# Interface Facets in Systems with Large Lattice Difference

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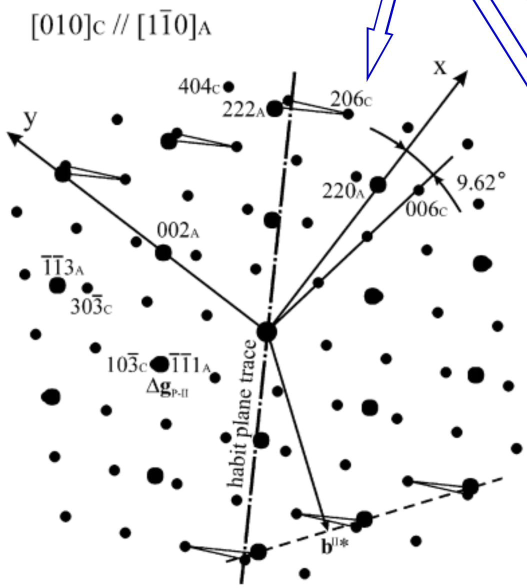
# Terminology

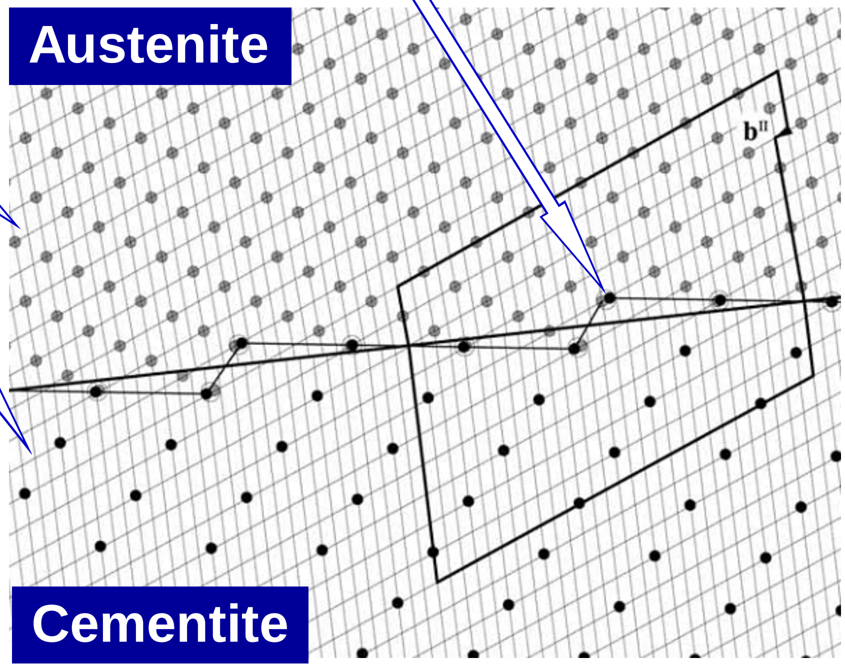
- **Lattice difference (misfit) vs Interfacial misfit**

Lattice misfit = Difference in lattice parameters

Interfacial misfit = Deviation from fit =a preferred state

T-H OR (diffraction pattern)






Ye and Zhang, 2002, Acta Mater.

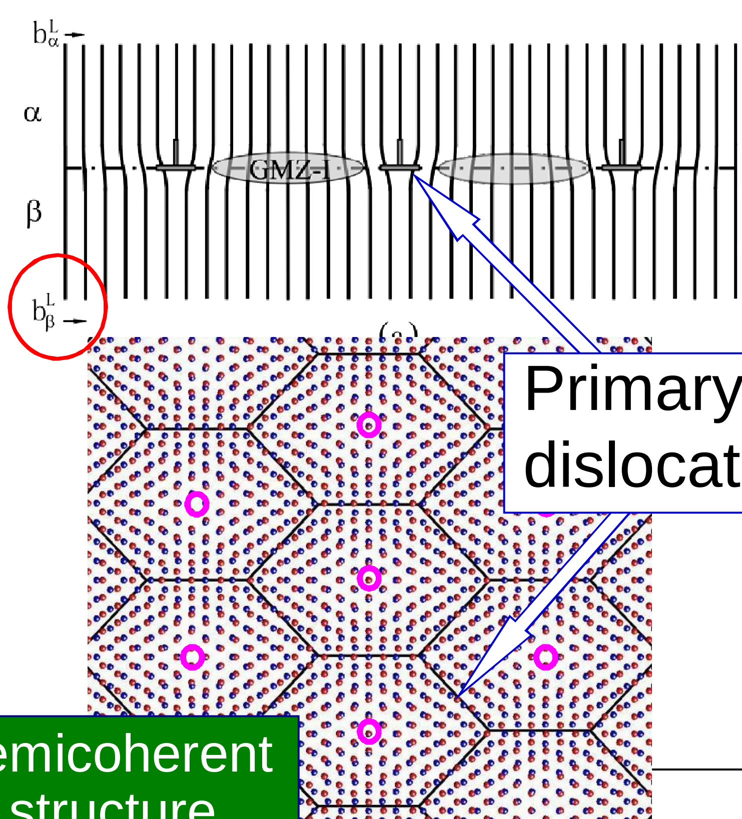
# Terminology

Bollmann, 1982, book

- **Primary preferred state** (PS) **vs Secondary PS**

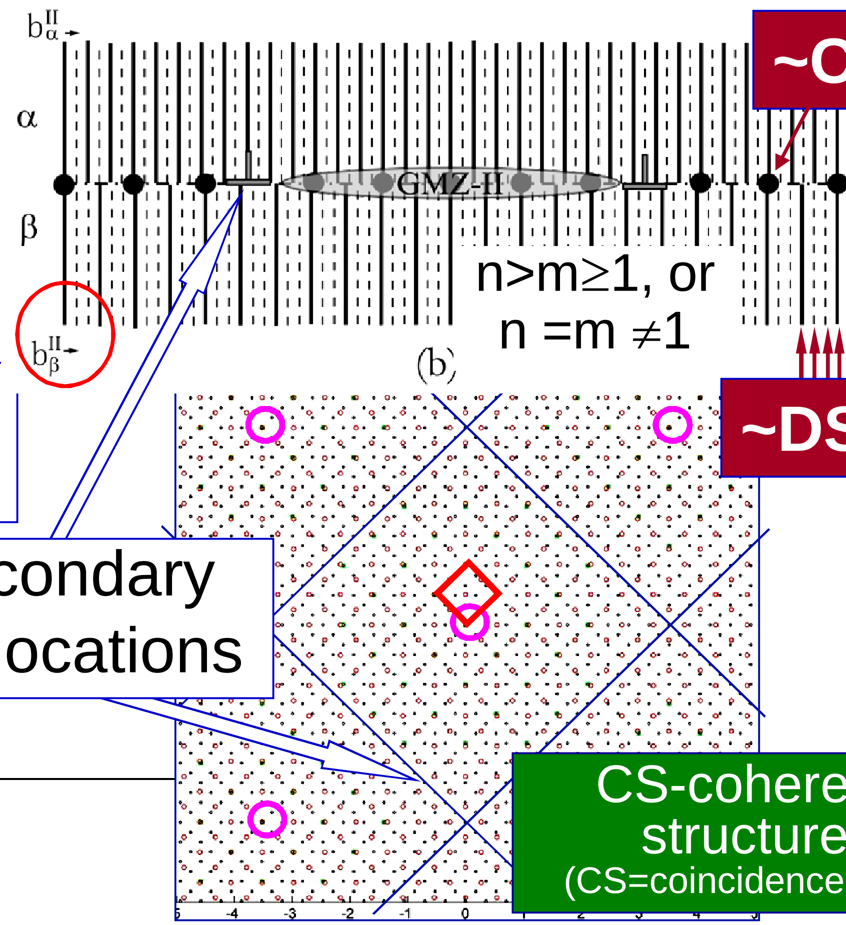
Primary PS = 1 to 1 fit

Secondary PS = n to m fit




Primary dislocations

semicoherent structure




~CSL

n>m≥1, or
n =m ≠1

~DSCL

Secondary dislocations

CS-coherent structure
(CS=coincidence site)

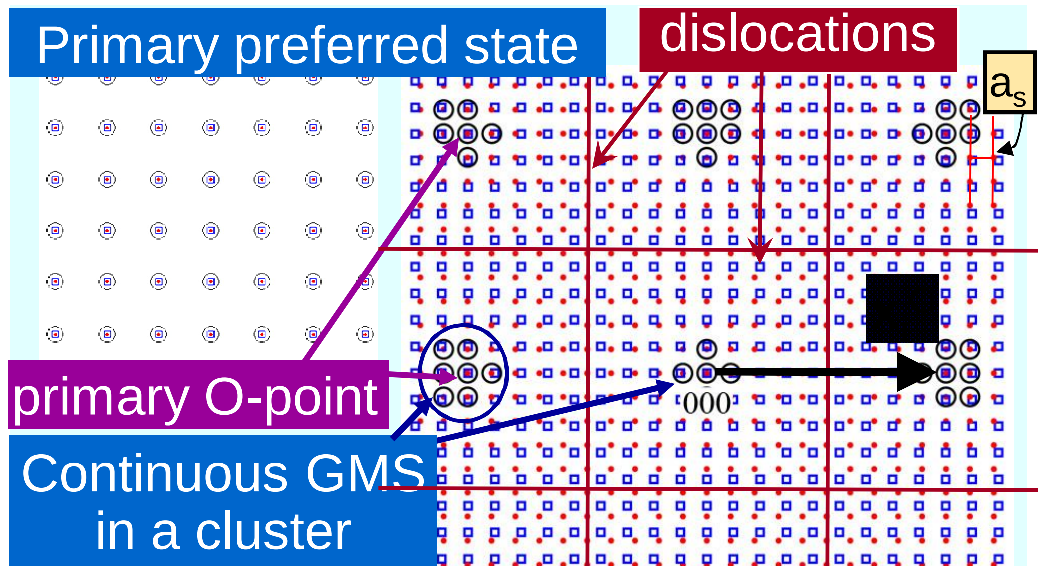
# Terminology

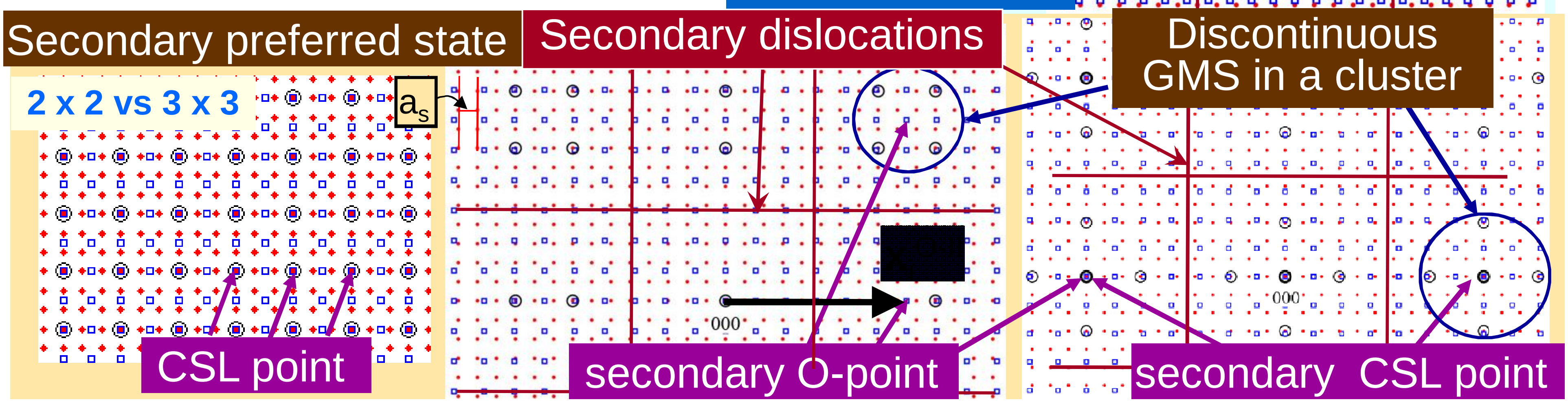
- **O-lattice (O-L) vs good matching sites (GMS)**

(A point is GMS: if $\Delta x < 15\% a_s$, modified from SL & NCS models)

O-L element = center of a cluster of GMS, where a preferred state holds

$\mathbf{x}_i^{O}$, $\mathbf{x}_i^{O\text{-}II}$ = principal O-L vector, cross by one dislocation



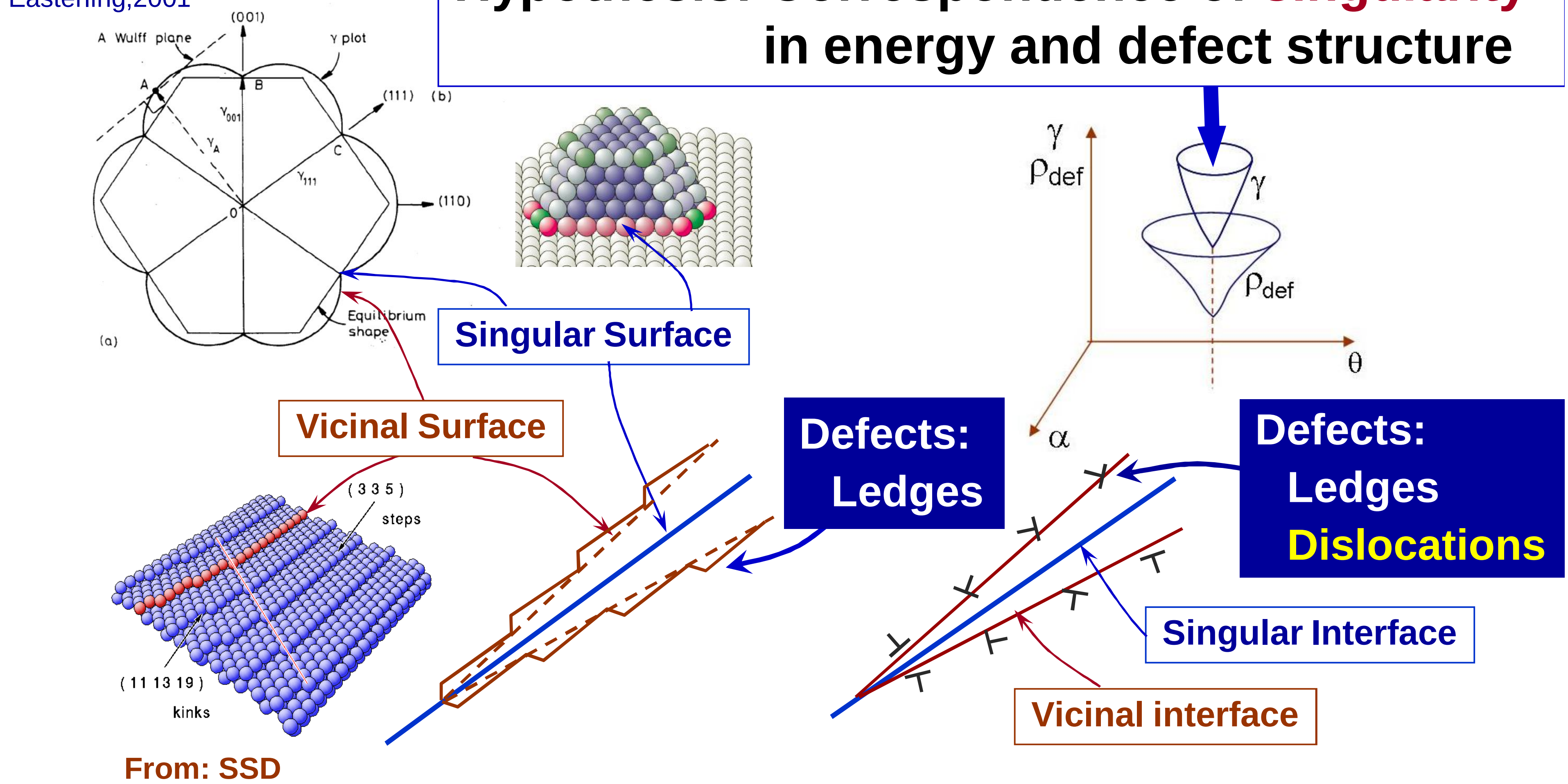



# Terminology

- **Singular interface vs Vicinal interface**

Porter and Easterling,2001

**Hypothesis: Correspondence of singularity in energy and defect structure**



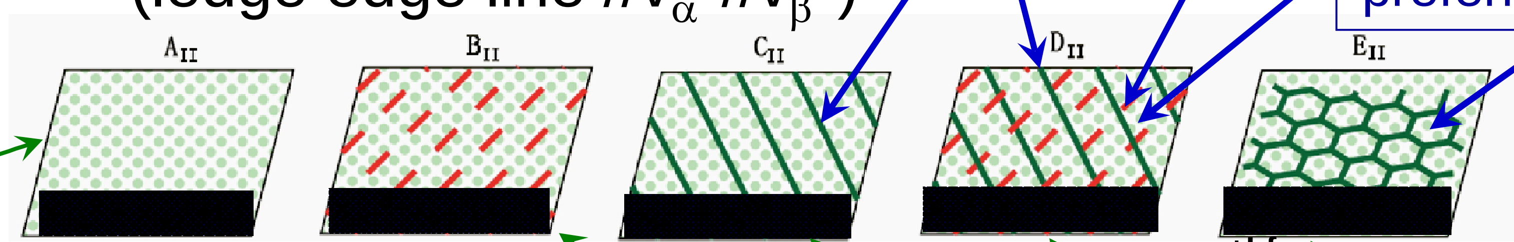

From: SSD

# Outline

- Introduction
- Understanding interface facets based on
  - Singular structures — in real space (defects)
  - $\Delta\mathbf{g}$ parallelism rules —in reciprocal space
  - Good matching site distribution — in real space
- Discussion and Summary

# Singular structures

- In terms of dislocation (disl.) defects, it contains two singular directions, defined by
  - Free of disl. = secondary invariant line, $\mathbf{x}_{in}^{II}$
  - 1 set of disl. = principal O-lattice vector, $\mathbf{x}_{i}^{O\text{-}II}$ (or major)
- In terms of ledge defects
  - Free of ledge
  - Kink-free ledge (ledge edge line $//v_{\alpha}^{L}//v_{\beta}^{L}$)

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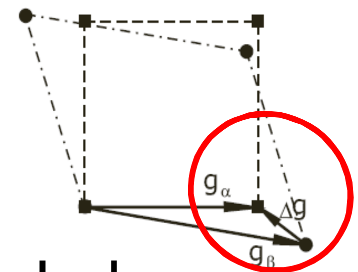
# Δg parallelism rules

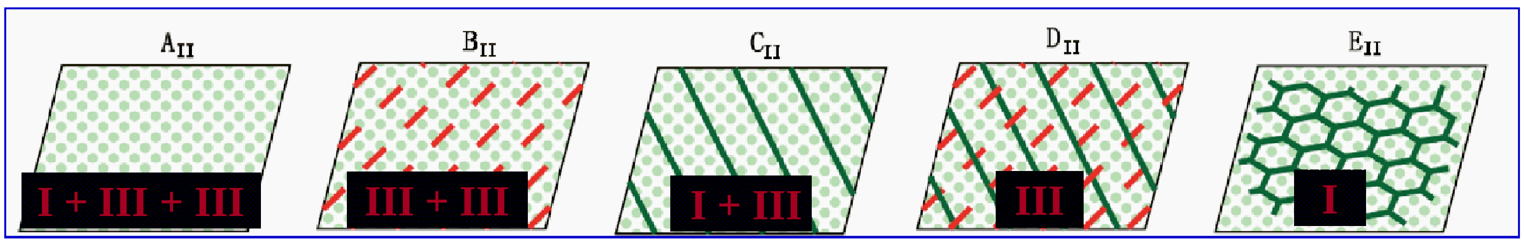
- **Orientation relationship (OR)** permitting a singular structure must obey one or more Δ**g** parallelism rules:




**I:** $\Delta g_{P\text{-}II} \,//\, g_\alpha \,//\, g_\beta \Rightarrow 2x_i^{II\text{-}O} + Lf$

**III:** $\Delta g_{P\text{-}II} // \Delta g_{Rel\text{-}CCSL} \Rightarrow x_{in}^{II}$ (or $x_{in}^{q}$) $+ x_i^{II\text{-}O}$

- $\mathbf{v}_\alpha^L // \mathbf{v}_\beta^L$ in ledge-free interface or along kink-free ledges
- A singular interface ⊥ parallel reciprocal vectors



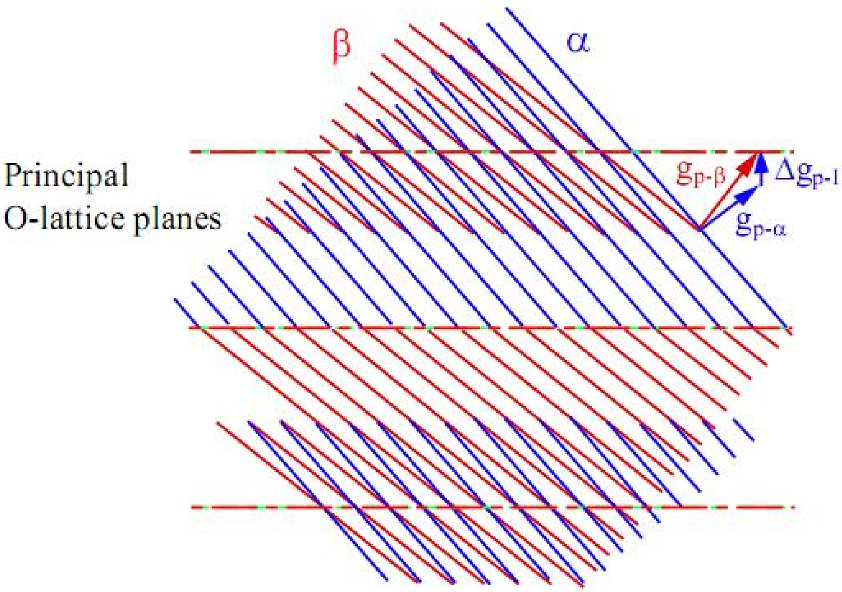

- OR following >1 rule is possible with special lattice param.

Principal 2dary O-lattice plane ⊥ $\Delta \mathbf{g}_{P\text{-}II}$, when it contains 2 of $x_i^{II\text{-}O}$ (or $x_{in}^{II}$)

Modified from Zhang and Weatherly, 2005, Prog. Mater. Sci.

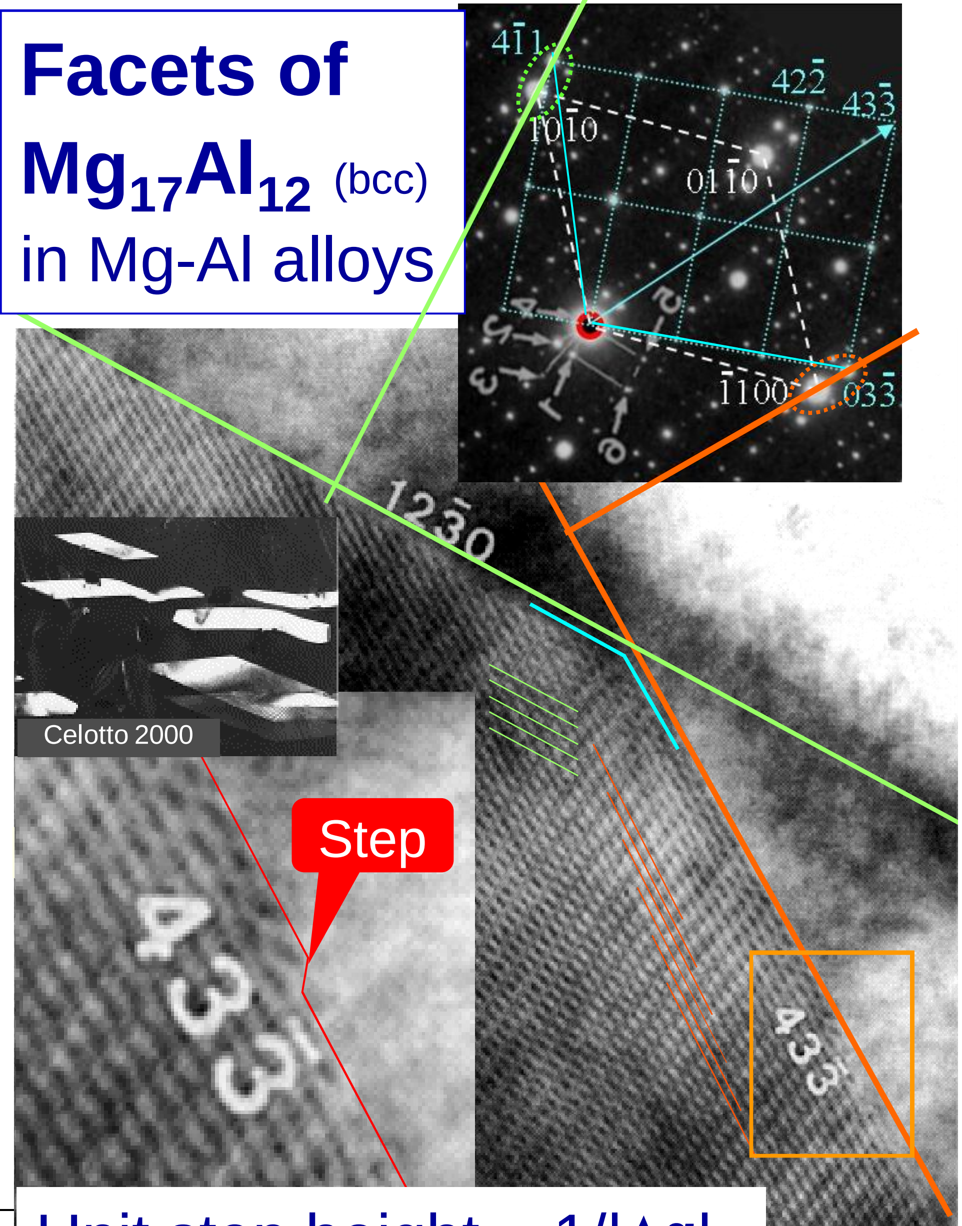
# Applications to morphologies of precipitates in Mg alloys

# Relation of Δg with Moiré planes




Edge to edge matching of two sets of planes in the interface parallel to the Moiré planes if two g's are not parallel

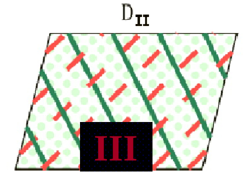
## Facets of $Mg_{17}Al_{12}$ (bcc) in Mg-Al alloys



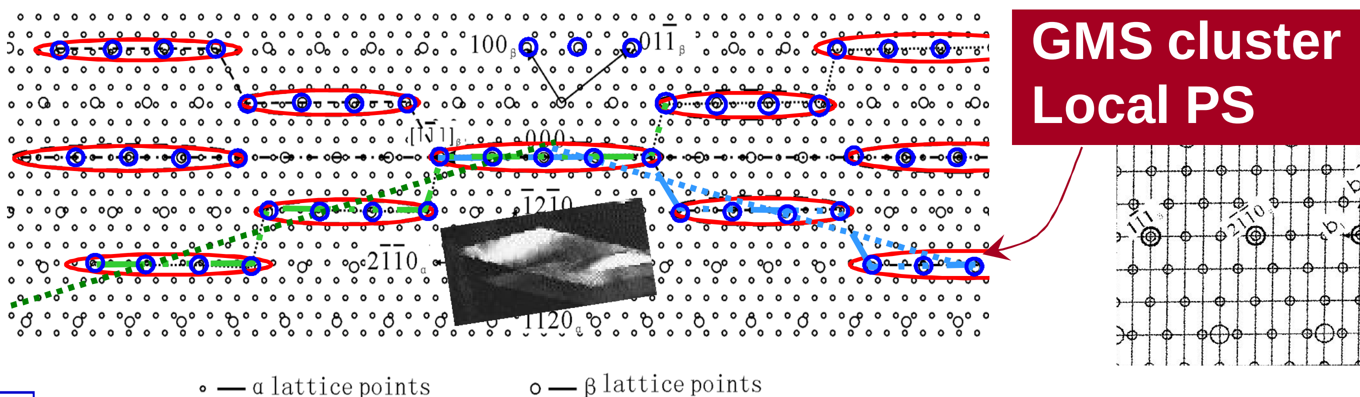

Unit step height = 1/|Δ**g**|

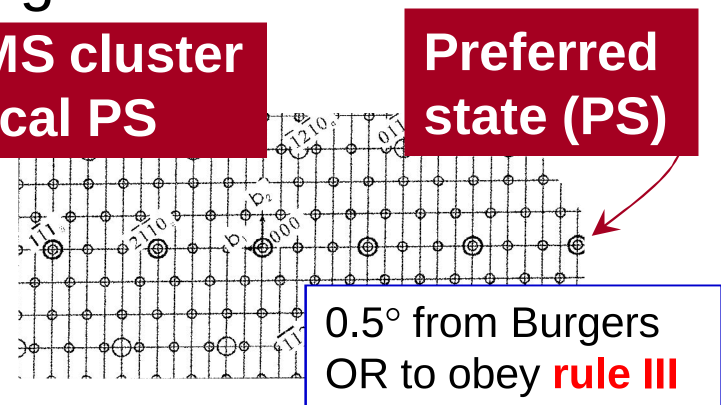
**Duly, Zhang & Audier, 1995, Phil. Mag.**

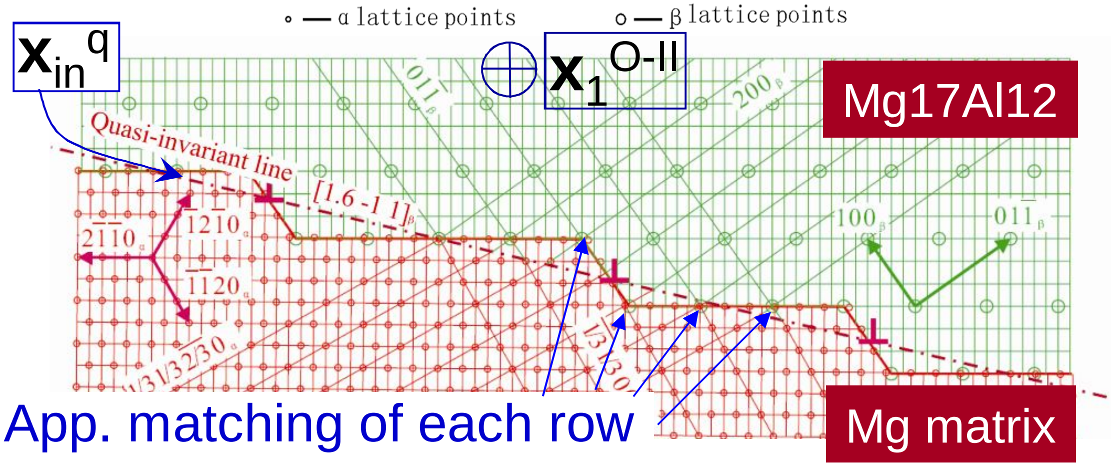
# Distribution of GMS



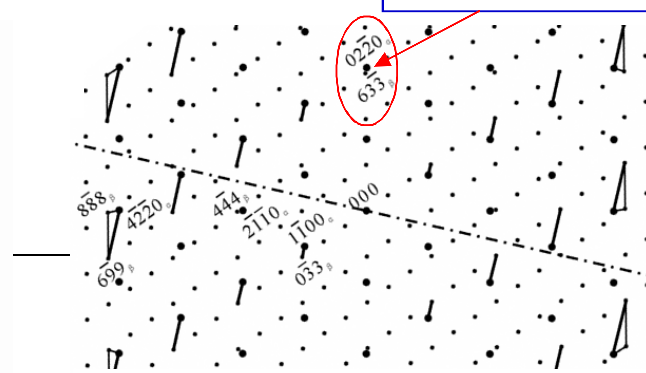

- Major side facet, free of long range strain
  - Exhibits singularity ($\mathbf{x}_1^{O\text{-}II}$($//v_\alpha^L//v_\beta^L$) & $\mathbf{x}_{in}^q$ lying in plane)
  - Obeys rule III ($D^{II}$) ~0.5° from Burgers OR
  - Contains continue and dense GMS clusters along $\mathbf{x}_{in}^q$
- Minor side facet (~$D^{II}$), carrying a slight residual strain



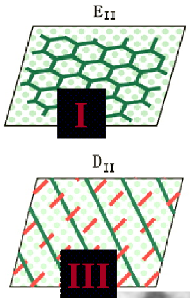

App. matching of each row



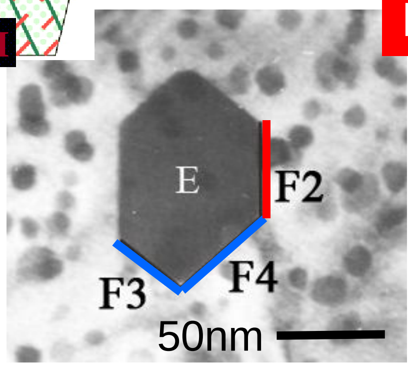

Zhang, Zhang, Ye, 2005, M. Trans

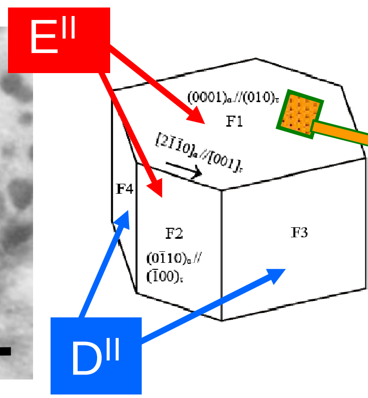
# Secondary CSL model ($\tau$-$Mg_{32}(Al, Zn)_{49}$, bcc)

## (with slight residual strain)




**Mg-Zn alloy**



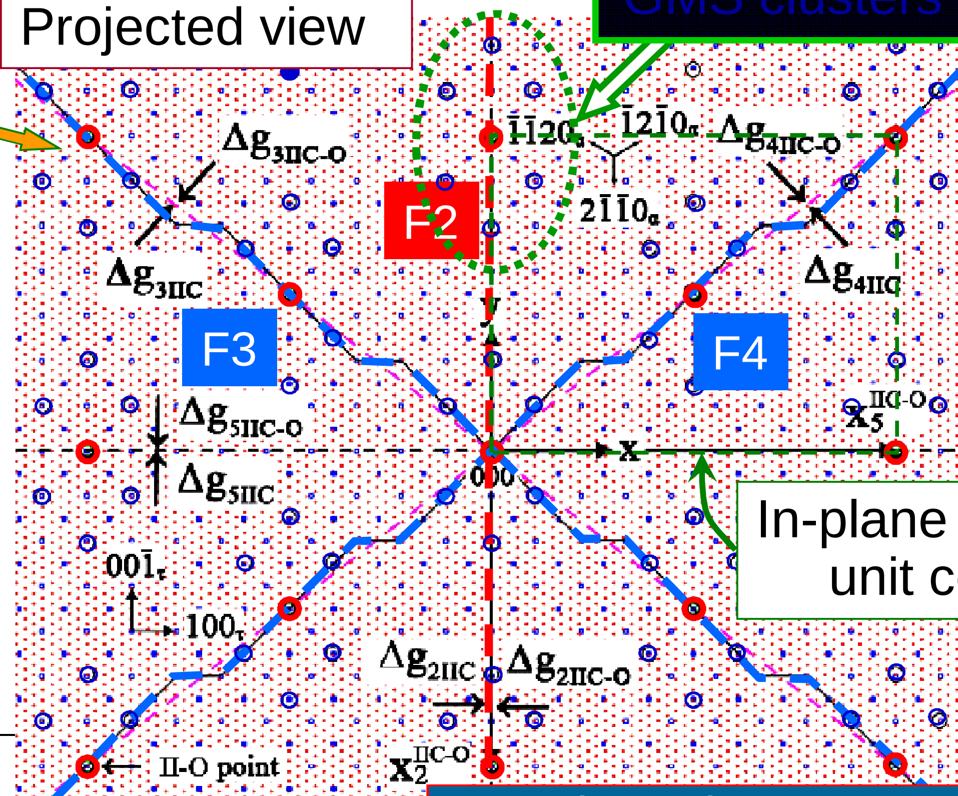




Rational OR (NEW):

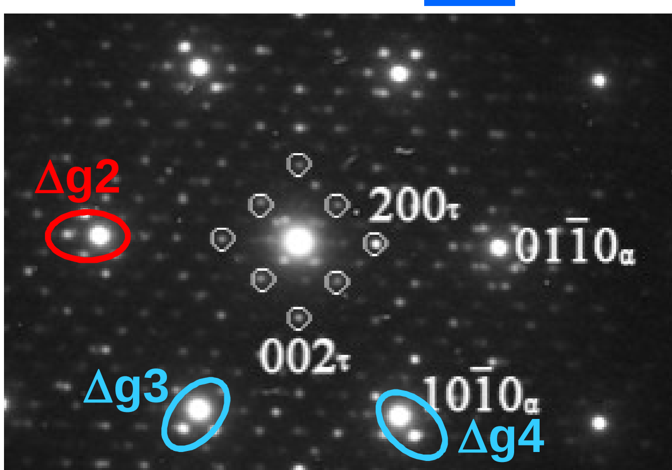
$[100]_\tau//[01\text{-}10]_\alpha$, $[010]_\tau//[0001]_\alpha$

Projected view

GMS clusters




In-plane unit cell




Shi, Zhang, 2011 Scripta Mater.

● = 2ndary CSL pts

○ = GMS

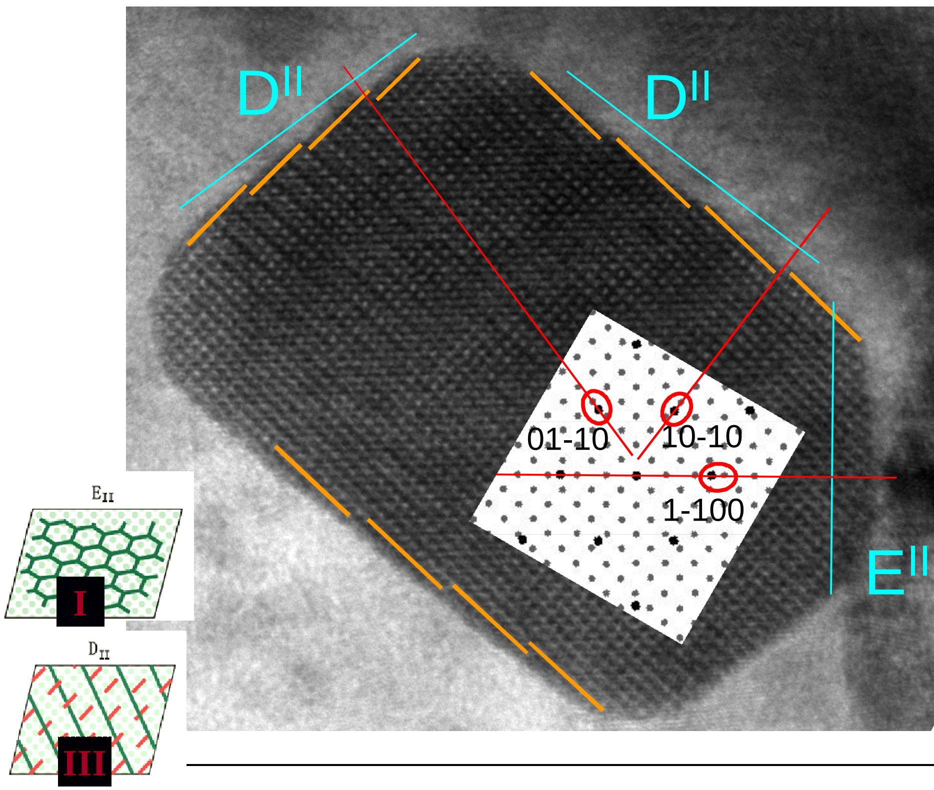
Less dense in F5 $(001)_\tau$ $//(2\text{-}1\text{-}10)_\alpha$, larger b$^{II}$ (E∝b$^2$)

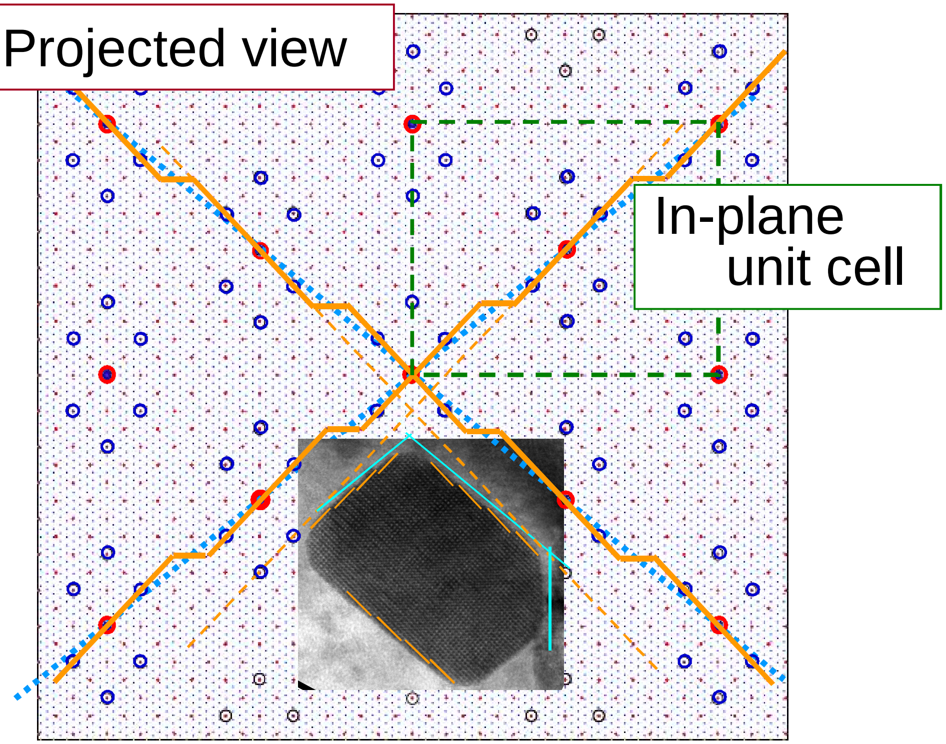
# Secondary CSL model ($Mg_{54}Ag_{17}$, bco)

## (with slight residual strain)

Mg-Sn-Ag-Zn-Mn alloy

Rational OR (NEW):
$(001)_P // (0001)_\alpha$; $[200]_P // [11\text{-}20]_\alpha$




X.-F. Huang, on going Ph. D work

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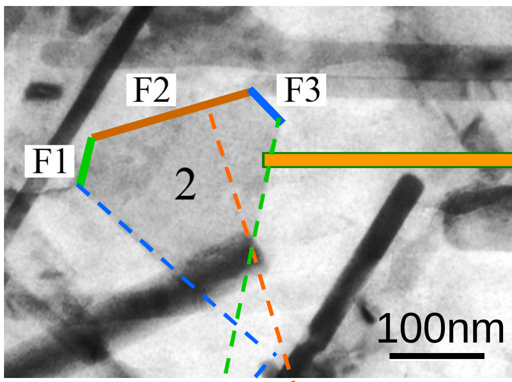
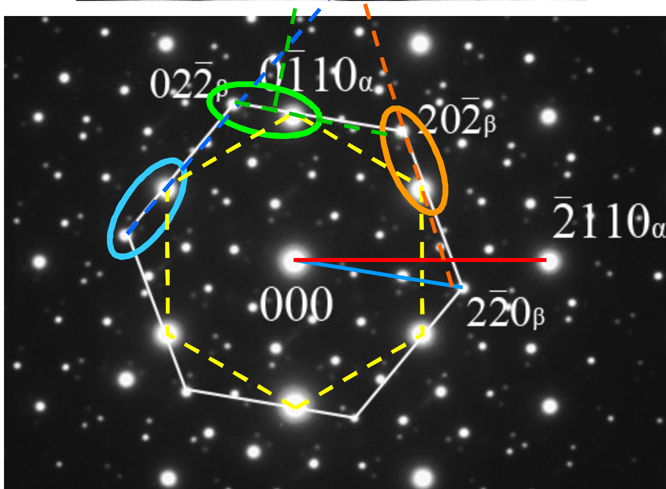
# Secondary CSL model ($\beta$- $Mg_2Sn$, fcc)

## (with slight residual strain)

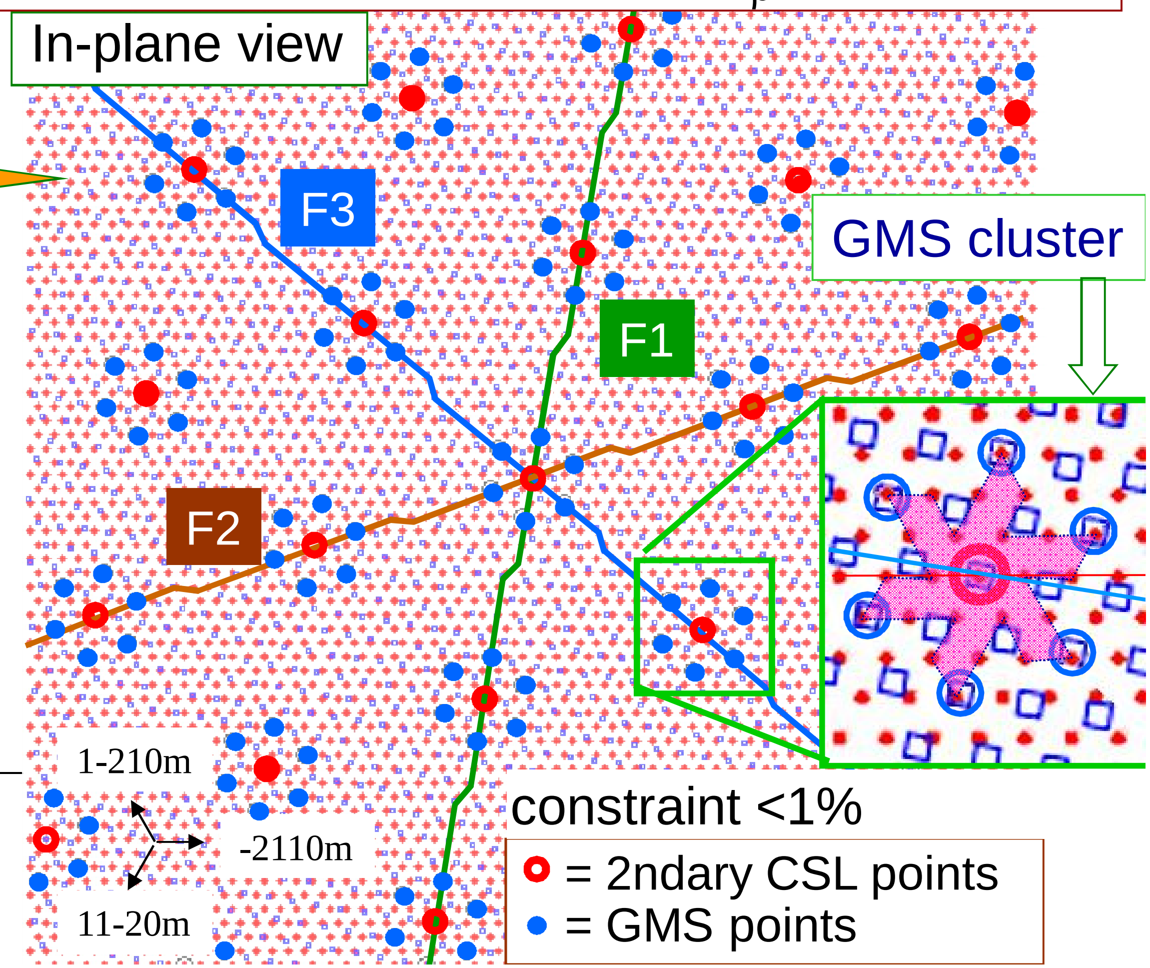
Irrational OR4: $(111)_\beta$ // $(0001)_\alpha$ , $[2\text{-}20]_\beta$ ^ $[2\text{-}1\text{-}10]_\alpha$ = 9.2º

Habit plane //$(111)_\beta$ ($E^{II}$)+ edge facets //$\{0.4\ 7\ \text{-}7.4\}_\beta$ ($D^{II}$)




Shi, Zhang, Zhang, 2010

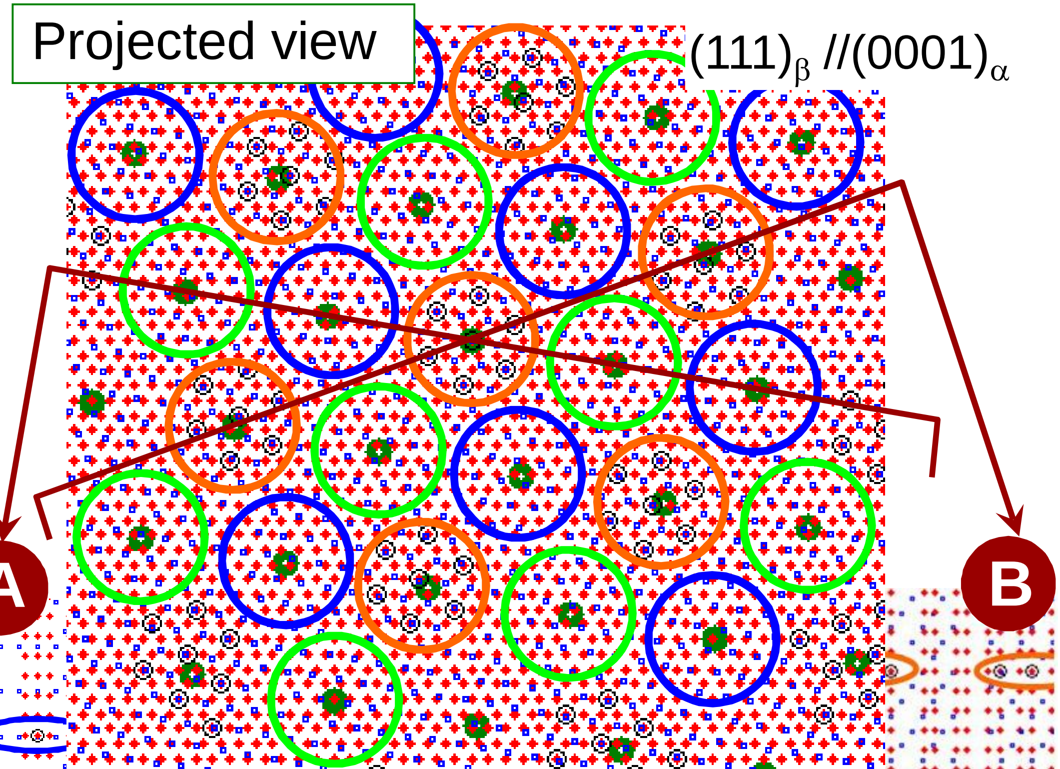


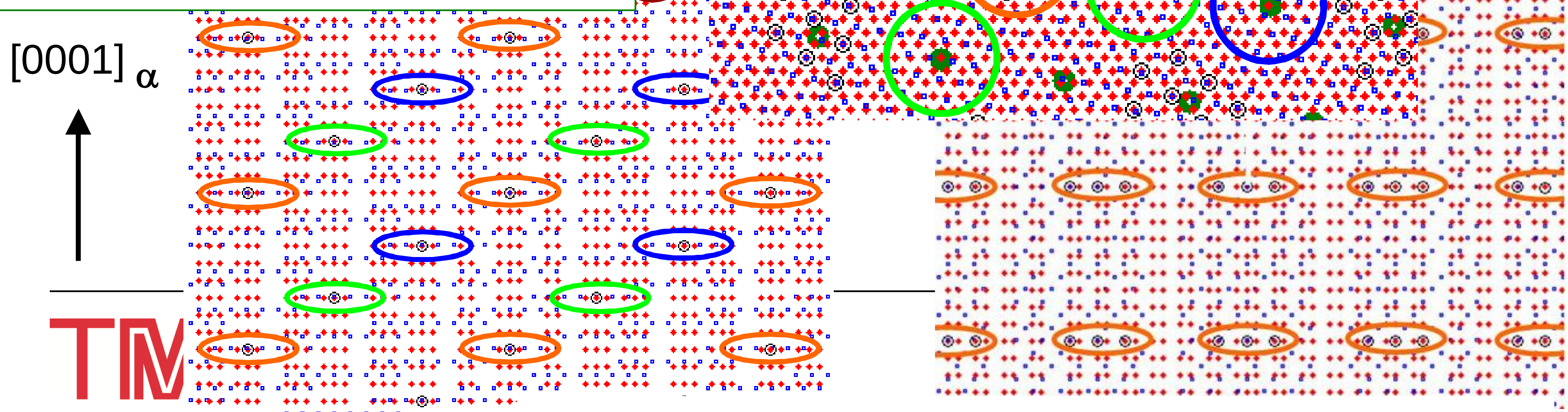
# Three GMS rules for facets—

what if they are conflict?

1. Dense GMS in a cluster
   (Priority: Preferred state) !
2. Dense GMS clusters
   (Prin. O-L plane ⊥ $\Delta g_{P-II}$)
3. Large GMS cluster
   (Small 2ndary misfit)

- Singular structures in A and B
- Overall GMS per unit area
  **B** (0.75) > **A** (0.31)



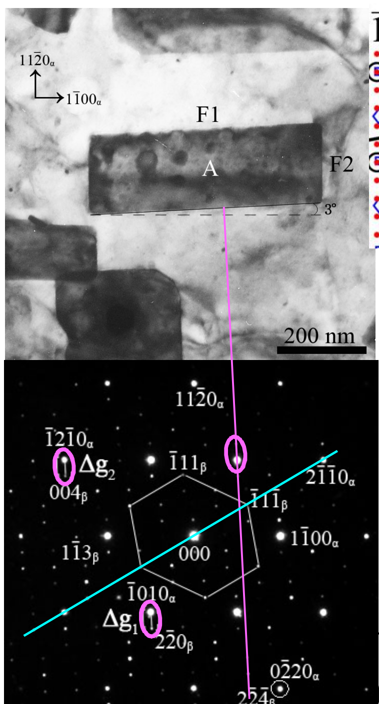



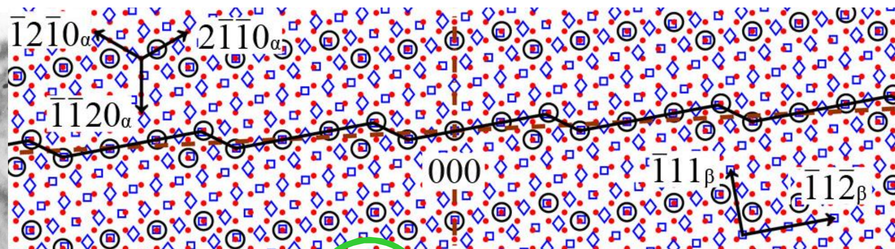

**Z.-Z. Shi, F.-Z. Dai, W.Z. Zhang submitted for publication**

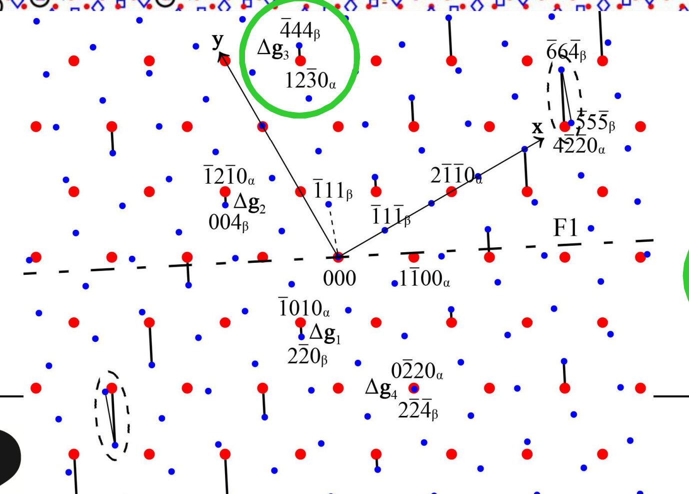
# Continuity of GMS clusters ($\beta$- $Mg_2Sn$, fcc)

OR2 ~Burgers: $(110)_\beta$ // $(0001)_\alpha$ , $[-11-1]_\beta$ ^ $[2-1-10]_\alpha$ = 0.22º
F1// $(-1\ 1\ 0.7)_\beta$ & F2 // $(-1\ 1\ -3.1)_\beta$ (both $E^{II}$)

F1 satisfies 1&2 GMS rules: Dense (continuous) clusters GMS resembling the preferred state



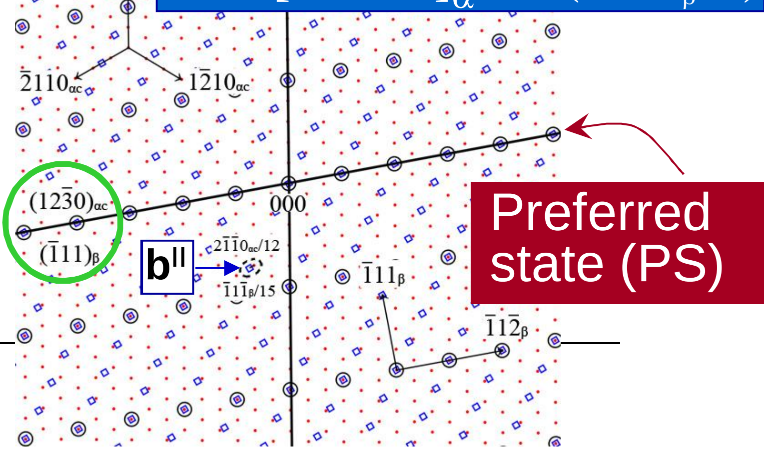




**GMS continuity criterion:**

$|\mathbf{b}^{II}|/2 \leq 15\%a_s$

$|\mathbf{b}^{II}|/2\ (=a_s/24) << 15\%a_s$

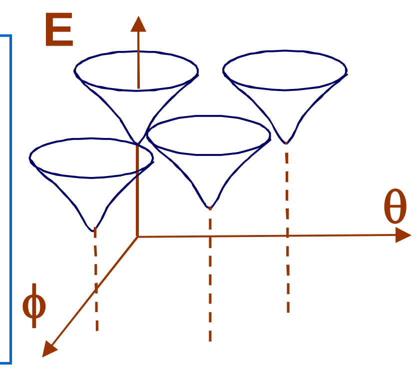
$\mathbf{b}^{II} = [2\text{-}1\text{-}10]_\alpha/12$ $([-11-1]_\beta/15)$

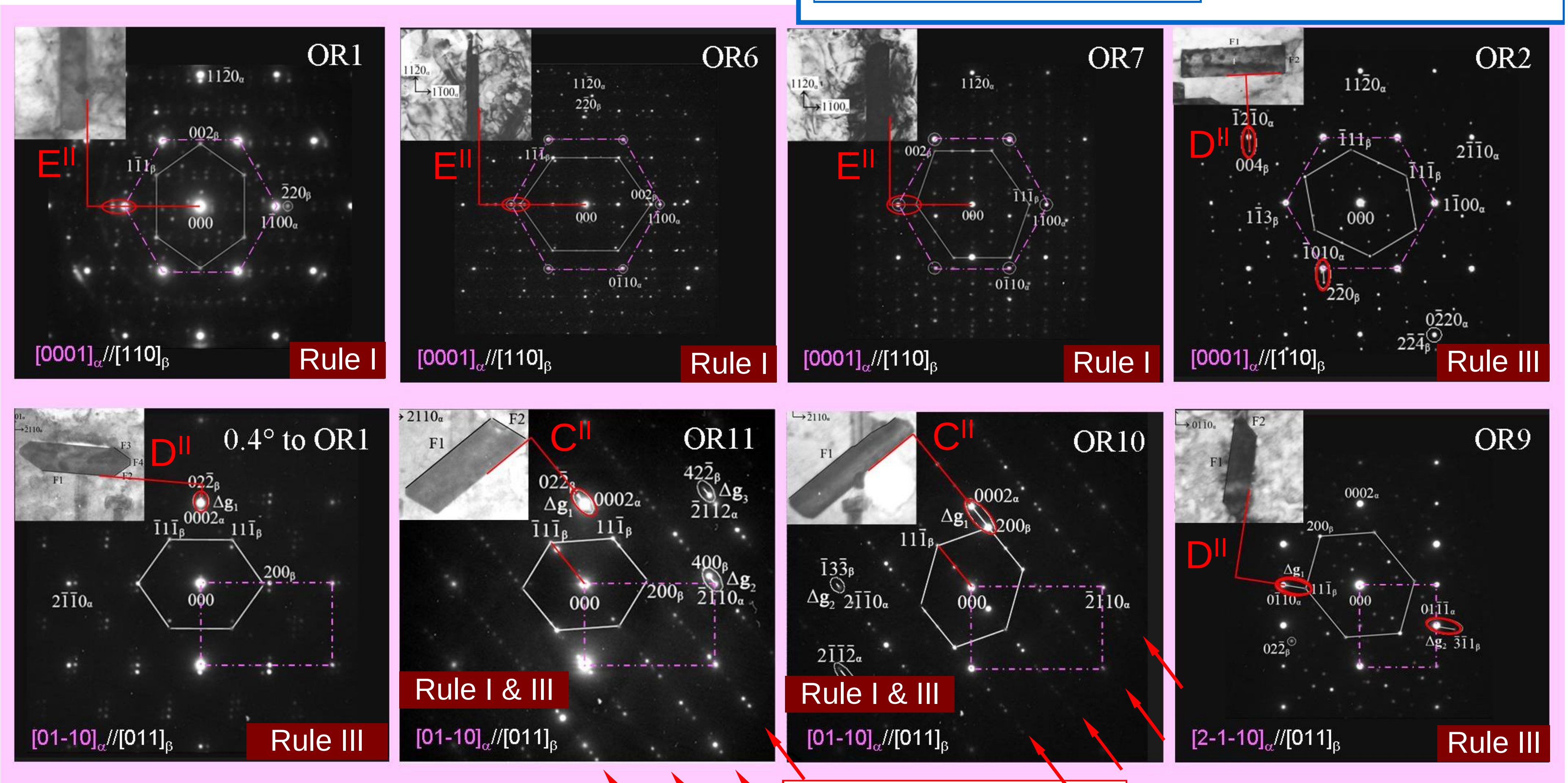



Shi, Zhang, Gu, 2012 Phil Mag.

# Multiple ORs for faceted $Mg_2Sn$ in $\alpha$(Mg-Sn,Mn…)

Multiple high & sharp energy cusps, associated with singular structures



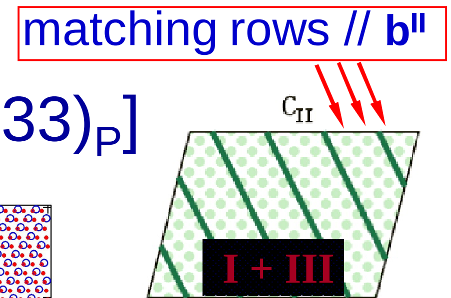



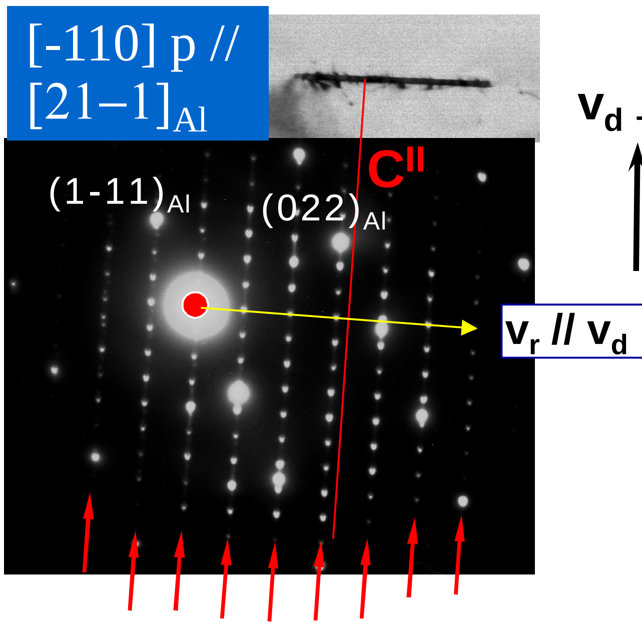

row matching

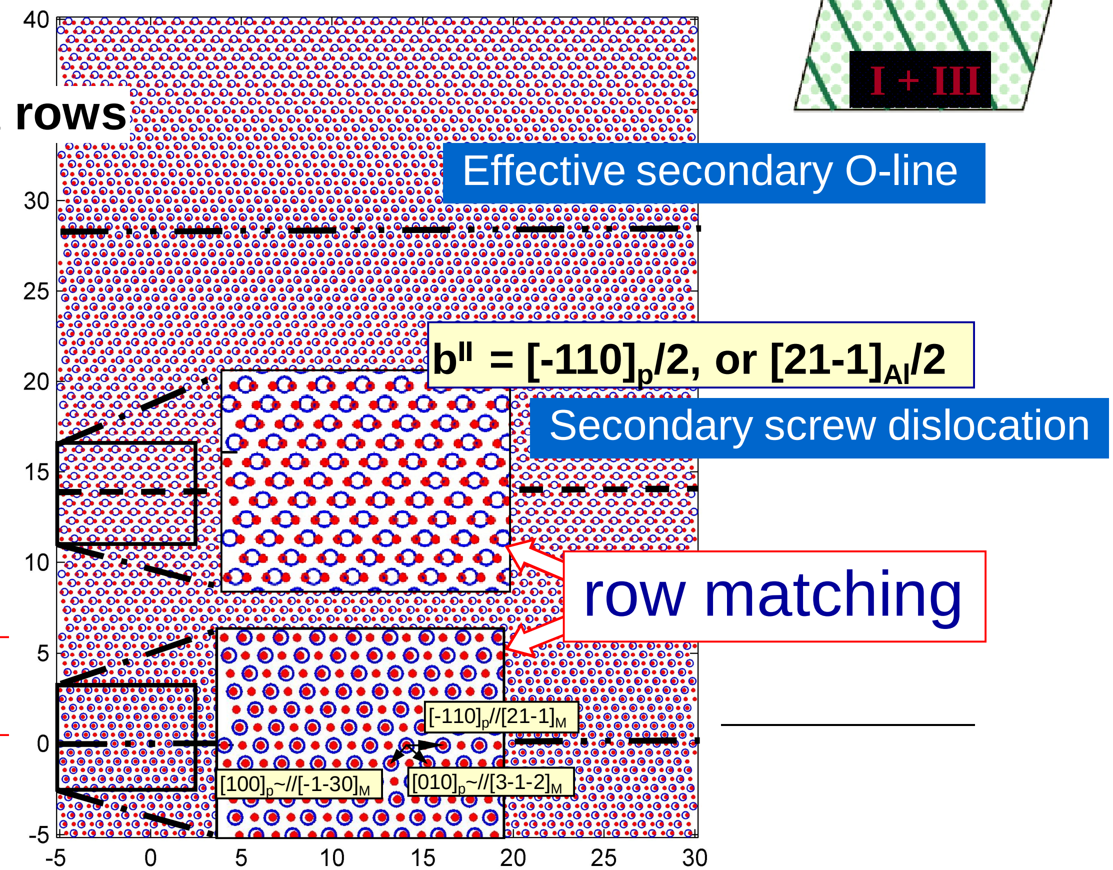
# Row matching in real and reciprocal space for type $C_{II}$ singular interface in Al alloys

**Habit plane normal of $Al_6(Fe,Mn)$//**

$(001)_p$ // $(3\text{-}15)_{Al}$ // $[(1\text{-}11)_{Al}–(113)_P]$ // $[(022)_{Al}–(\text{-}3\text{-}33)_P]$




row matching, **0.2% misfit**

**Y.J. Li et al. 2012**

# Facet of $Al_2CuMg$ in Al-Cu-Mg alloys—revisit

$\Delta \mathbf{g}_1 = \mathbf{g}_{(02\text{-}2)\alpha} - \mathbf{g}_{(062)s}$

$\Delta \mathbf{g}_2 = \mathbf{g}_{(020)\alpha} - \mathbf{g}_{(002)s}$

$\mathbf{g} = (0\ 4\ 3)_s$ (^0.28°)

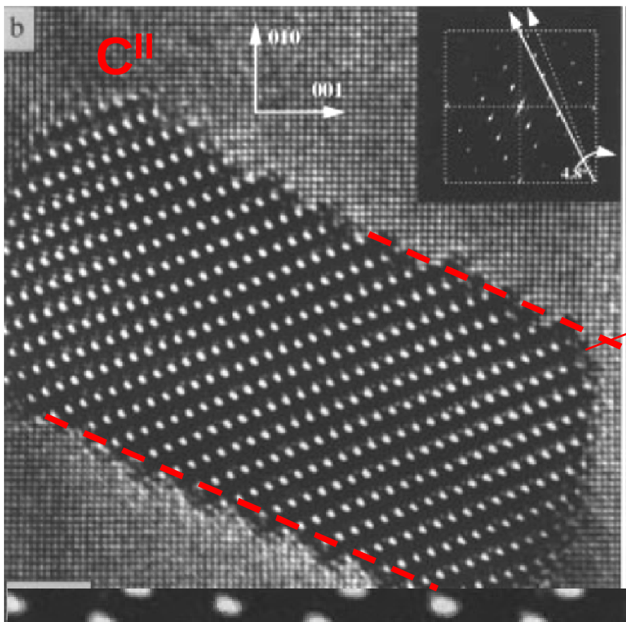
Reported OR (Type II) :

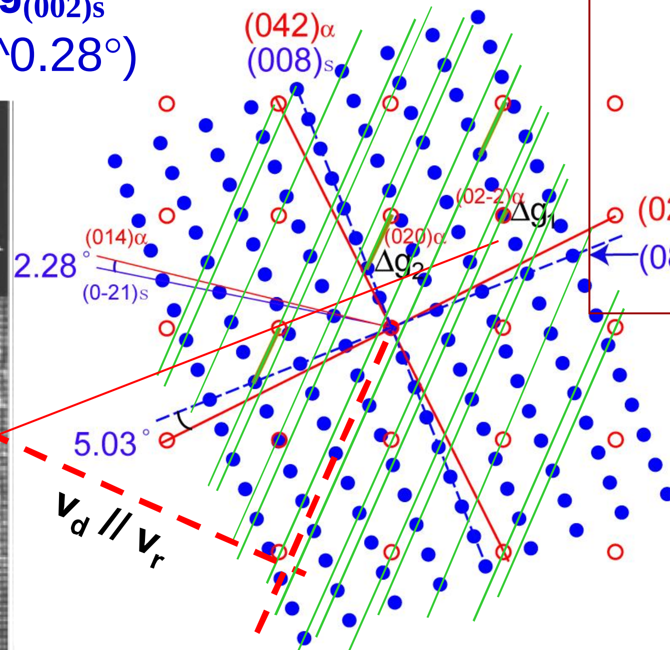
$[100]_s // [100]_\alpha$

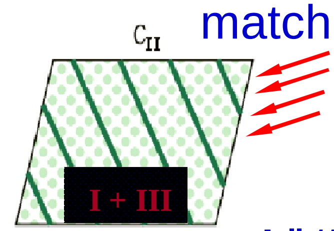
$(0\text{-}21)_s \sim // (014)_\alpha$

Reported facet:

$(0\ 4\ 3)s // (0\ 2\ 1)\alpha$

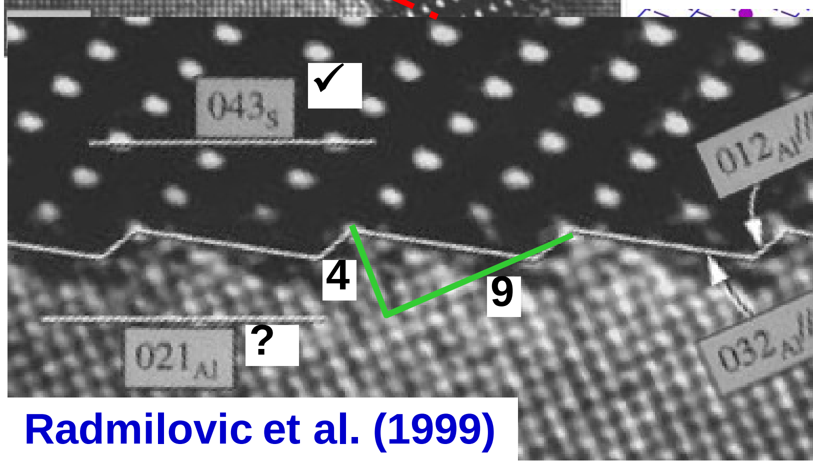


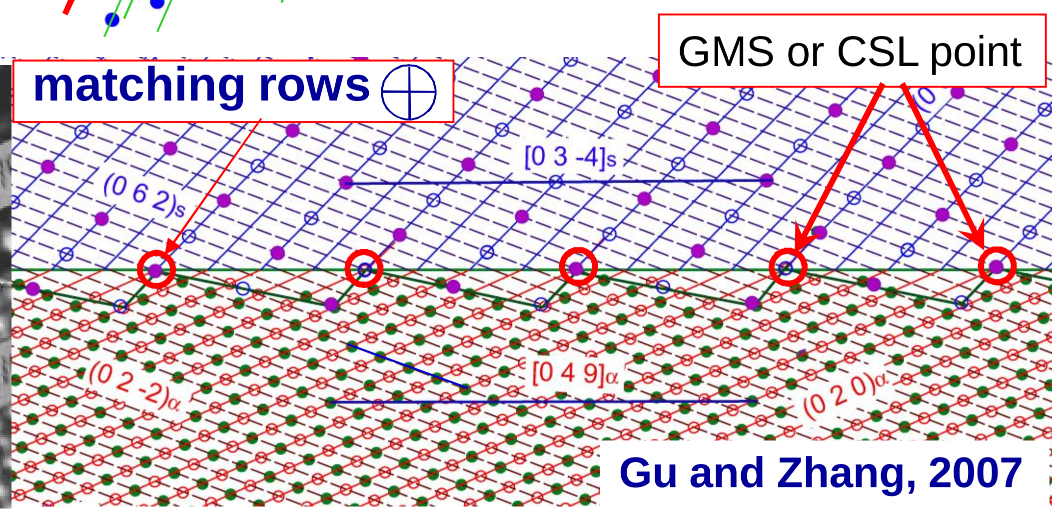




matching rows // b''

b'' //$[100]_s // [100]_\alpha$




Radmilovic et al. (1999)




Gu and Zhang, 2007

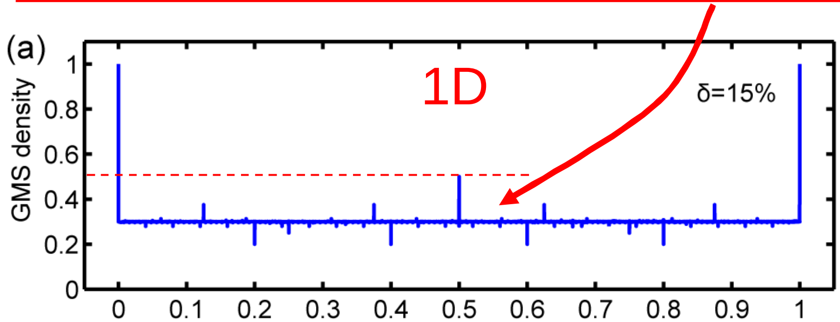
# A simple analysis of GMS for misfit in 1D, 2D and 3D from small to large lattice misfit

**Yang X.-P., ZHANG W.-Z. "A Systematic Analysis of Good Matching Sites between Two Lattices" SCIENCE CHINA Technological Sciences, in press**

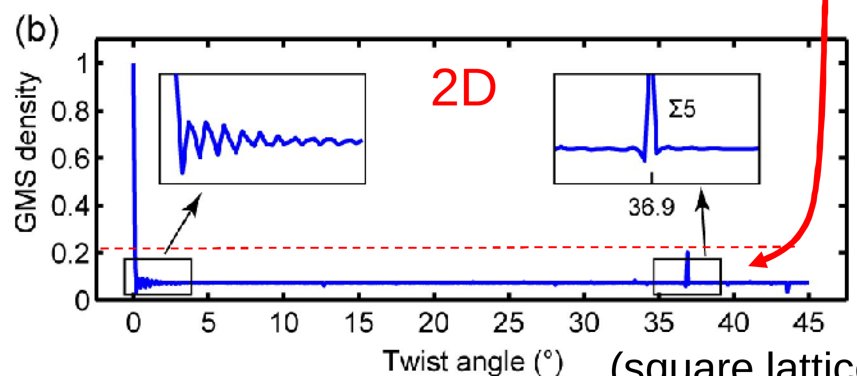
# Singularity in distribution of GMS

Near constant GMS density for nD, except for presence of CSL, independent of lattice misfit !!! (counted in larger lattice)

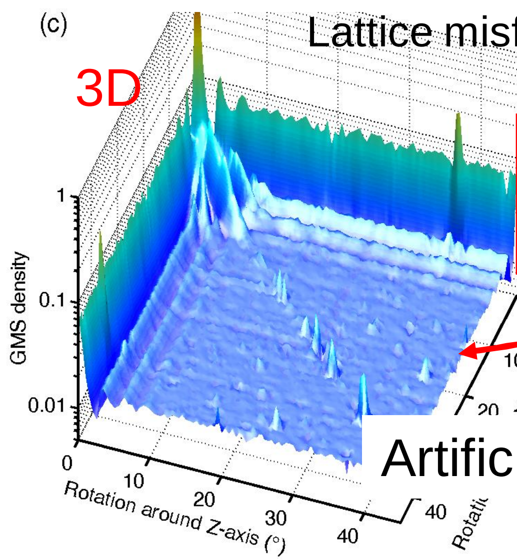
GMS density ~30% (=2$\delta$)




GMS density ~7% (~$\pi\delta^2$)



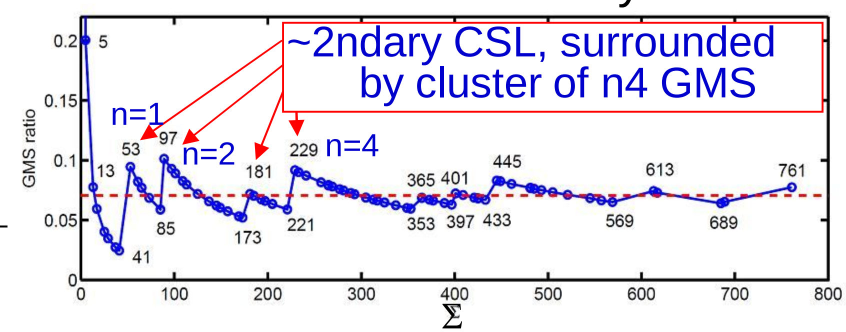

(square lattice)




GMS density ~1.6% (~$4\pi\delta^3/3$)

Artificial grain boundaries

Variation of GMS density with $\Sigma$



# GMS Density in Large Lattice Misfit systems

- GMS density in facet in 2ndary pref. state depends on:
  - $1/\Gamma_\beta$ = Density of CSL points in plane of preferred state
  - No. of $\mathbf{x}_{in}^{II}$ & $\mathbf{x}_i^{II\text{-}O}$ in the interface, or
  - $1/\Gamma_\beta^{II}$ (2ndary CSL) x No. in GMS cluster (e.g. 7/63~11% >7%)
  - $|\mathbf{b}_\alpha^{II}|$ compared with $a_\alpha$

(under Isotropic assumption)

| Misfit dimension | 0 | 1 | 2 | 3 |
|---|---|---|---|---|
| ~ GMS density | $1/\Gamma_\beta$ | $\sim 30\% a_\alpha/(\Gamma_\beta \lvert \mathbf{b}_\alpha^{II} \rvert)$ | $\sim 7\% a_\alpha^2/(\Gamma_\beta \lvert \mathbf{b}_\alpha^{II} \rvert^2)$ | ~1.4% |
| Singular vectors | $\mathbf{x}_{in1}^{II} + \mathbf{x}_{in2}^{II}$ | $\mathbf{x}_{in}^{II} + \mathbf{x}_i^{II\text{-}O}$ | $\mathbf{x}_1^{II\text{-}O} + \mathbf{x}_2^{II\text{-}O}$ | $\mathbf{x}_1^{II\text{-}O}$ or $\mathbf{x}_{in}^{II} \leq 1$ |
| Singular interf. $\perp$ | 3$\Delta\mathbf{g}_{II}$'s | 2$\Delta\mathbf{g}_{II}$'s | 1$\Delta\mathbf{g}_I$ | 0 |

$\mathbf{b}_\alpha^{II}$ must be large ($<a_\alpha/3$) for cluster feature (singularity) to be prominent

**+**

$a_\alpha^2/(\Gamma_\beta |\mathbf{b}_\alpha^{II}|^2) \approx 1$
$(\Gamma_\beta/\Gamma_{DSC\alpha}=1)$

$\Rightarrow$ $\boxed{\Gamma_\beta \leq 4}$

# Summary

- Faceted interfaces are often observed in systems consisting between intermetallic compounds and metal matrix. They can be interpreted in terms of singularity in interfacial structure, possible only at special OR and interface orientations
- Parameters to describe structure singularity include
  - Dislocation structure—identified by $\mathbf{x}_i^{II\text{-}O}$ and/or $\mathbf{x}_{in}^{II}$
  - $\Delta\mathbf{g}$ arrangement—parallelism rule I &/or III (app. rowing matching)
  - Distribution of GMS—discrete density values
- Special properties, compared to primary preferred state (I)
  - Multiple preferred states (I: one), & corresponding OR and facets
  - Alignment of GMS rows in almost all facets (I: no always)
  - Existence of slight long-range strain, for more singular features (I: no often)

# *Thank you*

**Support of NSFC**