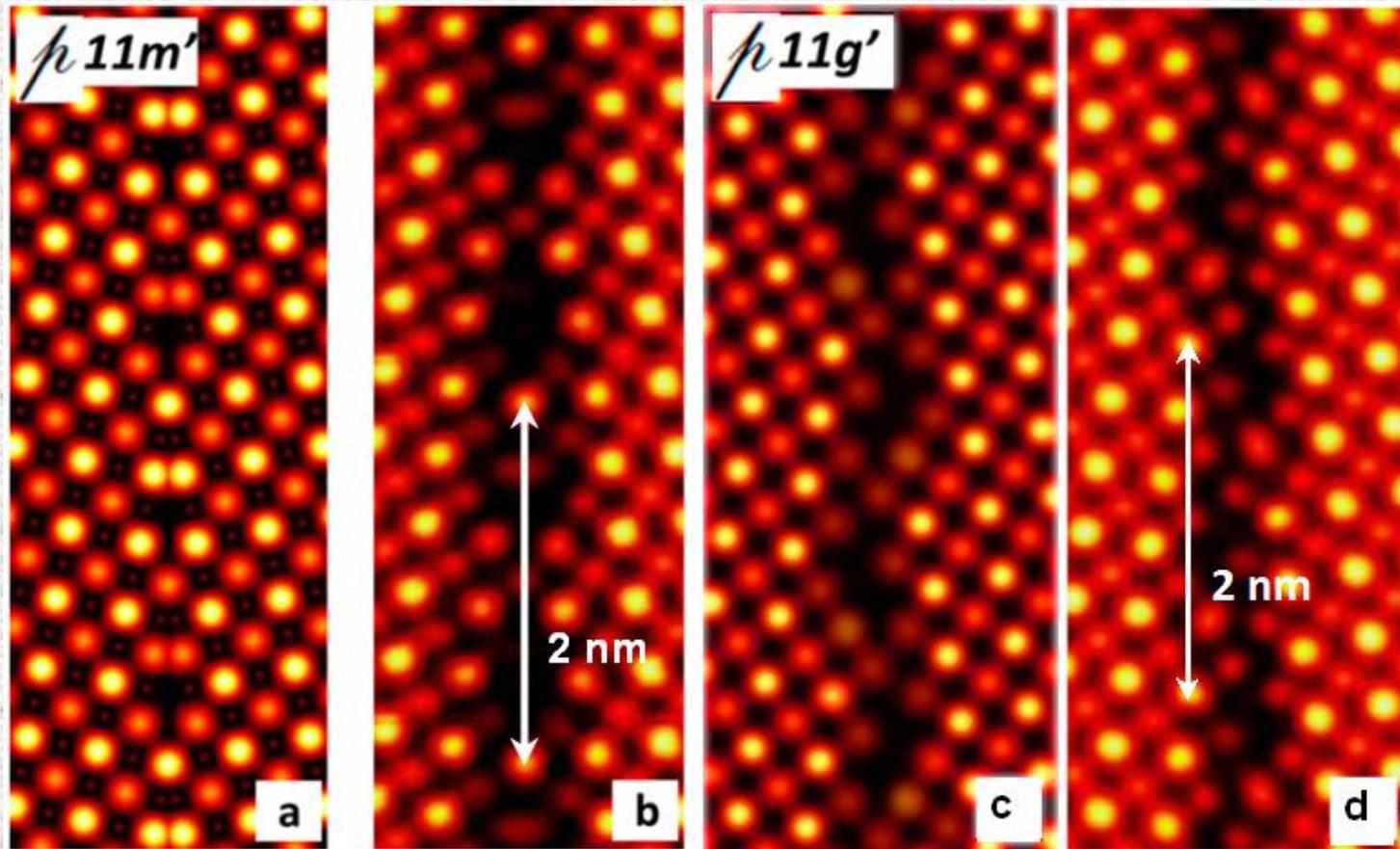
experimental confirmation for  $\Sigma$  13a SrTiO<sub>3</sub> (510): H. Yang et al.  
Phil Mag. **93** (2013) 1219-1229



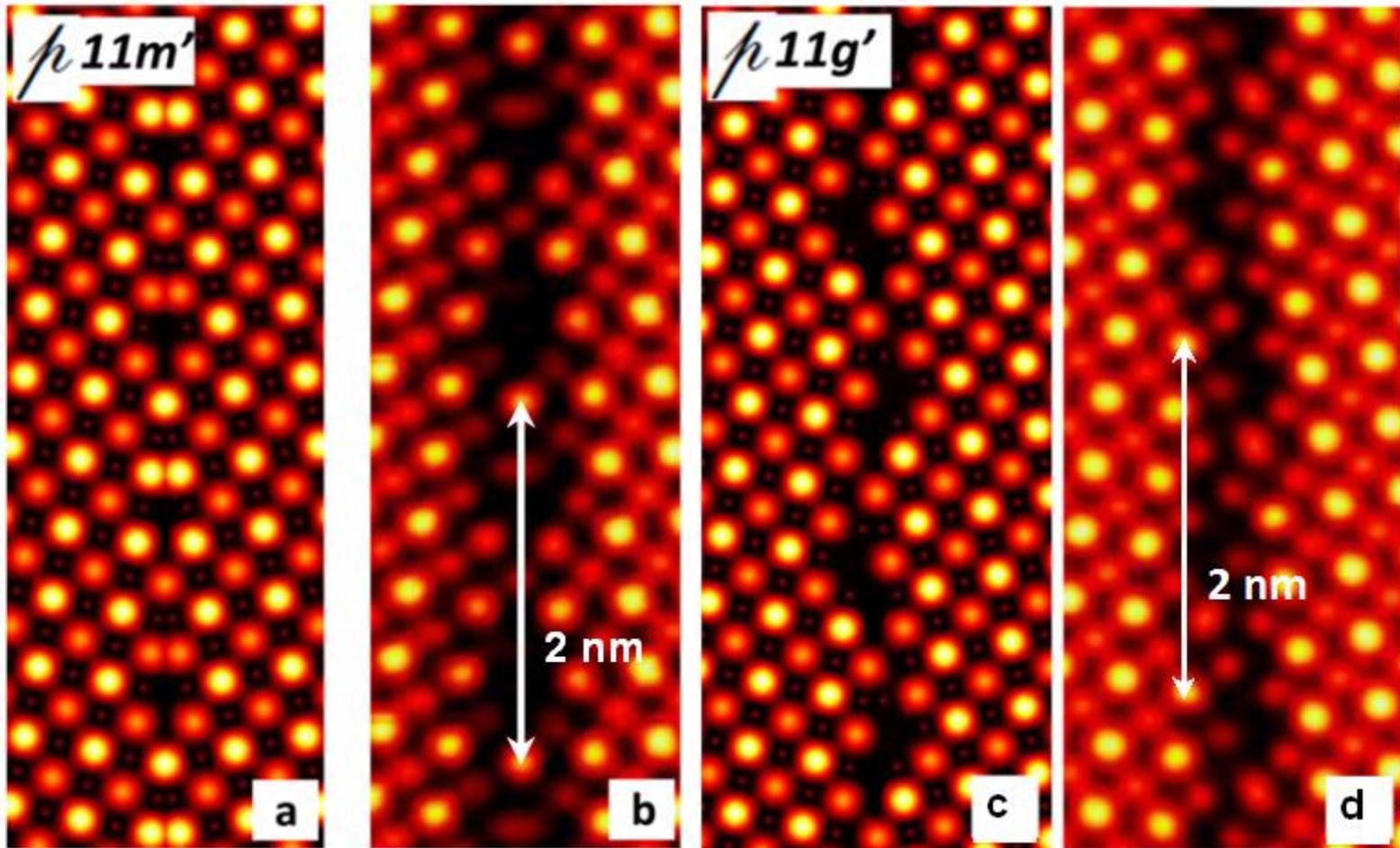
Figures a, c are predicted structures, Figures b, d are probe corrected Z-contrast STEM images

P. Moeck et al. Cryst. Res. Technol. **49** (2014) 708-720

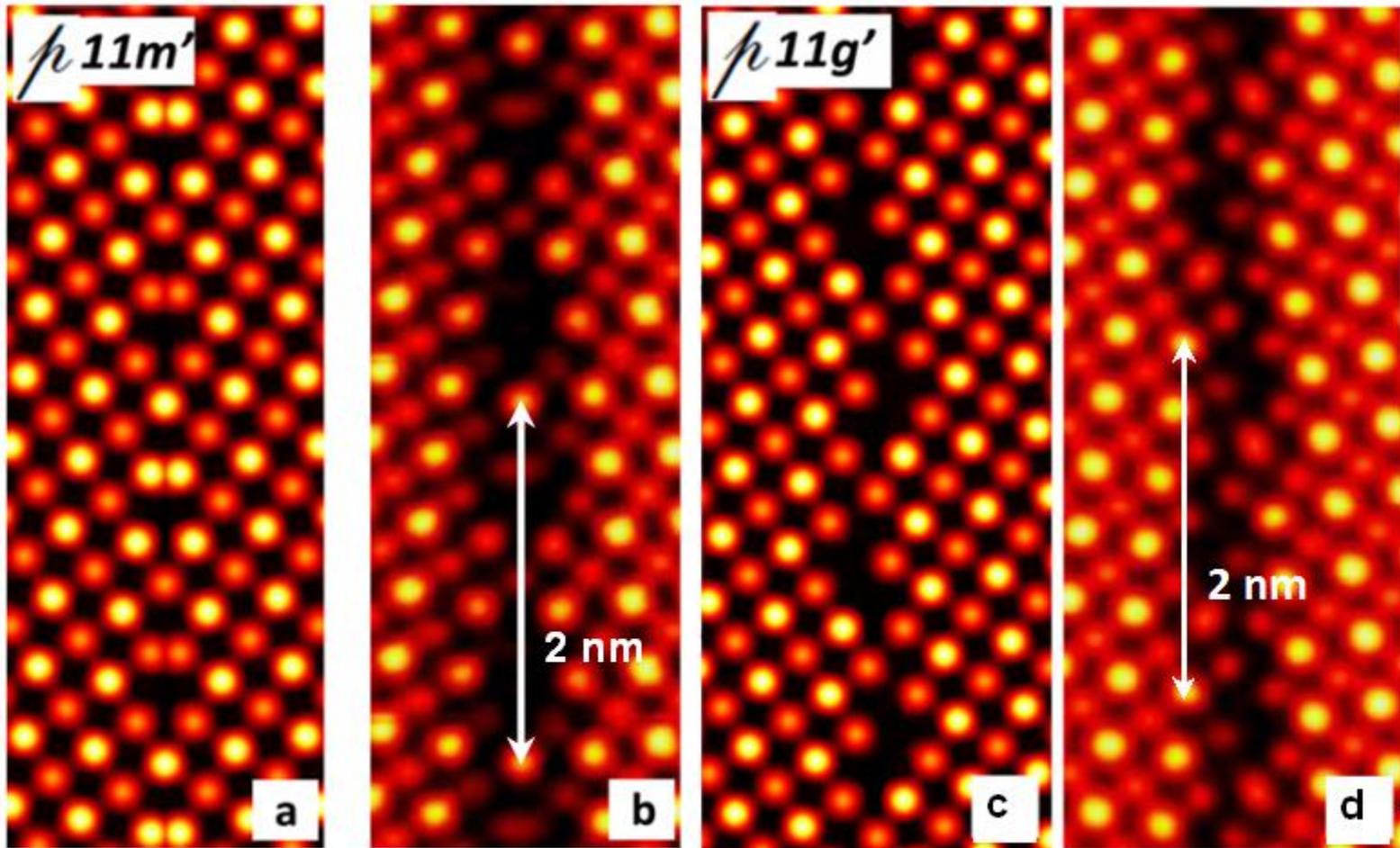
experimental confirmation for  $\Sigma$  13a SrTiO<sub>3</sub> (510): H. Yang et al.  
Phil Mag. **93** (2013) 1219-1229



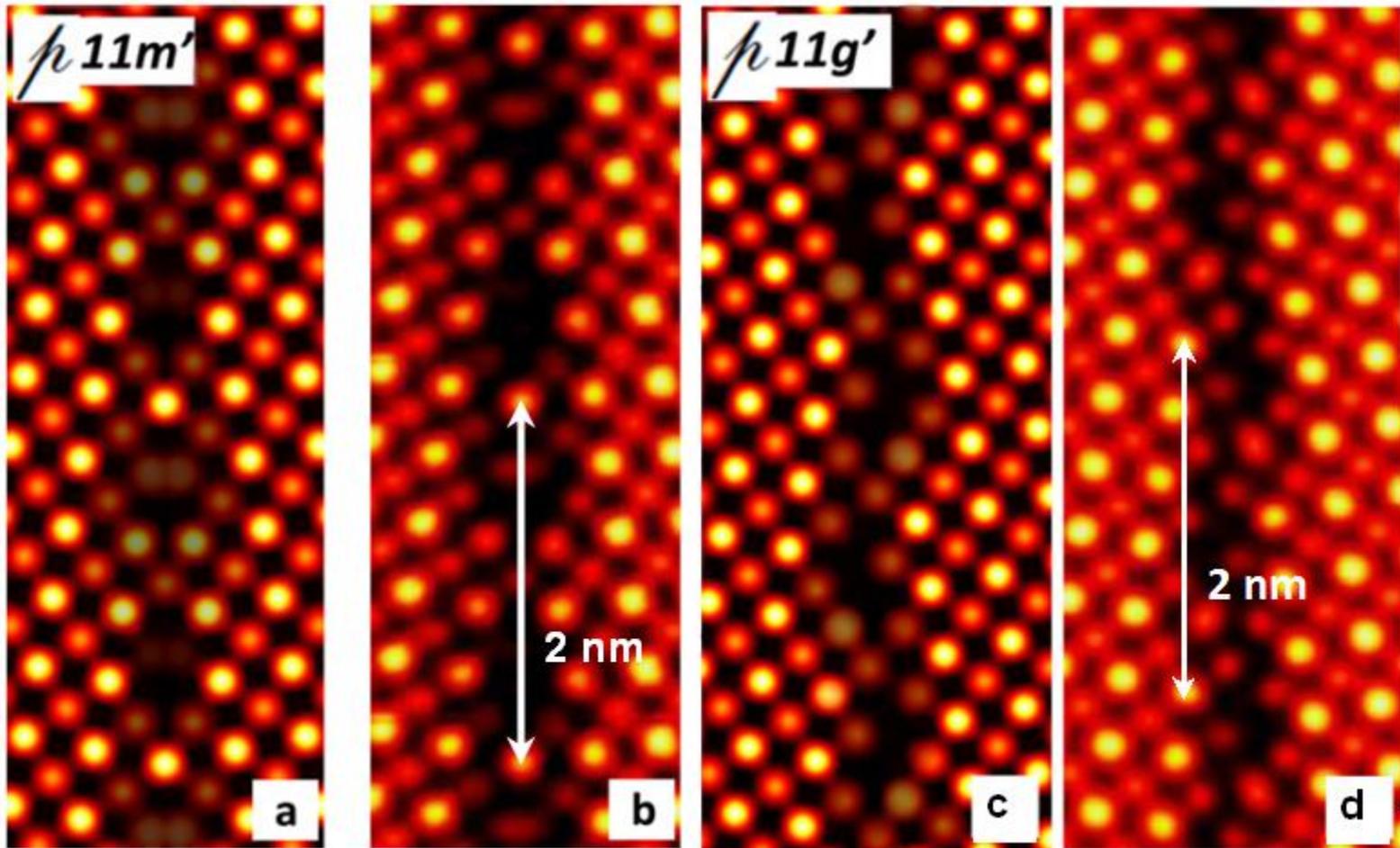
Figures a, c are predicted structures, Figures b, d are probe corrected Z-contrast STEM images



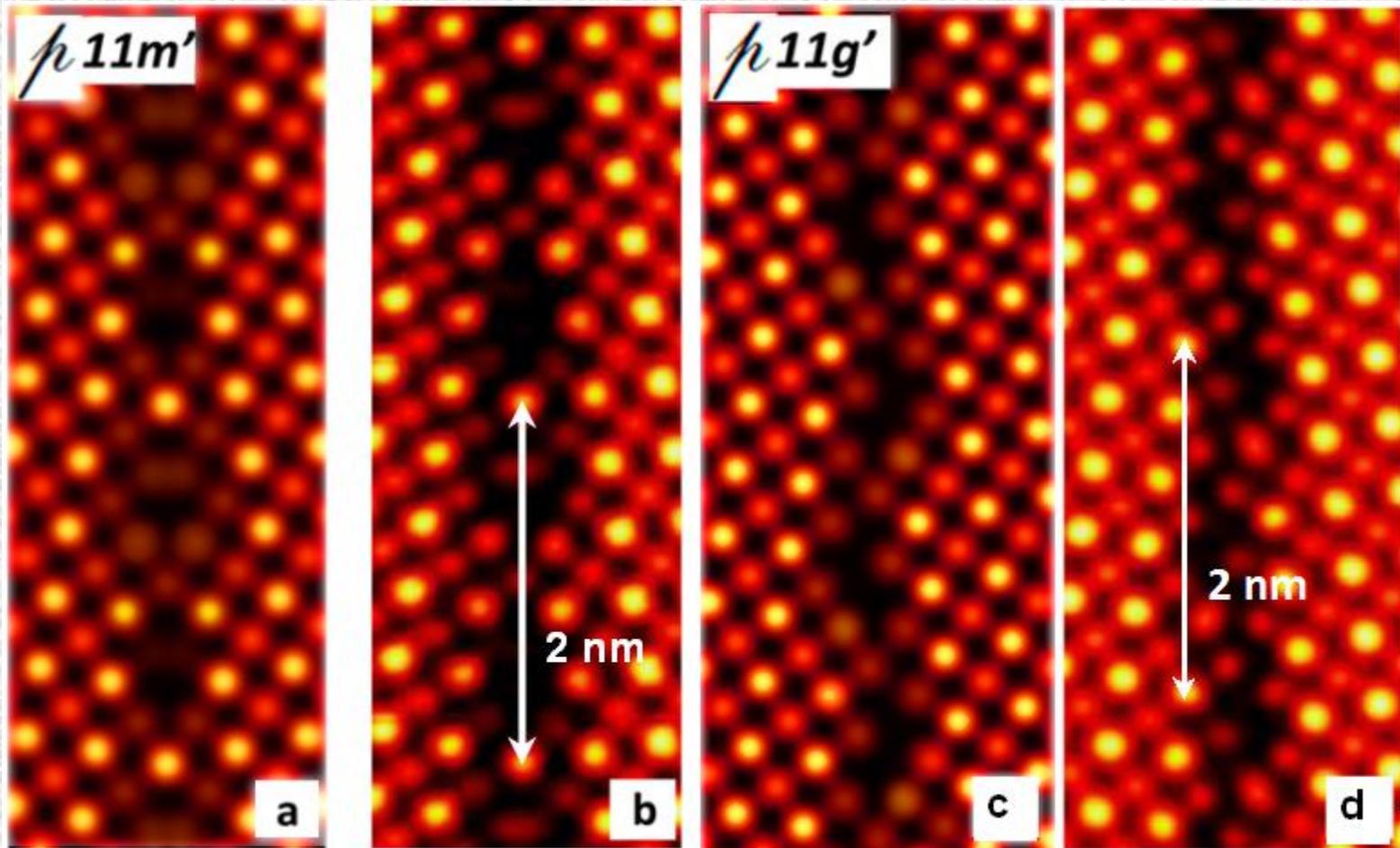
now watch out for the mirror symmetric variant of this grain boundary (left hand side)



now watch out for the mirror symmetric variant of this grain boundary (left hand side)



now watch out for the mirror symmetric variant of this grain boundary (left hand side)



Bicrystallography predictions in both cases close to the real structure as seen experimentally in aberration corrected Z-STEM

*“... the geometric properties of grain boundaries can be described in exactly the same way for general and coincidence lattice boundaries; the fundamental symmetries are given by a six-dimensional space group uniquely defined by the actual crystal structure and independent of the orientation of the two crystals.”*

D. Gratias & A. Thalal, ***Hidden symmetries in general grain boundaries***, Phil. Mag. Lett. **57** (1988) 63-68

# The interface region of a general planar grain boundary (with irrational interface indices) is actually quasicrystalline!

So far not considered in International Tables, ignored by almost all grain boundary textbooks, D. Romeu, *"Interfaces and Quasicrystals as competing crystal lattices. Towards a crystallographic theory of interfaces"*, Phys. Rev. B. **67**, 24202 (2003).

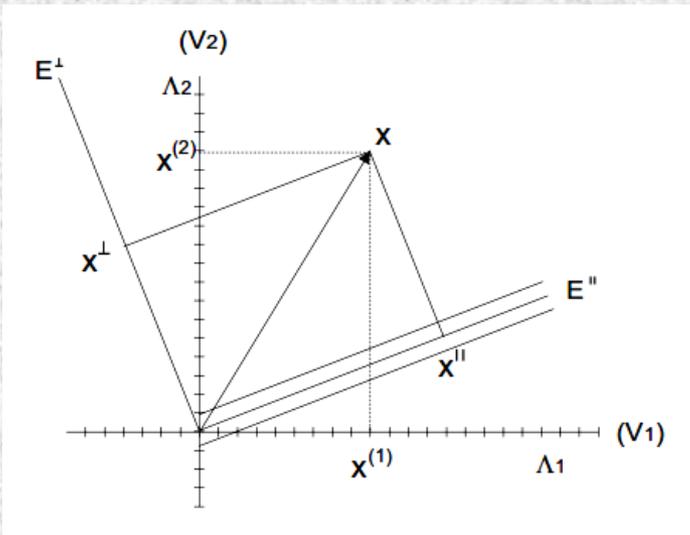
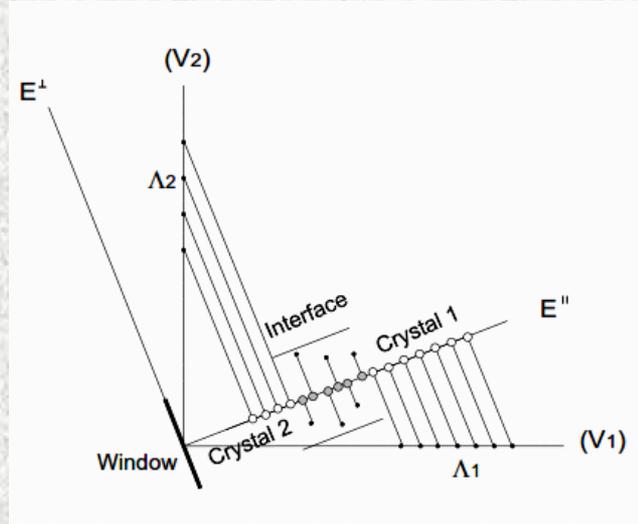


FIG. 1: Schematic representation of the projection of a 2D hyperlattice into the 1D orthogonal subspaces  $E^{\parallel}$  and  $E^{\perp}$ . Top: The hyperpoint  $x$  results of the embedding of the lattice points  $x^{(1)}$ ,  $x^{(2)}$ , and projects into the points  $x^{\parallel}$ ,  $x^{\perp}$ . Only points within the region around  $E^{\parallel}$  bounded by the strip are projected. Bottom: The projection of a complete bicrystal: interfacial points arise from the projection of the hyper-points inside the strip that lie within the region of conflict. Crystals 1 and 2 are recovered by projecting the hyper points  $(x^{(1)}, 0)$  and  $(0, x^{(2)})$ .



Luis David F.  
**Romeu Casajuana**

5 pages on quasicrystallinity in Sutton and Baluffi's classical text

combines (predictive) bicrystallography (Pond, Bollmann, Vlachavas, Kalonji, ...) with predictable grain boundary structure of 3D CSLs with sequences of "structural units" (Sutton, Vitek, ...), which are only genuine units for rational grain boundaries, i.e. approximants to quasicrystalline general grain boundaries, **Price: higher dimensional crystallography, no big deal for computers**

# Summary and Conclusions

bicrystallography helps keeping track with grain boundary parameters, accounts for 6 of the 9 free parameters, in 2D projection it becomes a simple drawing procedure

is just about predicting atomic position at and around an interface, alternative approach to both “structural units” and dislocations, but completely general

if bulk structures are related in any way (Bärnighausen trees), their ideal grain boundaries with the same set of 6 free parameters will be related as well, so structural units and ideally needed dislocations will be similar as a result

in disagreement with the current wisdom of the textbooks, **grain boundaries** are not really 2D defects in an ideal crystal, they **have their own ideal** (strain energy minimized) **structure** with respect to which one should define deviations as defects – real promise of Romeu’s work since 2003

Utilizing appropriate layer group symmetry and asymmetric unit results in significant shortening of CIF for grain boundary energy minimization calculations, prediction of physical properties over Curie’s symmetry principle, 3D print file creation programs, ...

experiments have shown that real atomic positions (3 more degrees of freedom) are not far from ideal atomic positions (sure some atoms may be missing, substituted, ...)

classical approaches unified by Romeu 2003 for description of general grain boundaries (with quasicrystalline interface and arbitrary large  $\Sigma$  as approximants) in 6 dimensions (shall become more popular in future when the SG in 6D have been enumerated and made available on the internet together with the algorithmic tools do deal with them properly ...)



$\Sigma$	$\theta$ (°)	uv w	$\phi_1, \Phi, \phi_2$			$\rho$			$\mathbf{q}$			
3	60	111	45	70.53	45	1/3	1/3	1/3	0.288	0.288	0.288	0.866
5	36.87	100	0	90	36.86	1/3	0.0	0.0	0.000	0.000	0.316	0.948
7	38.21	111	26.56	73.4	63.44	0.2	0.2	0.2	0.188	0.188	0.188	0.944
9	38.94	110	26.56	83.62	26.56	0.25	0.25	0.0	0.000	0.236	0.236	0.943
11	50.47	110	33.68	79.53	33.68	1/3	1/3	0.0	0.000	0.302	0.302	0.904
13a	22.62	100	0	90	22.62	0.2	0.0	0.0	0.000	0.000	0.196	0.981
13b	27.79	111	18.43	76.66	71.57	0.143	0.143	0.143	0.139	0.139	0.139	0.971
15	48.19	210	19.65	82.33	42.27	0.4	0.2	0.0	0.000	0.183	0.365	0.913
17a	28.07	100	0	90	28.07	0.25	0.0	0.0	0.000	0.000	0.243	0.970
17b	61.9	221	45	86.63	45	0.4	0.4	0.2	0.171	0.343	0.343	0.858
19a	26.53	110	18.44	89.68	18.44	1/6	1/6	0.0	0.000	0.162	0.162	0.973
19b	46.8	111	33.69	71.59	56.31	0.25	0.25	0.25	0.229	0.229	0.229	0.918
21a	21.78	111	14.03	79.02	75.97	1/9	1/9	1/9	0.109	0.109	0.109	0.982
21b	44.41	211	22.83	79.02	50.91	1/3	1/6	1/6	0.154	0.154	0.308	0.926
23	40.45	311	15.25	82.51	52.13	1/3	1/9	1/9	0.104	0.104	0.313	0.938
25a	16.26	100	0	90	16.26	0.143	0.0	0.0	0.000	0.000	0.142	0.99
25b	51.68	331	36.87	90	53.13	1/3	1/3	1/9	0.100	0.300	0.300	0.9
27a	31.59	110	21.8	85.75	21.8	0.2	0.2	0.0	0.000	0.193	0.193	0.962
27b	35.43	210	15.07	85.75	31.33	0.285	0.143	0.0	0.000	0.136	0.272	0.953
29a	43.6	100	0	90	43.6	0.4	0.0	0.0	0.000	0.000	0.393	0.928
29b	46.4	221	33.69	84.06	56.31	0.286	0.286	0.143	0.131	0.263	0.263	0.919
31a	17.9	111	11.31	80.72	78.69	1/11	1/11	1/11	0.09	0.09	0.09	0.988
31b	52.2	211	27.41	78.84	43.66	0.4	0.2	0.2	0.180	0.18	0.359	0.898
33a	20.1	110	12.34	83.04	58.73	0.125	0.125	0.000	0.000	0.123	0.123	0.985
33b	33.6	311	37.51	76.84	37.51	0.273	0.091	0.091	0.087	0.087	0.261	0.957
33c	59.0	110	38.66	75.97	38.66	0.4	0.4	0.000	0.000	0.348	0.348	0.870
35a	34.0	211	16.86	80.13	60.46	0.25	0.125	0.125	0.119	0.119	0.239	0.956
35b	43.2	331	30.96	88.36	59.04	0.272	0.272	0.091	0.083	0.253	0.253	0.93

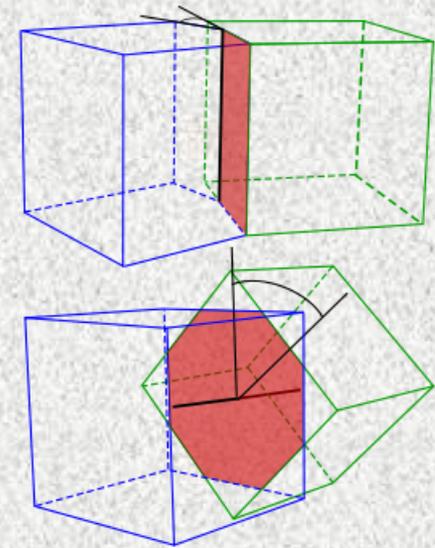
Table of CSL values in axis/angle, Euler angles, Rodrigues vectors, and quaternions

# The bigger picture

Two crystallites with their own structure meet at the interface. Up to the interface, their structure is considered ideal with local deviations that we call defects, at the interface both lattices compete with each other for space and a low energy structure forms,

but the interface structures are determined by both the orientation relationship (3 parameters) between the two crystals and the orientation and position of the grain boundary plane (an additional 3 parameters), the final 3 parameters are all microscopic and account for possible rigid body shifts

simplest cases tilt and twist boundaries



For orientation relationships with rational angles and axes (3 parameters), CSLs are formed. They are just the intersection of two lattices, e.g. two primitive cubic lattice (above), labeled  $\Sigma$  quoted together with orientation of grain boundary (2 more parameters)

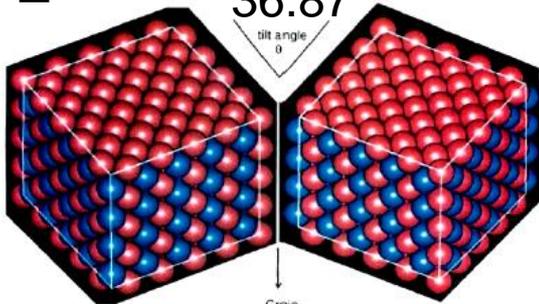
**but position of plane not accounted for**

$\sim 1000$  atoms (013)

$\Sigma 5$

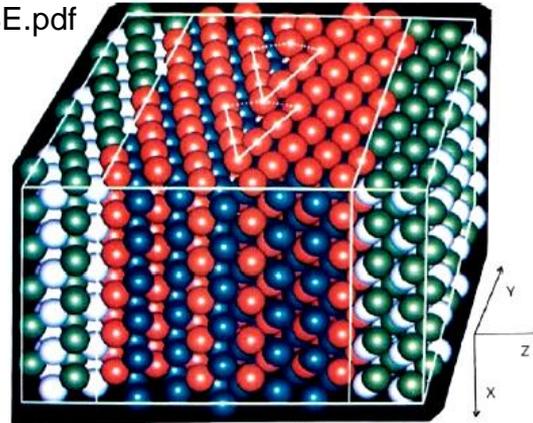
$36.87^\circ$

tilt angle  $\theta$



fcc metal, space group  $Fm\bar{3}m$

<https://nanohub.org/resources/20109/download/2013.11.13-Plimpton-CSE.pdf>



Freeware mercury from the CCDC does not understand layer symmetries but can at least do 3D print files



**Mercury 3.6 and higher**

$\Sigma 5 (310) [001] \text{CsCl}$

due to lack of understanding of layer symmetries, 152 atoms needed to be encoded for CsCl and a 2 x 2 x 1 unit cell grain boundary block - **instead of just 12 otherwise**