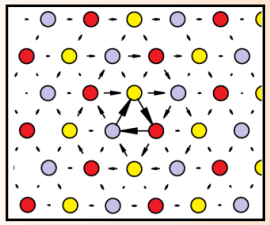
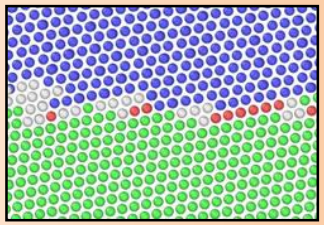
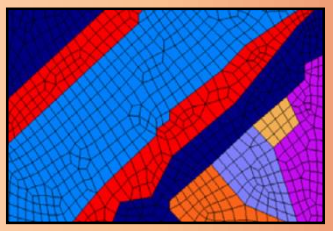
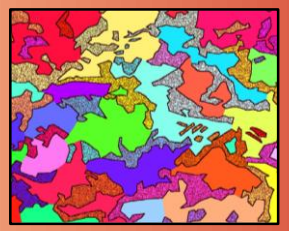
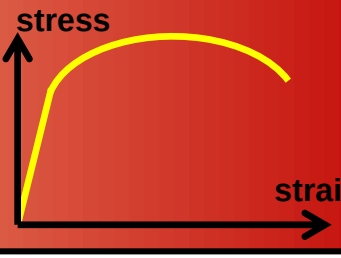

Contributions of austenite-martensite transformation to deformability of steels

From atomistic mechanisms to microstructural response

Francesco Maresca, William A. Curtin

LAMMM / Laboratory for Multiscale Mechanics Modeling

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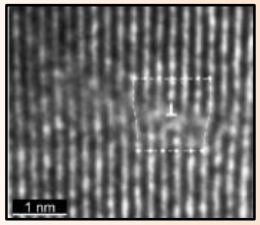
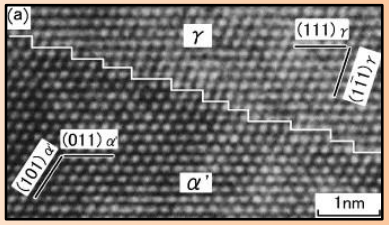
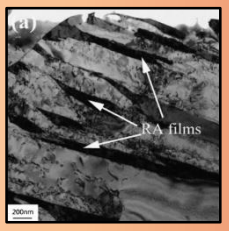
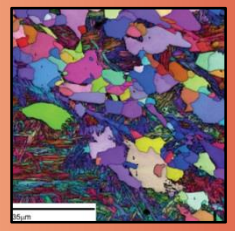
Funding from
European Research Council Advanced Grant Program for the project
"Predictive Computational Metallurgy" (W.A. Curtin)

10^{-10} 10^{-9} 10^{-6} 10^{-3} 1 m

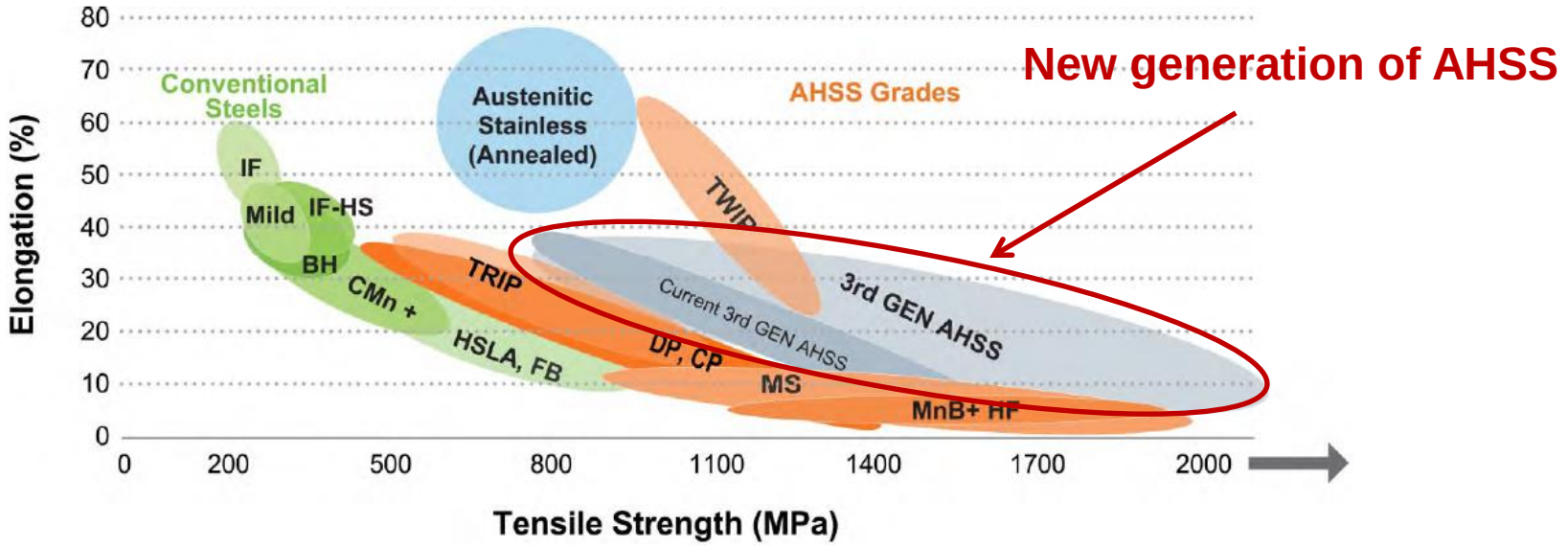









Advanced High Strength Steels: Nanolaminate Martensite/Austenite Microstructures



(World Auto Steel, AHSS application guidelines 2014 – V5.0)

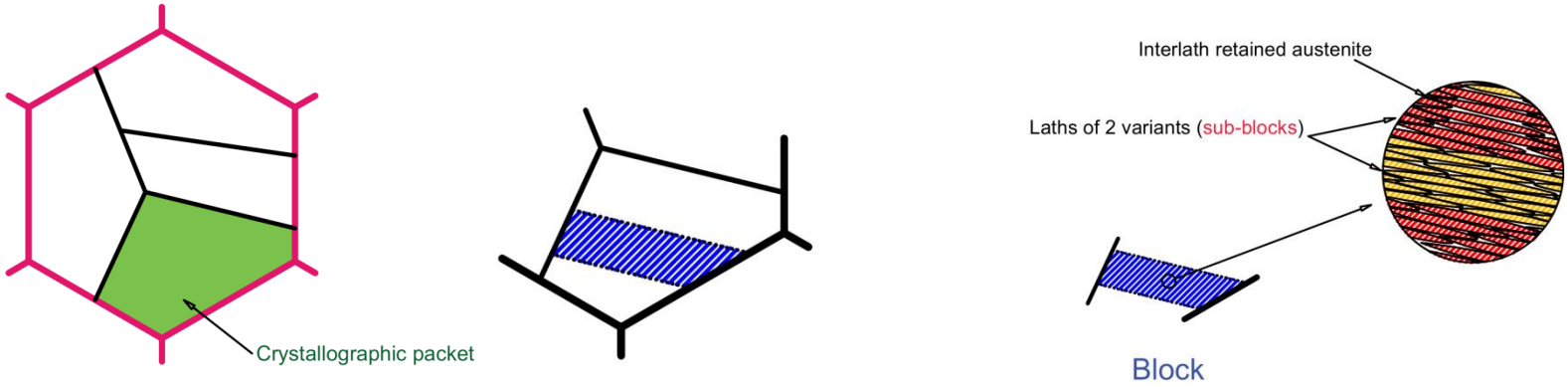
Nanolaminate martensite/austenite prevalent in

- Quenched and partitioned (Q&P) steels;
- TRIP steels;
- Bainitic
- Nanobainitic
- …

High strength (1-2 GPa) and elongation (10-30%)

Nano-/micro-scale determines Macroscale response!

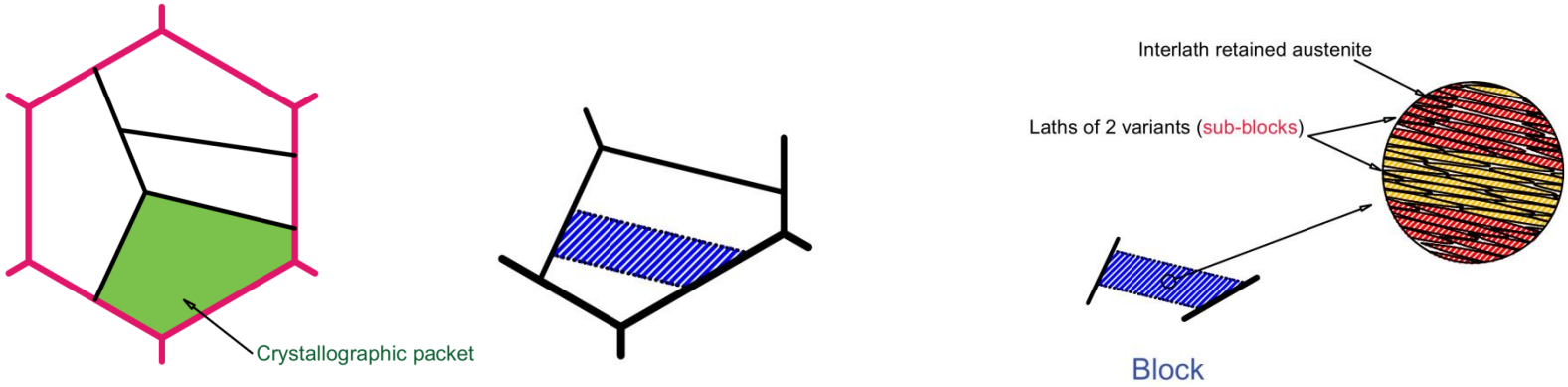
Hierarchical microstructure over multiple length scales



i. **Prior austenite** (10-500 μm) ii. **Packets** (10-100 μm) iii. **Blocks** (3-30 μm) iv. **Subblocks** (1-10 μm)

v. **Laths** (100-500 nm) vi. **Interlath retained austenite** (5-50 nm)

Hierarchical microstructure over multiple length scales



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martensite-austenite laminate (block/sub-block model):

1) $\boldsymbol{F}_L = \xi \boldsymbol{F}_M + (1-\xi)\boldsymbol{F}_A$ Laminate def. = phase average deformation

2) $\boldsymbol{P}_L = \xi \boldsymbol{P}_M + (1-\xi)\boldsymbol{P}_A$ Laminate stress = phase average stress

constraints:

3) $\boldsymbol{F}_M \cdot (\boldsymbol{I} - \boldsymbol{p} \otimes \boldsymbol{p}) = \boldsymbol{F}_A \cdot (\boldsymbol{I} - \boldsymbol{p} \otimes \boldsymbol{p})$ Phase compatibility

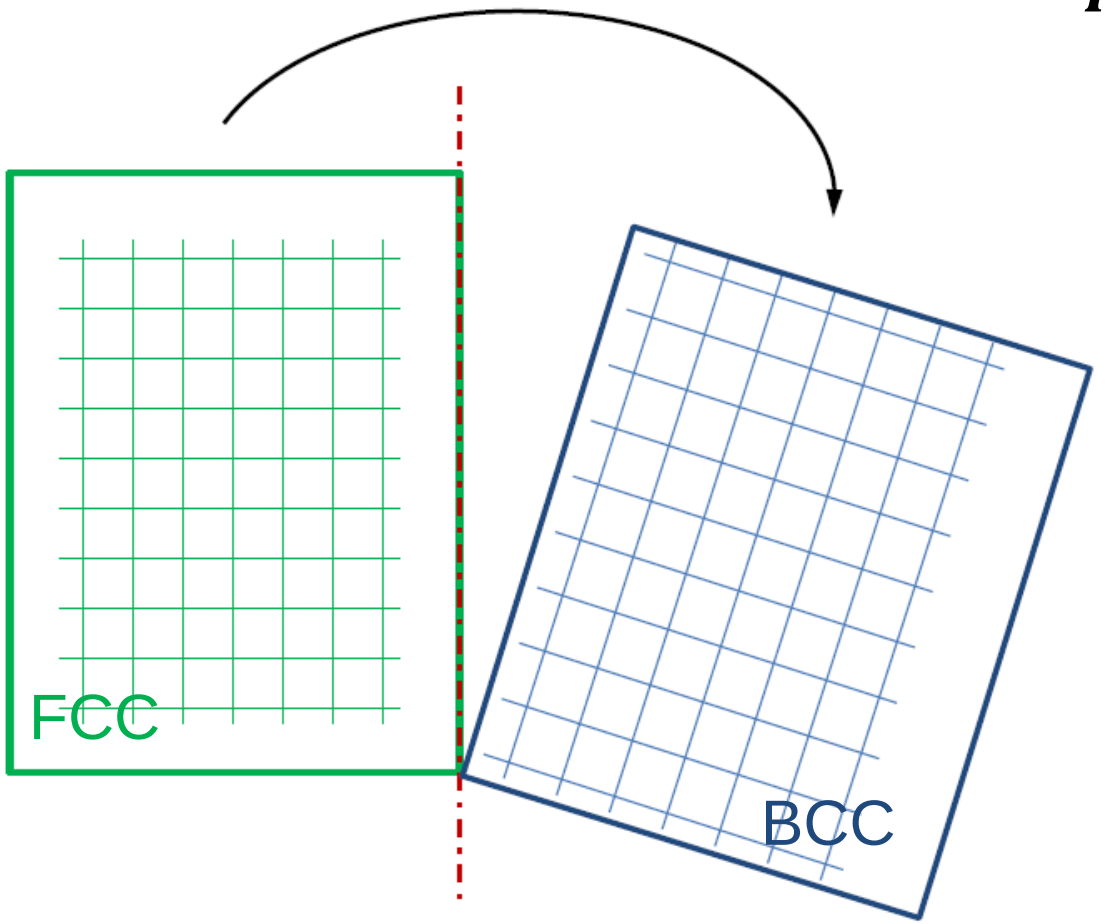
4) $\boldsymbol{P}_M \cdot \boldsymbol{p} = \boldsymbol{P}_A \cdot \boldsymbol{p}$ Interface equilibrium

phase constitutive equations: $\boldsymbol{P}_A = \mathcal{F}(\boldsymbol{F}_A)$ $\boldsymbol{P}_M = \mathcal{G}(\boldsymbol{F}_M)$

Austenite-martensite phase transformation model

Lattice transformation

$$\boldsymbol{S} = \boldsymbol{R} \cdot \boldsymbol{B}$$



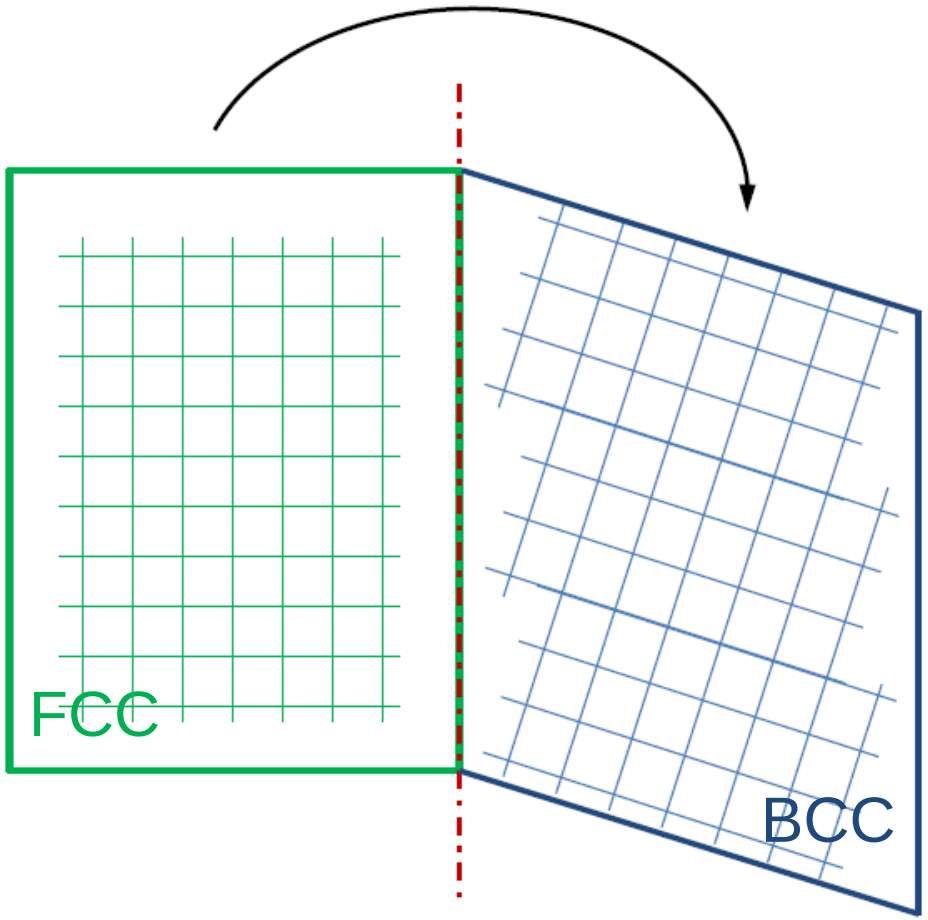
Orientation relationship

$$\boldsymbol{R} = \boldsymbol{R}_{\varphi} \cdot \boldsymbol{R}_{\psi}$$

Austenite-martensite phase transformation model

In situ transformation strain ("shape deformation")

$$\boldsymbol{P}^{(1)} = \boldsymbol{S} \cdot \boldsymbol{P}^{(3)} \cdot \boldsymbol{P}^{(2)}$$



Orientation relationship

$$\boldsymbol{R} = \boldsymbol{R}_{\varphi} \cdot \boldsymbol{R}_{\psi}$$

Lattice transformation

$$\boldsymbol{S} = \boldsymbol{R} \cdot \boldsymbol{B}$$

Lattice invariant shears

$$\boldsymbol{P}^{(2)} = \boldsymbol{I} + m^{(2)}\boldsymbol{s}^{(2)} \otimes \boldsymbol{n}^{(2)}$$

$$\boldsymbol{P}^{(3)} = \boldsymbol{I} + m^{(3)}\boldsymbol{s}^{(3)} \otimes \boldsymbol{n}^{(3)}$$

Atomistic interface *vs* experiments

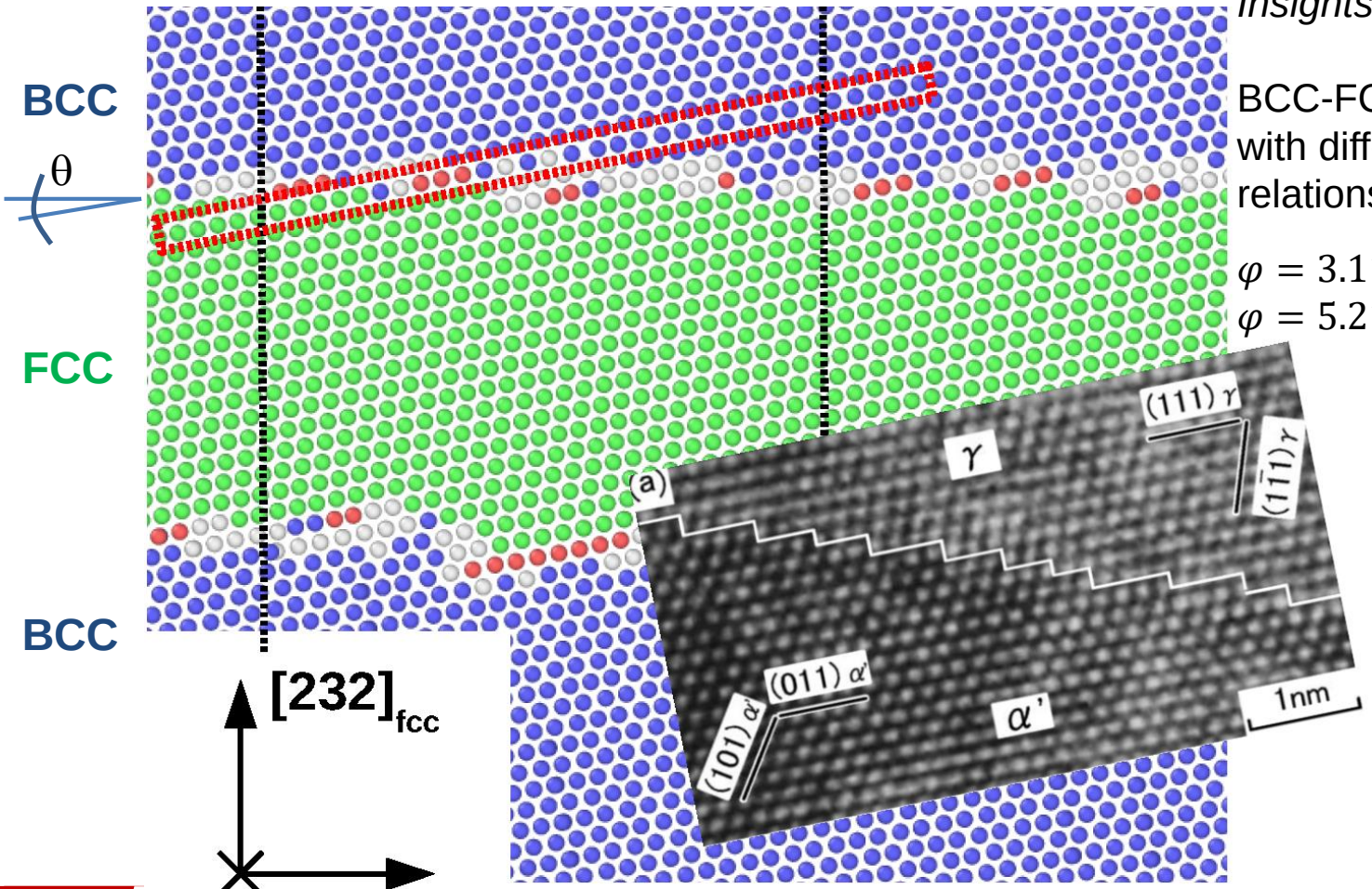
1) Interface orientation mismatch not important (local variations)
2) Phases aligned with experiments!
3) Interface steps like experiments
4) Same match on other orientation (not shown here)

[Molecular statics (T=0K) with MEAM-T Fe potential (Lee et al. 2012)]

Insights trascend the potential

BCC-FCC (periodic) bicrystals with different orientation relationships:

$\varphi = 3.11°$, $\varphi = 4.75°$,
$\varphi = 5.21°$ (~NW), $\varphi = 5.7°$



$\theta = 11°$
$\varphi = 4.75°$ interface

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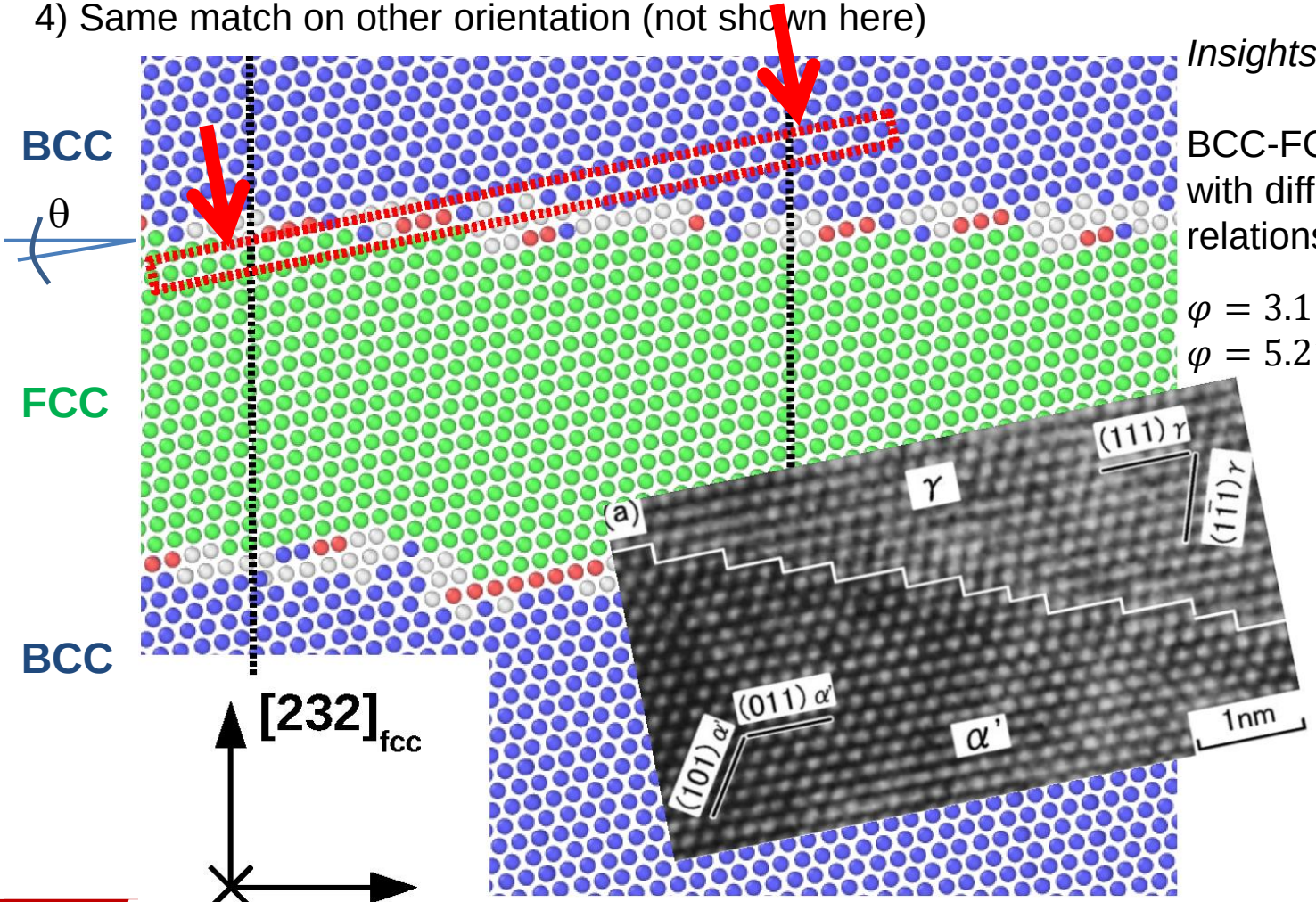
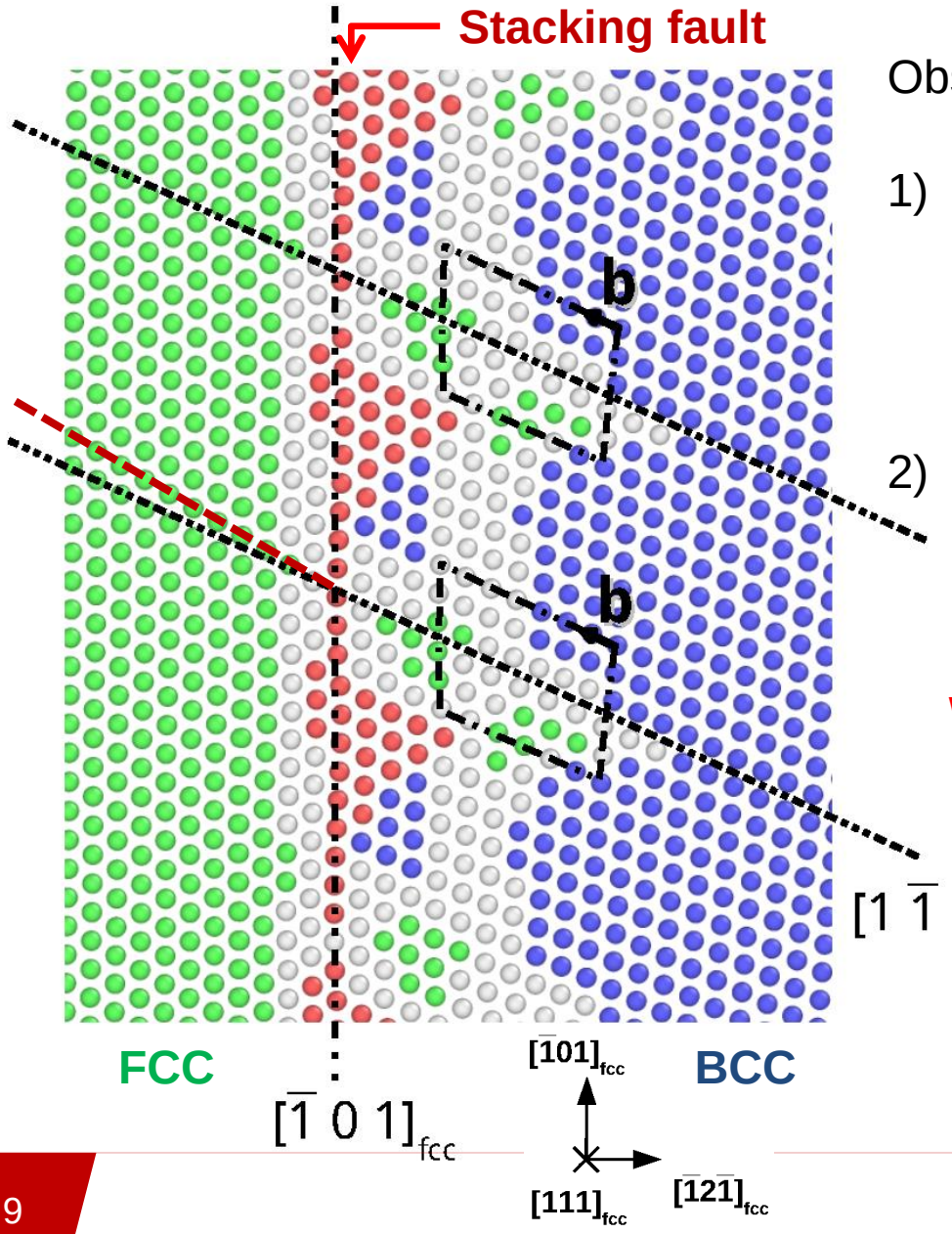


$\theta = 11°$
$\varphi = 4.75°$ interface

Atomistic interface defects



Observed interface structure:

1) $a_{fcc}/2\ [\bar{1}01]$ **screw** dislocations

gliding on $(111)_{fcc}$

2) $a_{bcc}/2\ [1\bar{1}1]$ **kinks in the bcc**

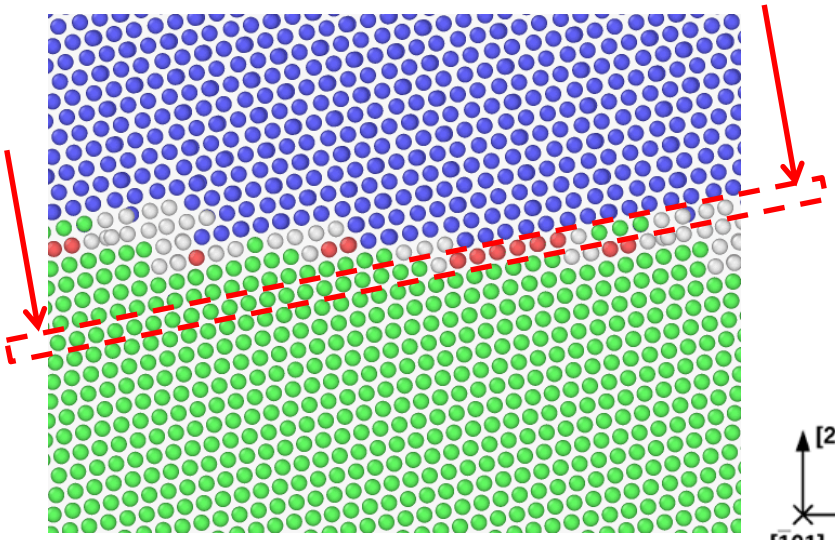
gliding on $(\bar{1}01)_{bcc}$

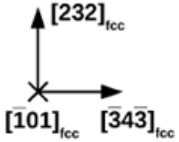
Why was this not considered before?

Thought that it could not be glissile: crossing dislocations

BUT there is no slip plane for these bcc segments to move into the fcc phase (misaligned)

Atomistic interface motion

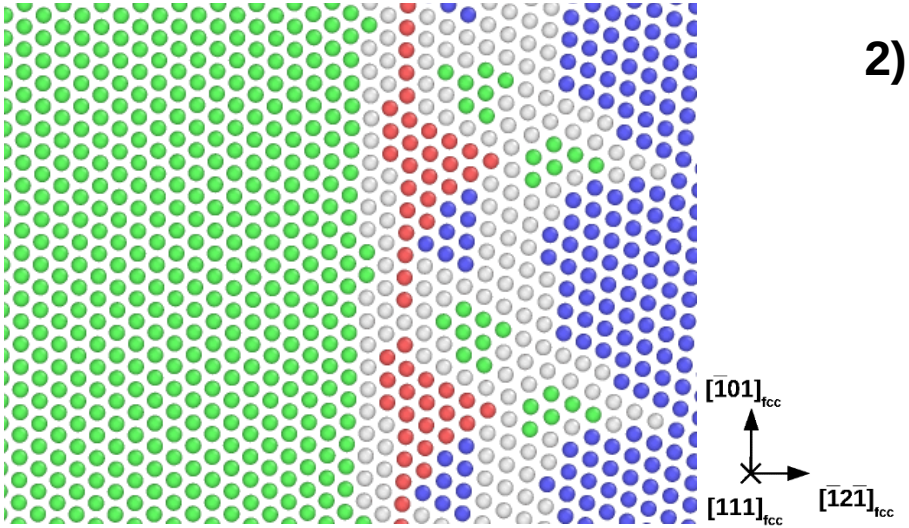




The interface can glide, at ~zero stress!

1) **Defects do not interact/cross**

2) **They glide in a cooperative manner**



Predictive theory of martensite crystallography

Determination of the shape deformation

$$\boldsymbol{P}^{(1)} = \boldsymbol{S} \cdot \boldsymbol{P}^{(3)} \cdot \boldsymbol{P}^{(2)}$$

where $\boldsymbol{S} = \boldsymbol{R} \cdot \boldsymbol{B}$ $\quad (\boldsymbol{R} = \boldsymbol{R}_{\varphi} \cdot \boldsymbol{R}_{\psi})$

$$\boldsymbol{P}^{(i)} = \boldsymbol{I} + m^{(i)} \boldsymbol{s}^{(i)} \otimes \boldsymbol{n}^{(i)} \qquad i = 1,2,3$$

1) Specify $\boldsymbol{P}^{(2)}, \boldsymbol{P}^{(3)}$

2) Calculate $\boldsymbol{P}^{(1)} = \boldsymbol{I} + m^{(1)} \boldsymbol{s}^{(1)} \otimes \boldsymbol{n}^{(1)}$

   a. Habit plane normal vector $\boldsymbol{n}^{(1)}$

   b. Shape deformation direction $\boldsymbol{s}^{(1)}$

   c. Shape deformation magnitude $m^{(1)}$

} Experimentally measurable **variables**

Predictive theory of martensite crystallography

From atomistics we see:

1) $\boldsymbol{P}^{(2)}$ is the shear due to $a_{\mathrm{bcc}}/2\ [1\bar{1}1]$ kinks on $(\bar{1}01)_{\mathrm{bcc}}$

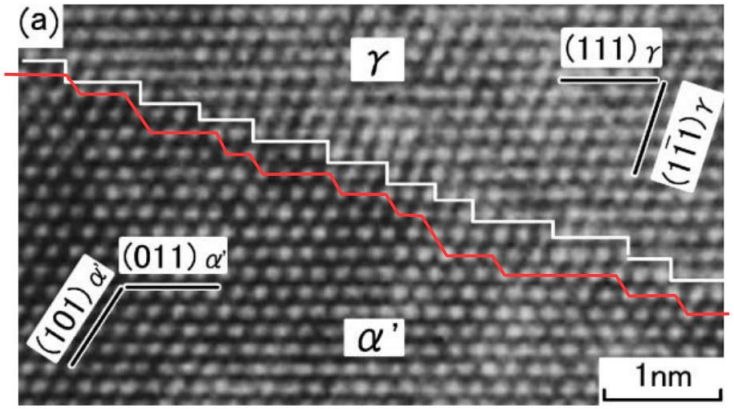
$$\boldsymbol{P}^{(2)} = \boldsymbol{I} + m^{(2)}\boldsymbol{s}^{(2)} \otimes \boldsymbol{n}^{(2)}$$

All known

2) $\boldsymbol{P}^{(3)}$ is the shear due to $a_{\mathrm{fcc}}/2\ [\bar{1}01]$ screw dislocations on $(111)_{\mathrm{fcc}}$

$$\boldsymbol{P}^{(3)} = \boldsymbol{I} + m^{(3)}\boldsymbol{s}^{(3)} \otimes \boldsymbol{n}^{(3)}$$

Unknown **Known**



$$m^{(3)} = \frac{b}{h_{\mathrm{ave}}}$$ (there is 1 screw per step!)

$$h_{\mathrm{ave}} = \beta\frac{a_{\mathrm{fcc}}}{\sqrt{3}} \qquad \beta \geq 1$$ (outcome of calculations)

Predictive theory of martensite crystallography

Calculation procedure:

Ogawa & Kajiwara (2004)

1) Guess $\beta \rightarrow \boldsymbol{P}^{(3)}$

2) Calculate $\boldsymbol{P}^{(1)} = \boldsymbol{S} \cdot \boldsymbol{P}^{(3)} \cdot \boldsymbol{P}^{(2)}$

3) Calculate right stretch tensor $\boldsymbol{U} = \sqrt{[\boldsymbol{P}^{(1)}]^T \cdot \boldsymbol{P}^{(1)}}$

4) Calculate the eigenvalues $\begin{pmatrix} \lambda_{\min} \\ \lambda_{\text{int}} \\ \lambda_{\max} \end{pmatrix}$

5) Tune β : iterate 1-4 until λ_{int}=1

→ $\boldsymbol{P}^{(1)}$ can be written in the form $\boldsymbol{P}^{(1)} = \boldsymbol{I} + m^{(1)} \boldsymbol{s}^{(1)} \otimes \boldsymbol{n}^{(1)}$

where $m^{(1)}$, $\boldsymbol{s}^{(1)}$ and $\boldsymbol{n}^{(1)}$ are functions of $(\lambda_{\min}, \lambda_{\max})$ and their eigenvectors $(\boldsymbol{e}_{\min}, \boldsymbol{e}_{\max})$

→ $\boldsymbol{R}_{\Delta}$ making contact with experiments

Theory validation on atomistic simulations

Theory with defects is consistent with all aspects of simulations!

	Simulations	Theory	Simulations	Theory
$\frac{a_{\mathrm{fcc}}}{a_{\mathrm{bcc}}}$	$\simeq 1.2537$	1.2537	$\simeq 1.2518$	1.2518
φ	4.75°	4.75°	3.11°	3.11°
β	1.5	1.515	1.46	1.552
$\boldsymbol{n}^{(1)}$	$(2\ 3\ 2)_{\mathrm{fcc}}$	$(2\ 3\ 2)_{\mathrm{fcc}}$	$(10\ 17\ 10)_{\mathrm{fcc}}$	$(10.5\ 17.6\ 10)_{\mathrm{fcc}}$
$\boldsymbol{s}^{(1)}$	$[\bar{1}\ 0\ 1]_{\mathrm{fcc}} + 19.5°$	$[\bar{1}\ 0\ 1]_{\mathrm{fcc}} + 19.5°$	$[\bar{1}\ 0\ 1]_{\mathrm{fcc}} + 19.9°$	$[\bar{1}\ 0\ 1]_{\mathrm{fcc}} + 20.4°$
$m^{(1)}$	0.59	0.57	0.55	0.56
$d\theta$	0.34°	0.28°	0.49°	0.34°
$d\varphi$	0° (constrained)	−0.15°	0° (constrained)	0.017°
$d\chi$	0° (constrained)	−0.003°	0° (constrained)	0.021°
η	0° (constrained)	0.38°	0° (constrained)	3.5°
s_η	----	37.9 nm	----	4.1 nm

Defined input

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$\boldsymbol{s}^{(1)}$	$[\bar{1}\ 0\ 1]_{\mathrm{fcc}} + 19.5°$	$[\bar{1}\ 0\ 1]_{\mathrm{fcc}} + 19.5°$	$[\bar{1}\ 0\ 1]_{\mathrm{fcc}} + 19.9°$	$[\bar{1}\ 0\ 1]_{\mathrm{fcc}} + 20.4°$
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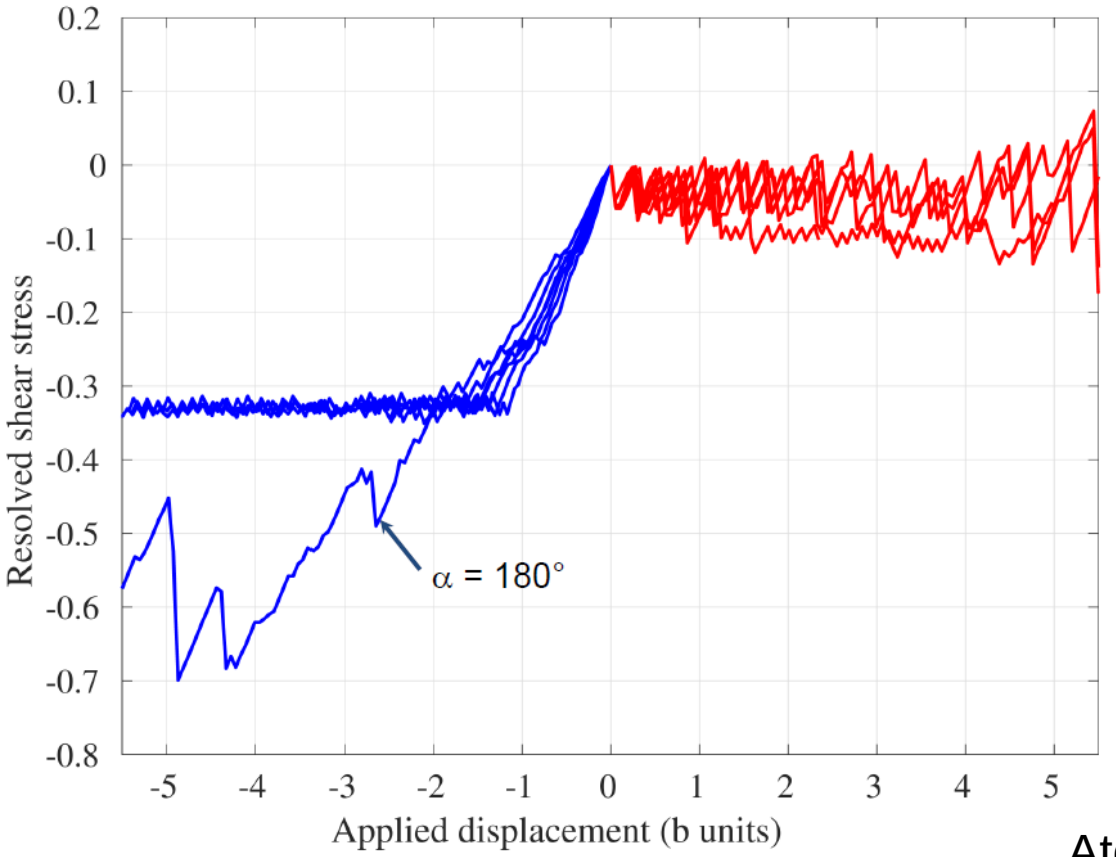
Defined input

Activation criterion for transformation



$$\tau = \boldsymbol{\Sigma}: \left(\boldsymbol{s}^{(1)} \otimes \boldsymbol{n}^{(1)}\right)$$

evaluated for all α at which transformation (forward/reverse) occurs.

← All curves overlap (except $\alpha = 180°$)

→Transformation initiated as slip in crystal plasticity

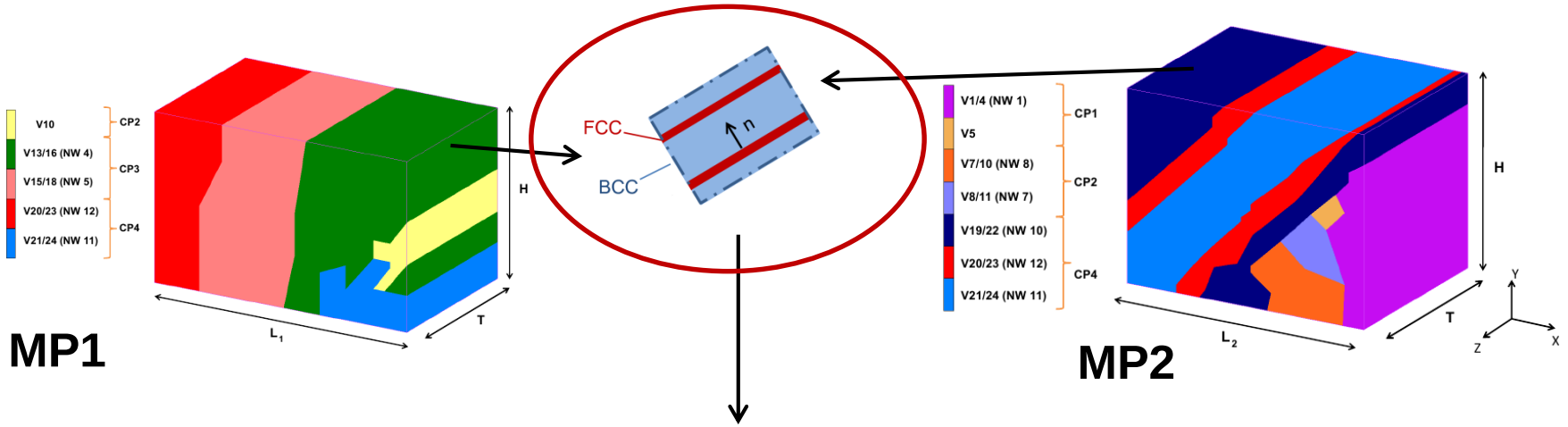
$$f = |\tau| - \tau_c \leq 0 \quad \dot{\varepsilon}_{tr} \geq 0 \quad f\dot{\varepsilon}_{tr} = 0$$

↓

Atomistic justification of Patel-Cohen criterion for phase transformations!

f transformation criterion
τ_c critical resolved shear stress at which transformation starts
$\dot{\varepsilon}_{tr}$ transformation rate (∝ normalized interface speed)

Continuum model for austenite-martensite laminate



martensite-austenite laminate:

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2) $\boldsymbol{P}_L = \xi \boldsymbol{P}_M + (1-\xi)\boldsymbol{P}_A$ Laminate stress = phase average stress

constraints:

3) $\boldsymbol{F}_M \cdot (\boldsymbol{I} - \boldsymbol{p} \otimes \boldsymbol{p}) = \boldsymbol{F}_A \cdot (\boldsymbol{I} - \boldsymbol{p} \otimes \boldsymbol{p})$ Phase compatibility

4) $\boldsymbol{P}_M \cdot \boldsymbol{p} = \boldsymbol{P}_A \cdot \boldsymbol{p}$ Interface equilibrium

phase constitutive equations: $\boldsymbol{P}_A = \mathcal{F}(\boldsymbol{F}_A)$ $\boldsymbol{P}_M = \mathcal{G}(\boldsymbol{F}_M)$

Continuum model for transformation

Single-phase models / constitutive assumptions and evolution laws

Elasticity: $\overline{\boldsymbol{S}} = \mathbb{C}: \boldsymbol{E}_e$ Hooke's law $(\boldsymbol{P} = \boldsymbol{F}_e \cdot \overline{\boldsymbol{S}} \cdot \boldsymbol{F}_i^{-T})$

Transformation (in Austenite)

$$\dot{\varepsilon}_{tr}^{\alpha} = \dot{\varepsilon}_0 \left(\frac{\tau^{\alpha}}{\tau_{tr}^{\alpha}} \right)^{1/m} \qquad \tau^{\alpha} = \langle (\boldsymbol{C}_e \cdot \overline{\boldsymbol{S}}) : \boldsymbol{s}^{(1)} \otimes \boldsymbol{n}^{(1)} \rangle \qquad \text{Ass.: } \xi = \xi_0, \quad \varepsilon_{tr,max} = \varepsilon_{tr}$$

Plastic slip (in Martensite)

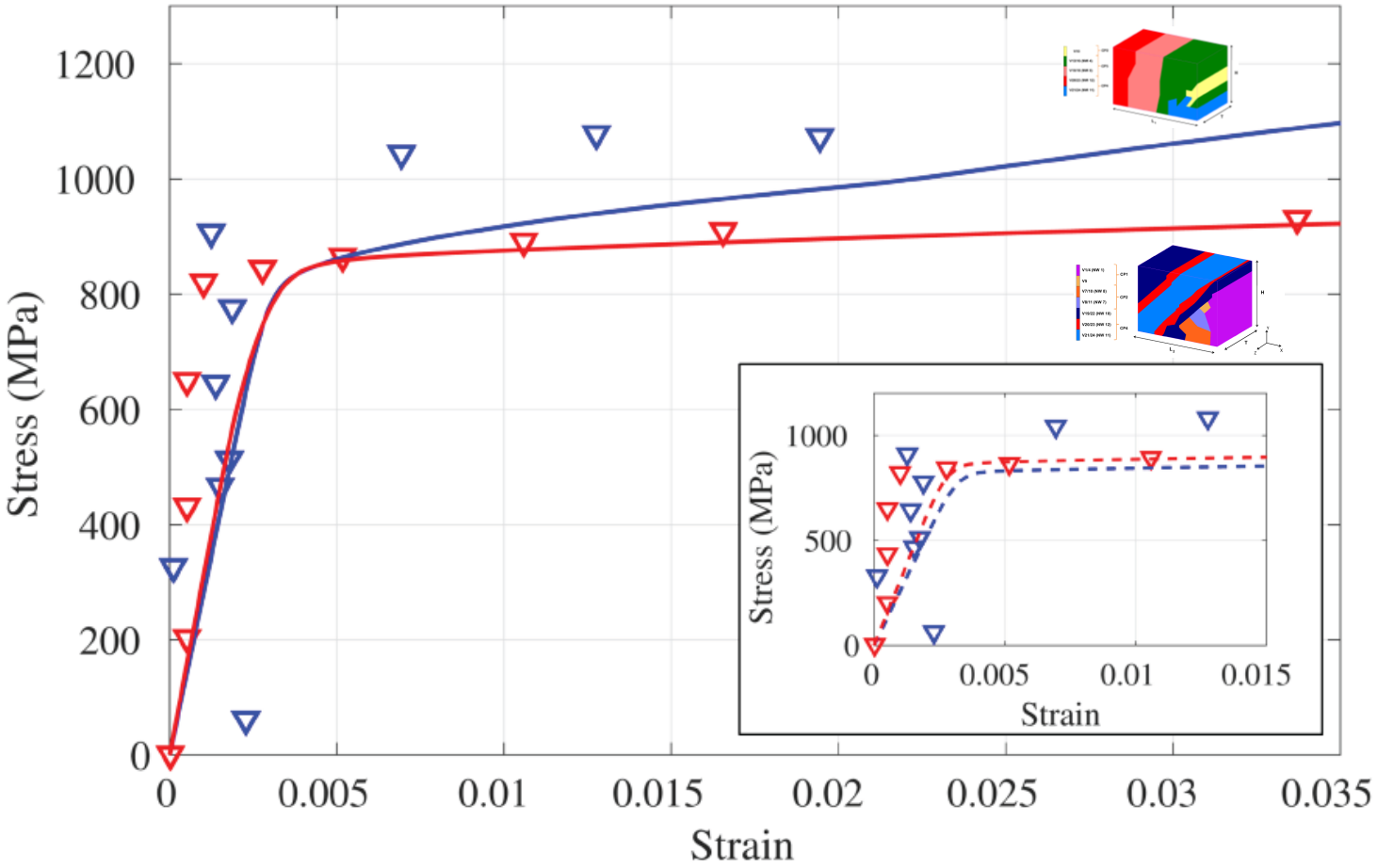
$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left(\frac{|\tau^{\alpha}|}{\tau_y^{\alpha}} \right)^{1/m} \text{sign}\,(\tau^{\alpha}) \qquad \tau^{\alpha} = (\boldsymbol{C}_e \cdot \overline{\boldsymbol{S}}) : \boldsymbol{s} \otimes \boldsymbol{n}$$

Material model parameters:

1) Initial phase fractions ξ and 1- ξ (from XRD for a specific material)
2) Elasticity $\mathbb{C}$ (from experiments)
3) Critical stresses for transformation τ_{tr}^{α} and slip τ_y^{α} ← Can be determined from solute strengthening theories/experiments

→ **No arbitrary, free-fitting parameters!**

Application: FeC martensite polycrystal



- Correct order (MP1 stronger than MP2) reproduced
- Inset: model without austenite films cannot reproduce correct strength difference

Conclusions: atomistic to continuum modeling of nano A/M

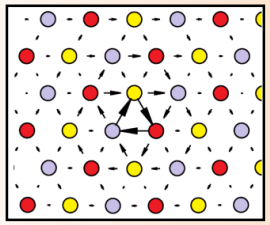
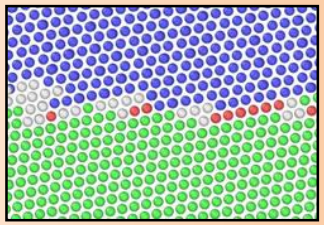
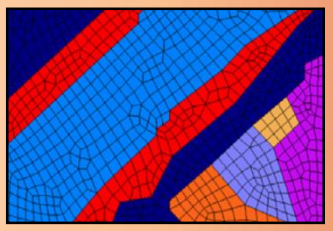
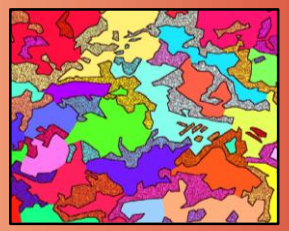
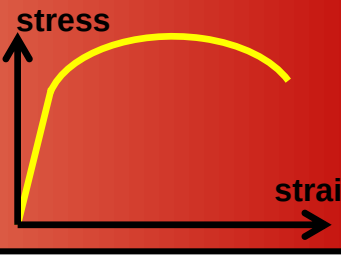
1) **Atomistic fcc austenite/bcc martensite interface**
   - reproduces all main aspects of experimental interfaces,
   - reveals (first time!) interface defects

2) ***Predictive* crystallographic theory for martensite**
   - reproduces simulation results and is consistent with experiments
   - can be used to explore potential of existing/new alloys

3) **Atomistic applied load simulations**
   - reveal Schmid-type response of interface
   - interface motion controlled by fcc/bcc screw dislocations (forward/reverse tr.)

4) **Continuum model of transformation**
   - kinematics of austenite controlled by apparent slip along transformation systems;
   - comparison with experiments show austenite films can contribute substantially to plastic deformation of nanolaminate austenite/martensite microstructures.

More details in:
Maresca & Curtin (2017), *Acta Materialia* 134:302
Maresca, Kouznetsova, Geers, Curtin, *Under review*

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European Research Council Advanced Grant Program for the project
"Predictive Computational Metallurgy" (W.A. Curtin)

10^{-10} 10^{-9} 10^{-6} 10^{-3} 1 m