Multiscale Mechanics in Metallic Alloys

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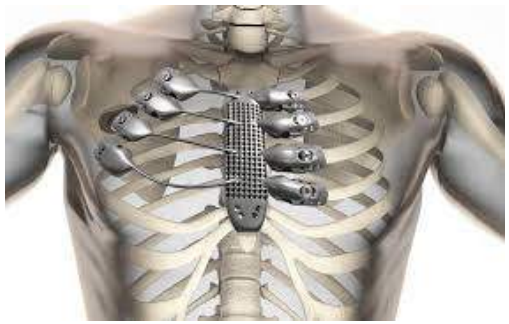
《工业中的多尺度力学方法》讲习班, 清华大学, 11/1/2021

Outline

- Metallic alloys: brief introduction
- Integrated Computational Materials Engineering (ICME) for metallic alloys
- Multiscale mechanics in metallic alloys – some cases
  - Mechanics at atomic scale
    - Twin boundary solute atom segregation Mg/Gd/Zn (DFT)
  - Bridging atomic scale to meso and macro scales
    - Precipitate hardening in Fe-Cu alloys. (DFT + Micromechanics)
    - Precipitate hardening in Mg and Al alloys. (DFT + Phase field)

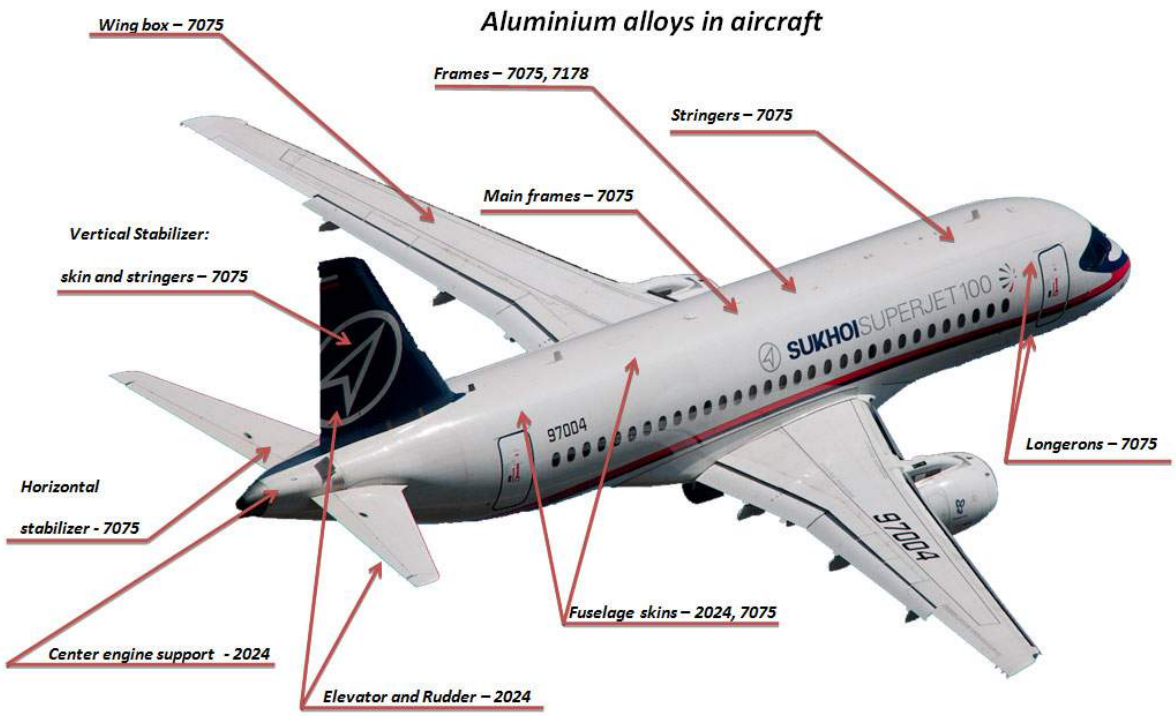
Metals: most commonly used structural material

- **Why metals?**
  - Metals represent the most versatile structural material used in modern society.
  - Metals provide the best combination of various mechanical properties needed in applications.



Metallic alloy: mixture of multiple elements

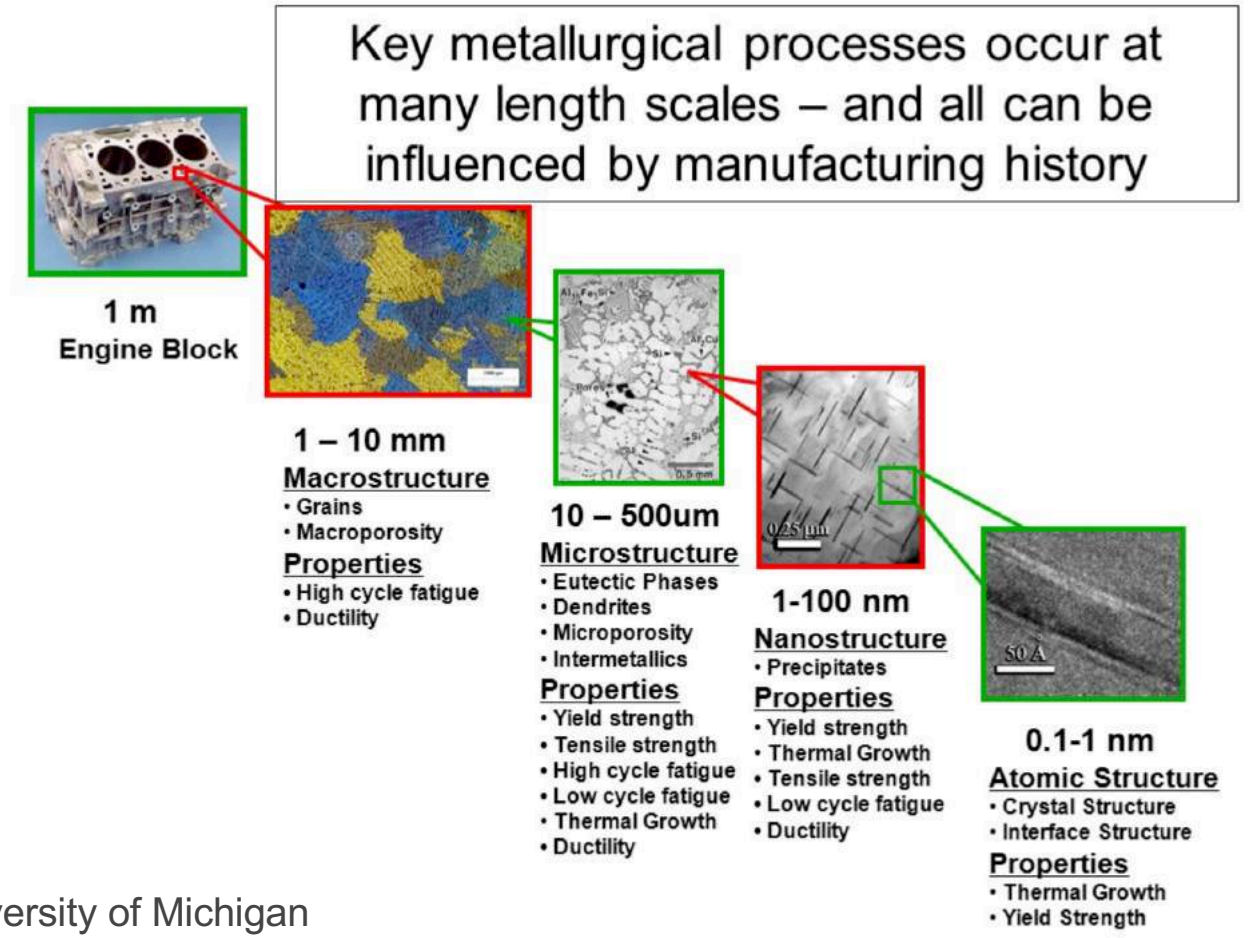
- Mixing multiple elements improves the mechanical and chemical properties of metals.
- But it takes **decades** to design/develop in engineering applications.



7075: Al(90.0)Zn(5.6)Mg(2.5)Cu(1.6)Cr(0.23)
2024: Al(92.0)Si(0.5)Fe(0.5)Cu(3.8-4.9)Mn(0.3-0.9)Mg(1.2-1.8)Cr(0.1)Zn(0.25)Ti(0.15)

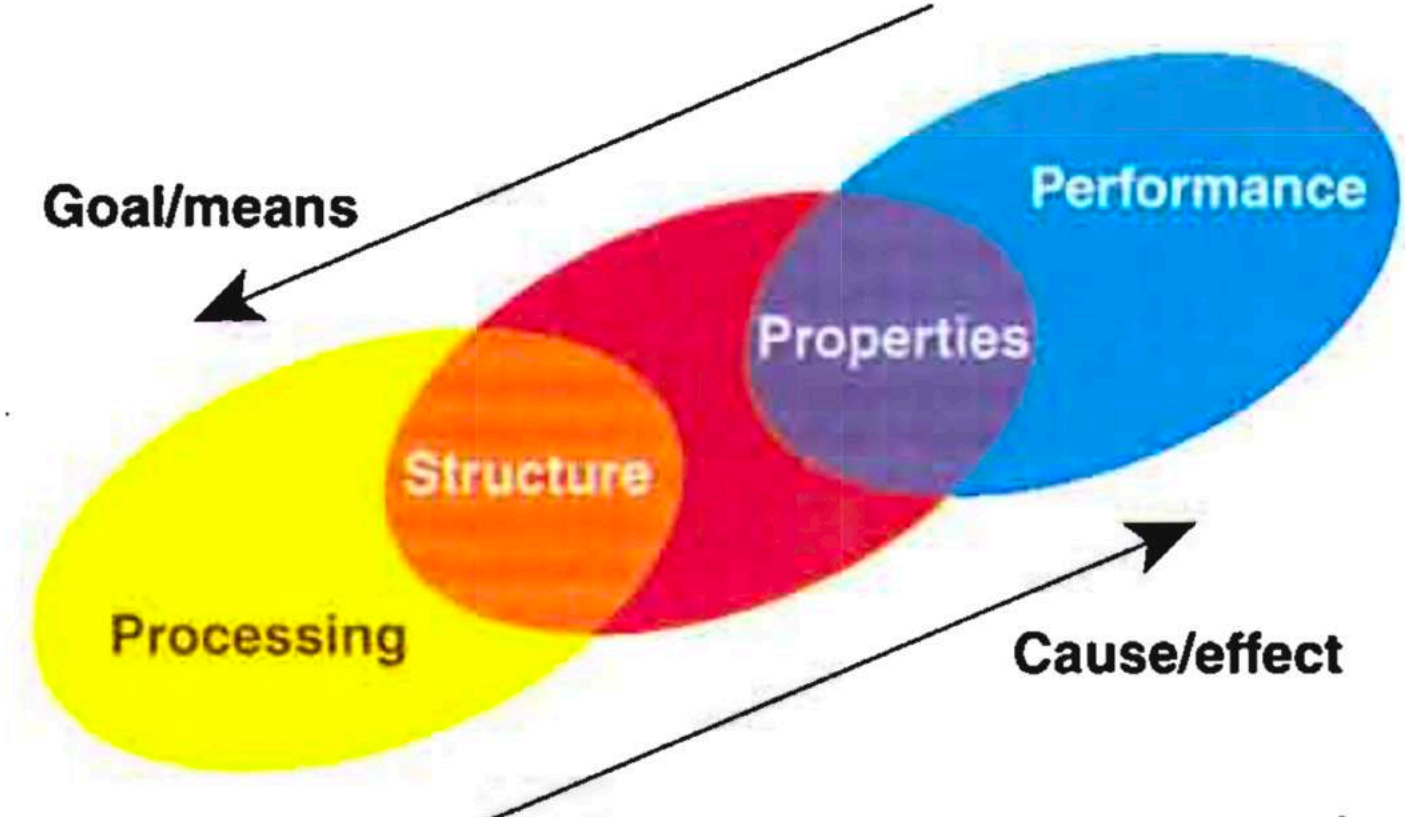
Complex microstructures on multiple length scales

- Mixing multiple elements together generates complex microstructures on multiple length scales, which determine mechanical properties.



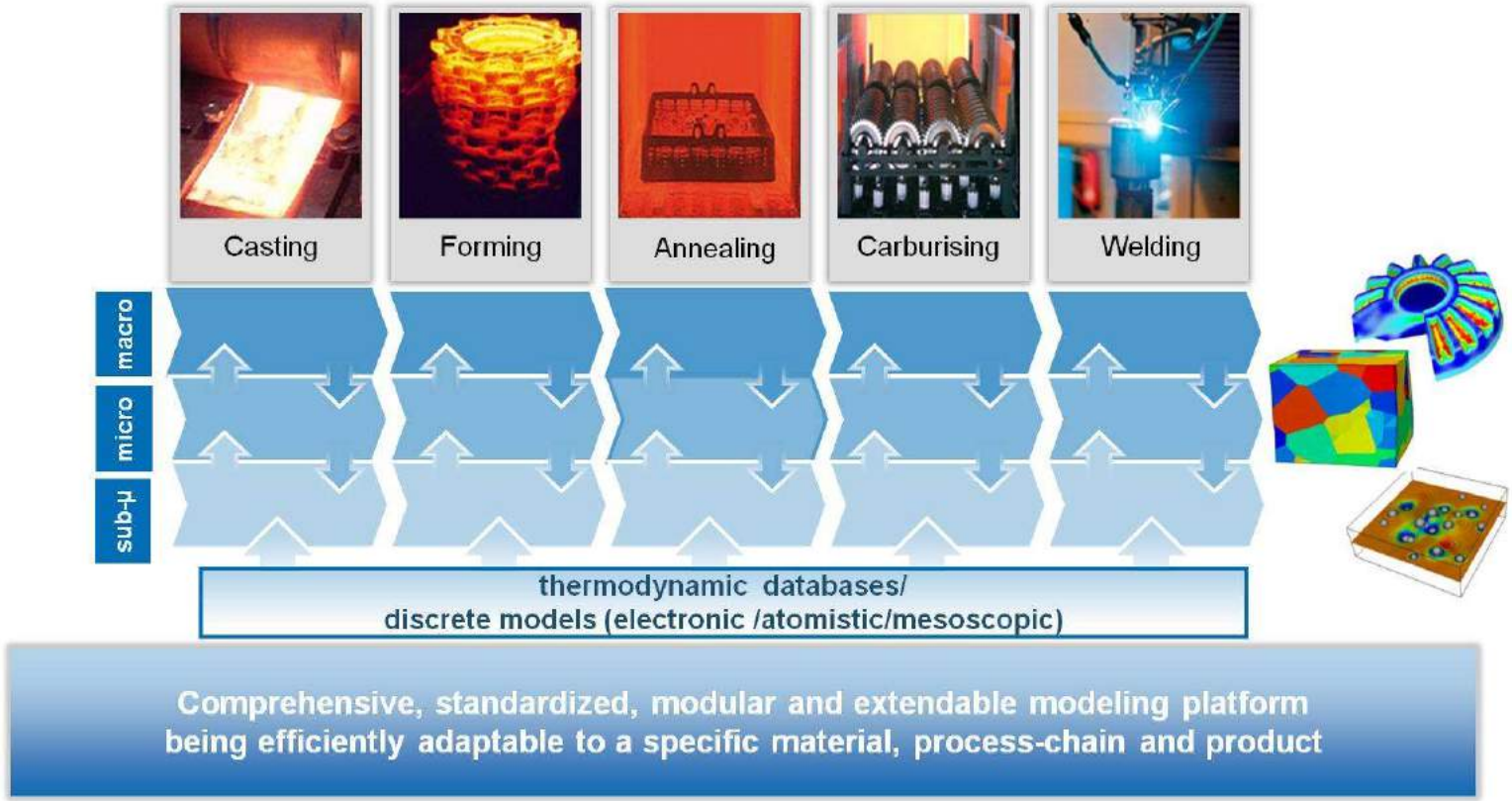
Processing-Structure-Property-Performance

- Essence of alloy design is processing-structure-property-performance relationship.
- Using trial-and-error experiments to design alloys (~ 5-10 elements and manufacturing dependent) costs time and money.



Integrated Computational Materials Engineering (ICME)

- **ICME** is an approach to design products, the materials that comprise them, and their associated materials processing methods by linking materials models at multiple length scales.
- ICME aims to half the cost and time for materials design.



http://www.icmeg.euproject.info

Successful story of ICME

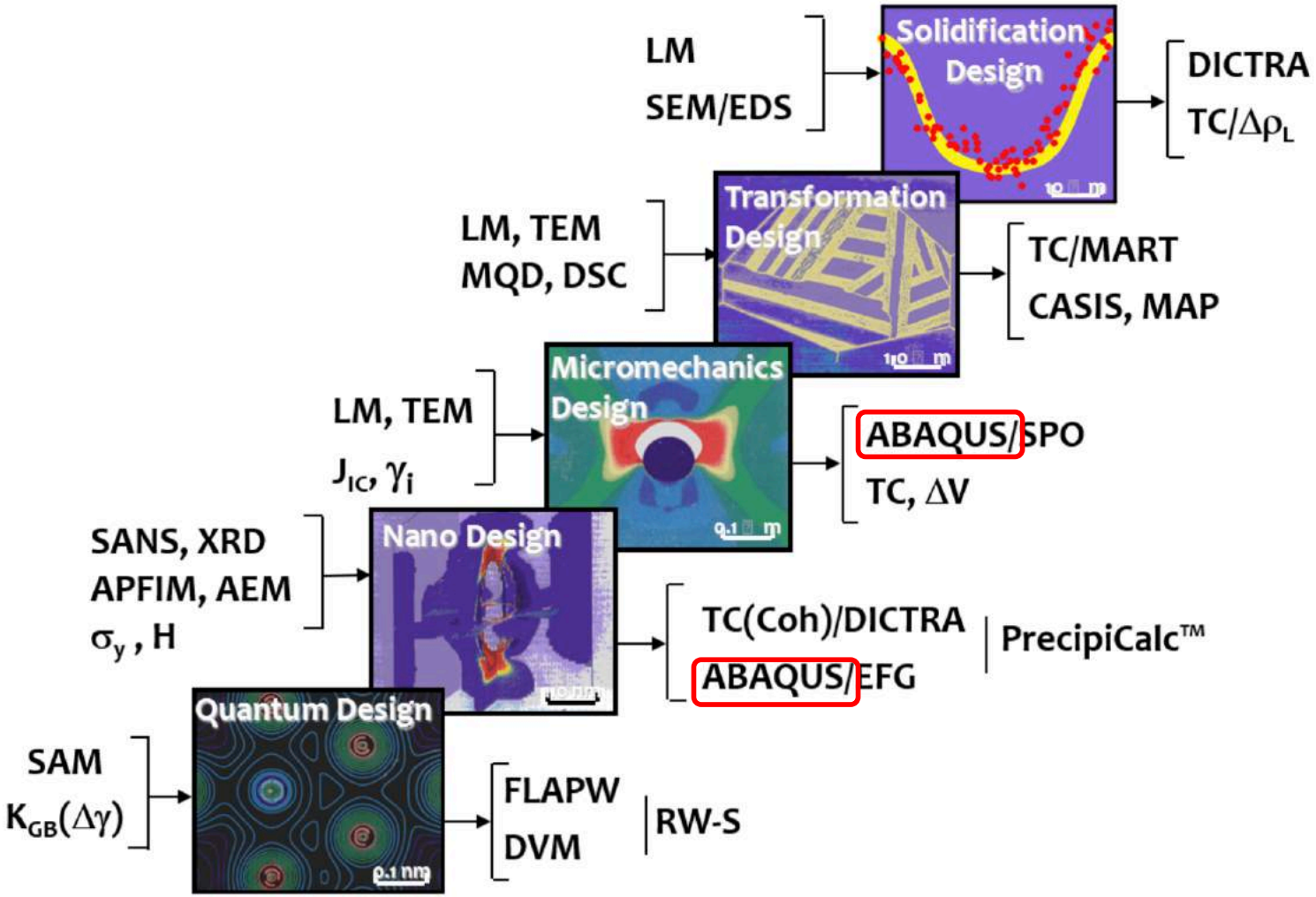
First Flight: QuesTek *Ferrium* S53®
T-38 main landing gear piston
December 17, 2010

8.5 years

Material approval:	**November 2009**
Component approval:	**August 2010**
Component installation:	**November 2010**
First flight:	**December 2010**

QUESTEK® INNOVATIONS LLC

Hierarchical Structure Needs Hierarchy of Methods

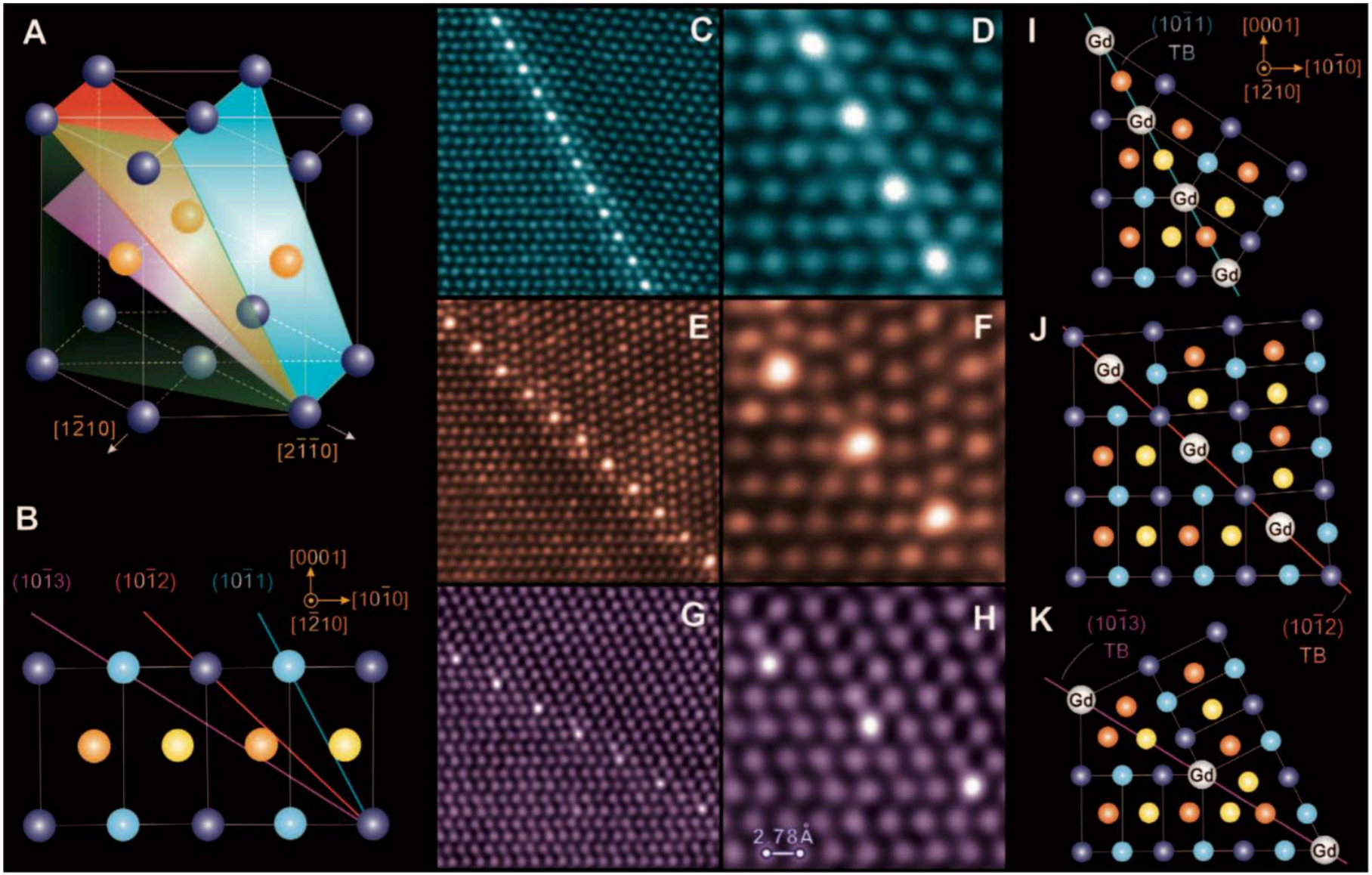


- Multiscale mechanics is essential in the hierarchy of design models.

Twin boundary segregation in Mg-Gd,Zn alloys

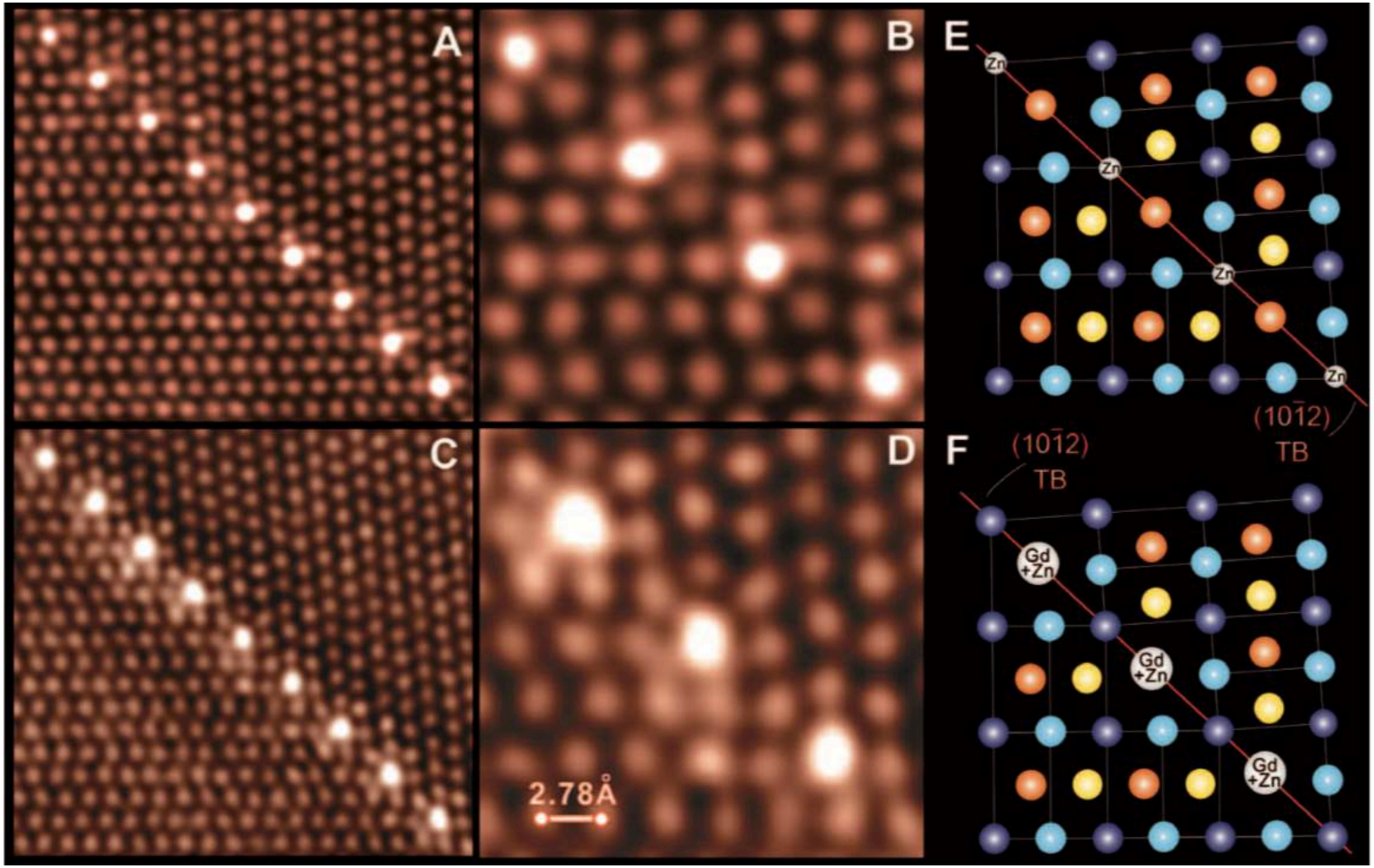
- Unexpected segregation in fully coherent TBs
- **Strain energy minimization** as driving force (DFT)
- Predicted enhanced mechanical strength confirmed in experiments (DFT)

Segregation of Gd Atoms to Mg Twin Boundary

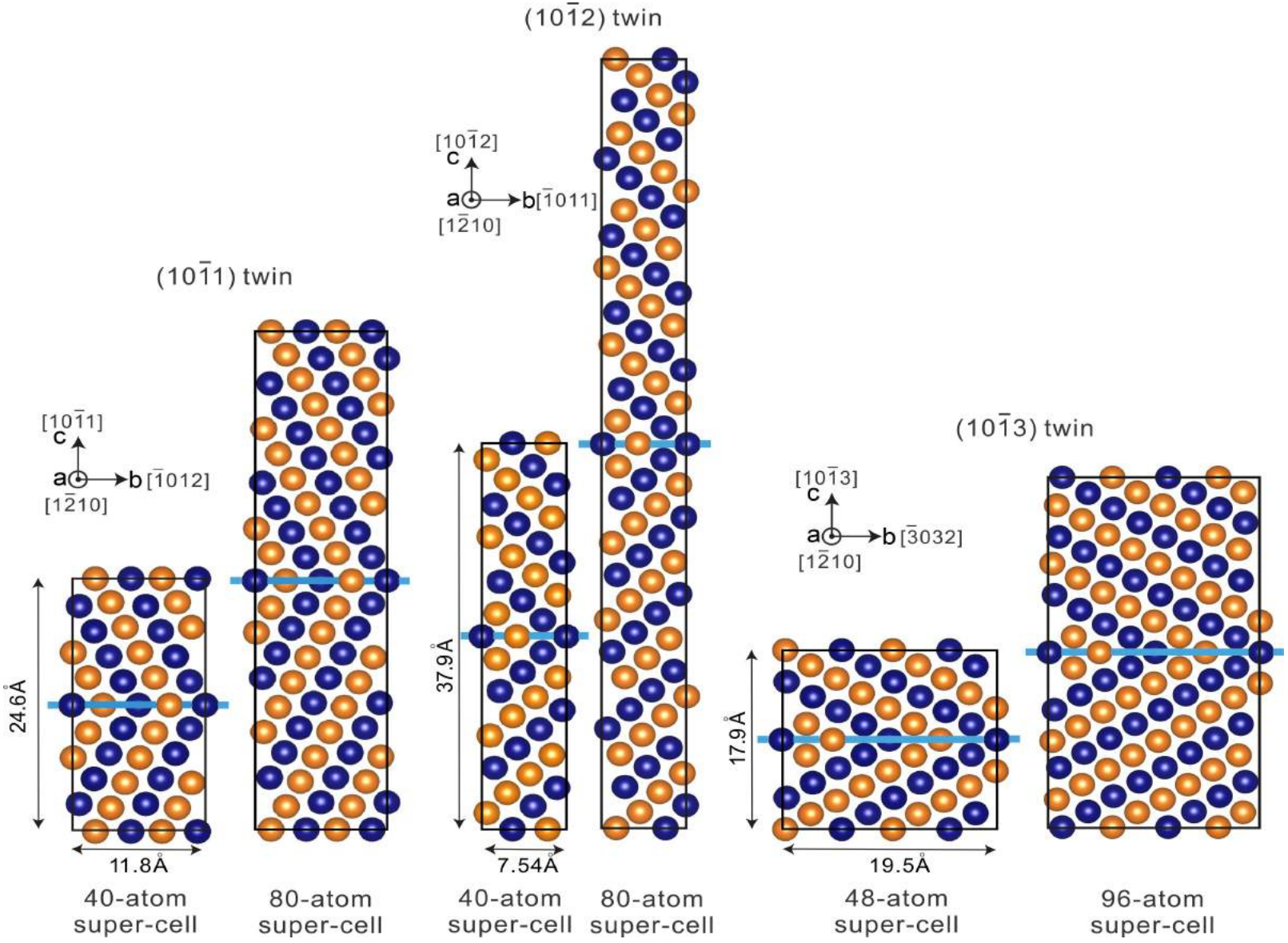


Nie et al. Science 340, 957 (2013)

Segregation of Gd and Zn to Mg Twin Boundary

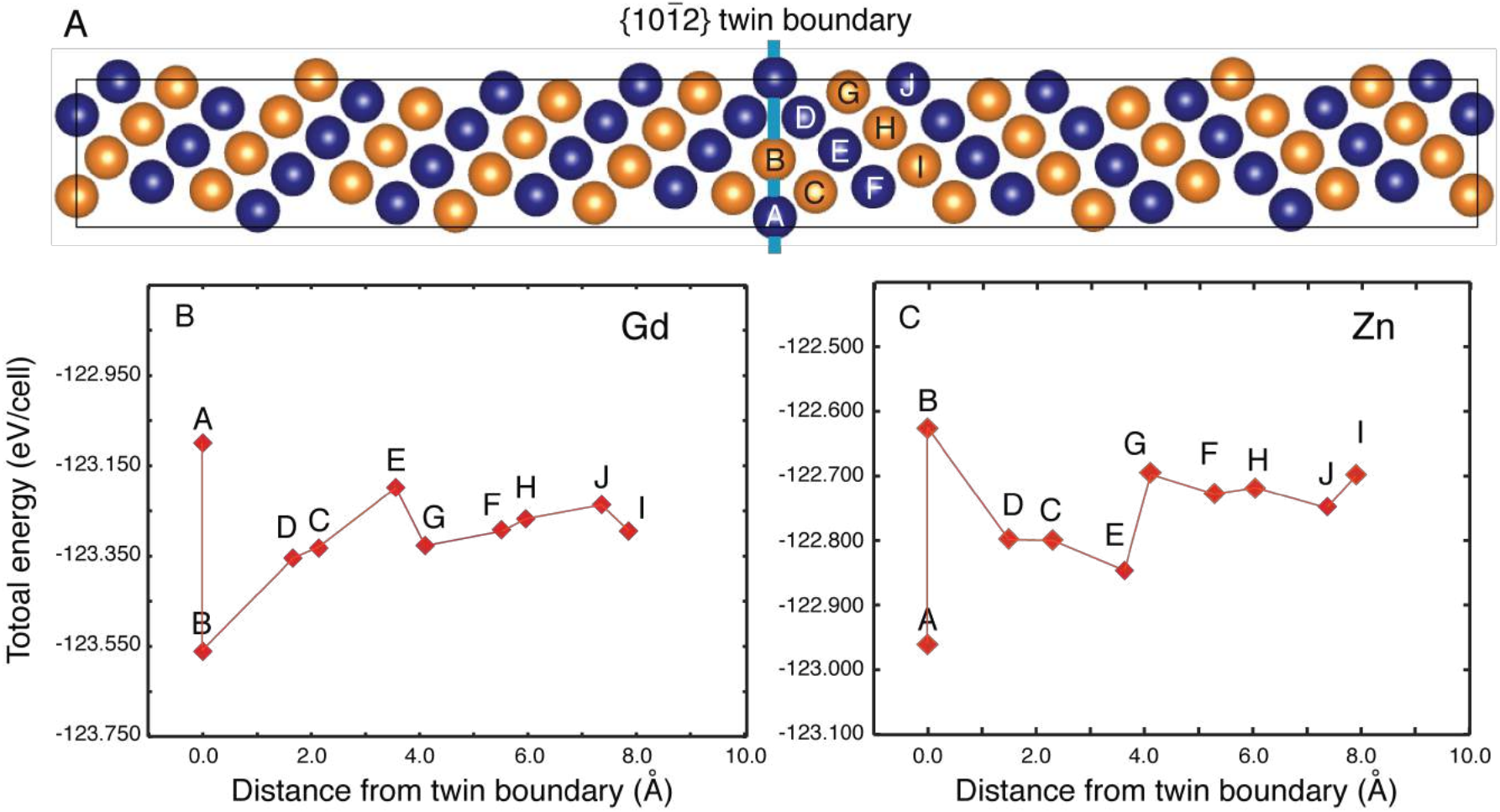


Twin Supercells

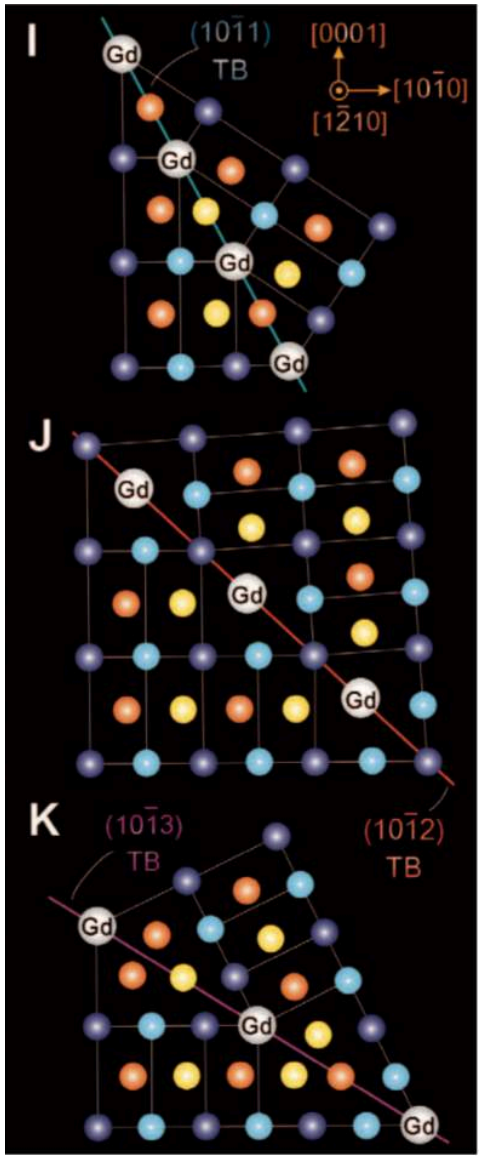


Segregation Energy of Gd and Zn atoms

- **DFT calculation for supercells**



Strain at atomistic scale?



- Inspection of lattice structure shows the two lattice sites A and B occupy different volumes. Lattice strain?
- How could we define atomic strain at an interface defect?
  - Can we define strain at atomistic scale?
  - How could we define a strain free state at the interface?
- Atomic local strain invariant from Ju Li et al.

$$\mathbf{M}_i = \sum_j \mathbf{q}_{ij}\mathbf{q}_{ij}^T \qquad \mathbf{q}_{ij} = \mathbf{q}_j - \mathbf{q}_i$$

Nearest neighbor position vector

$$\boldsymbol{\eta}_i = \frac{1}{2}(\mathbf{M}_i^T / d_0 - \mathbf{I})$$

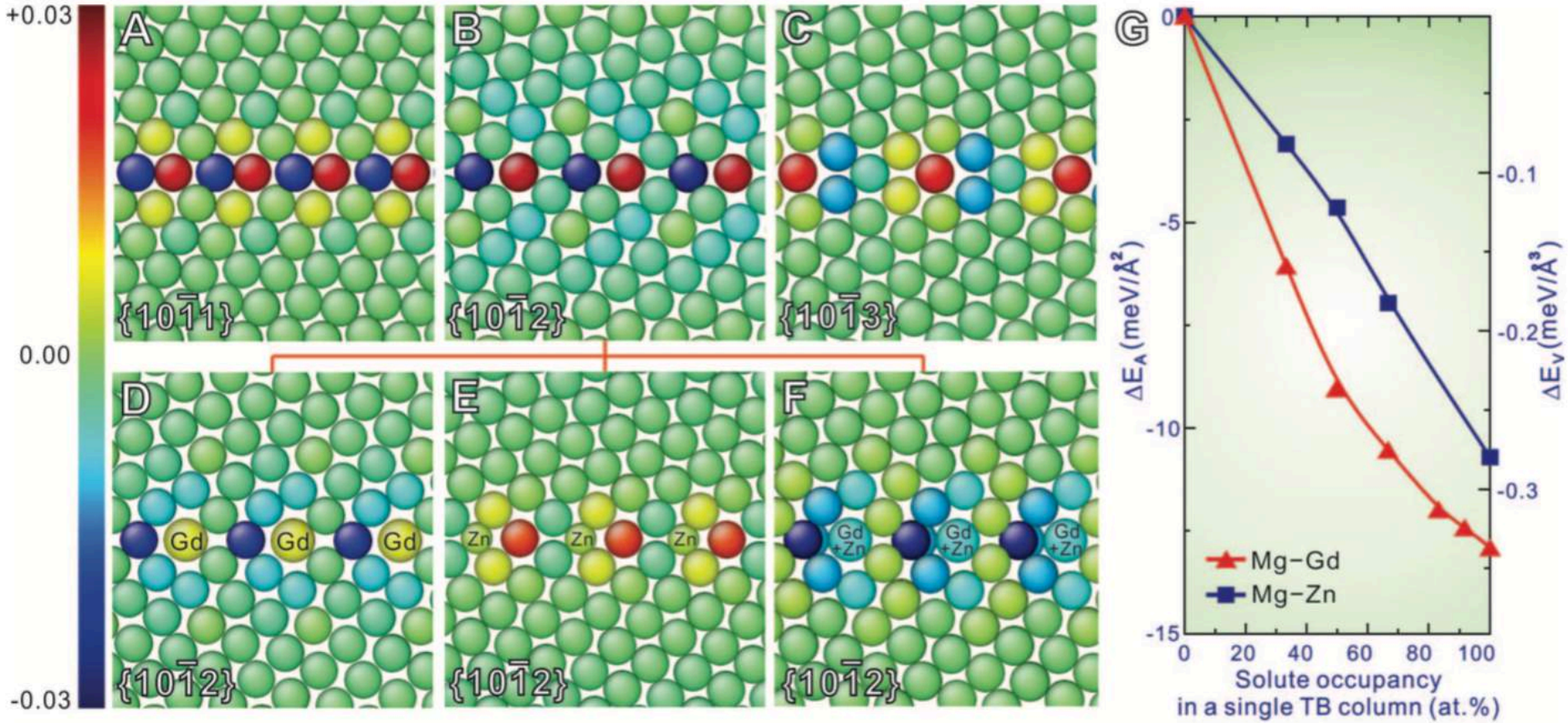
Local Lagrangian strain

$$\eta_m = \frac{1}{3}\mathrm{Tr}\boldsymbol{\eta} = \frac{1}{6}\left(d_0^{-1}\mathrm{Tr}\mathbf{M}_i - 3\right)$$

Hydrostatic invariant

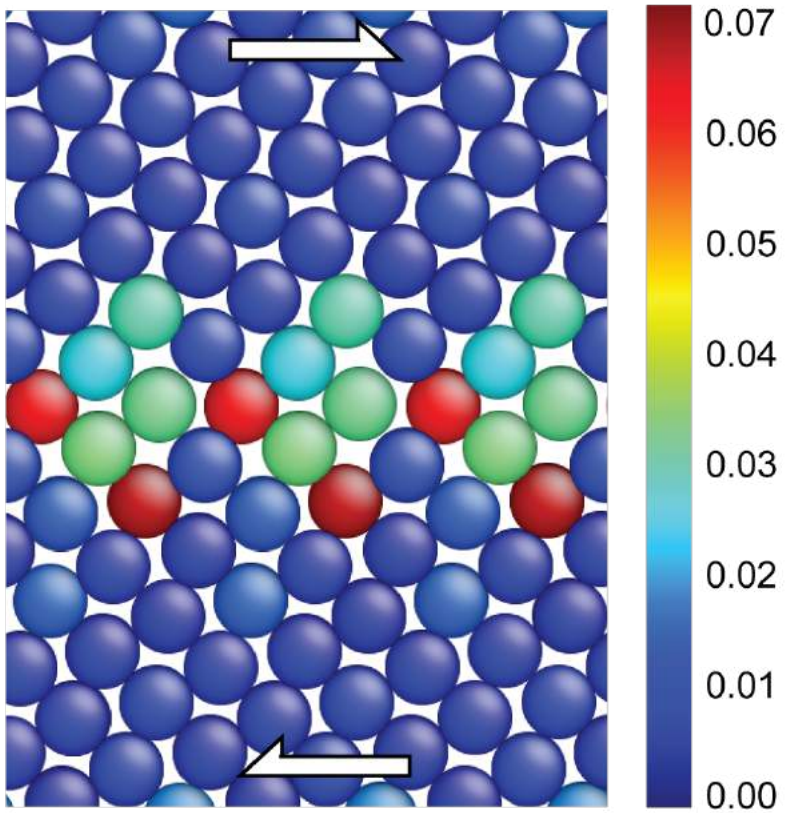
Strain Minimization Induced Solute Atom Segregation

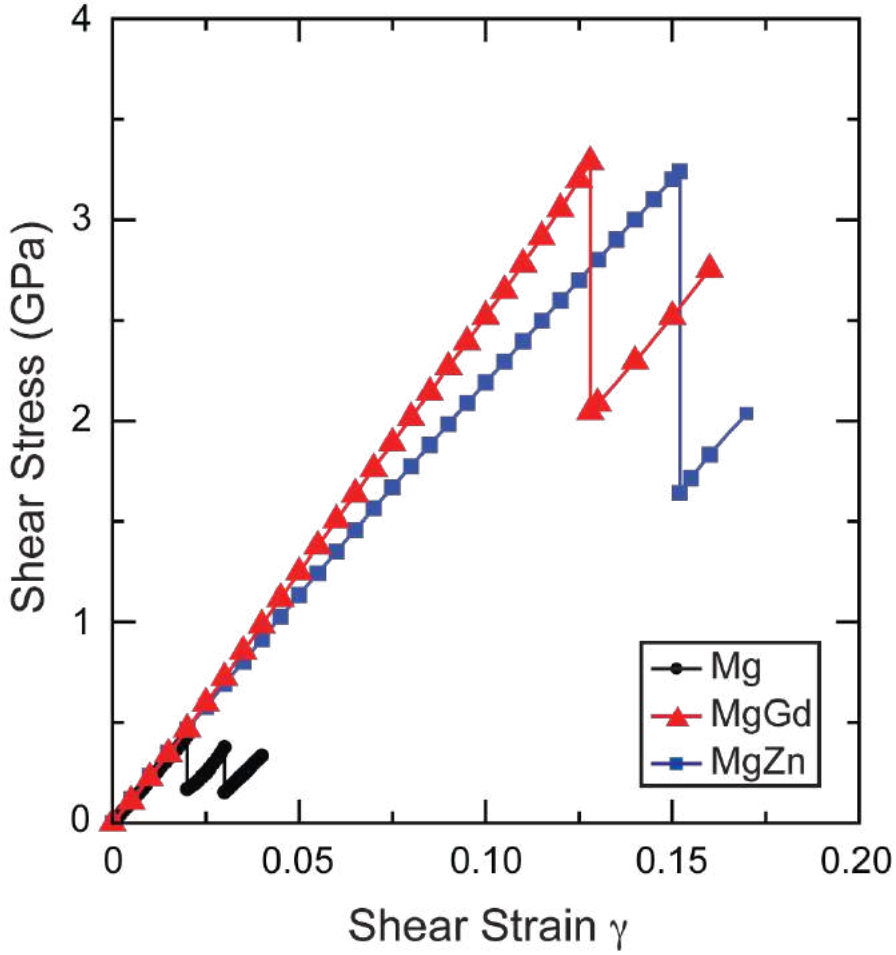
- Local atomic strain hydrostatic invariant reduces after segregation.
- The estimated strain energy reduction from Eshelby model agrees with DFT total energy quite well, e.g., -249 meV vs. -226 meV for Mg-Zn.



Strengthening effect prediction from DFT

Local atomic strain shear invariant

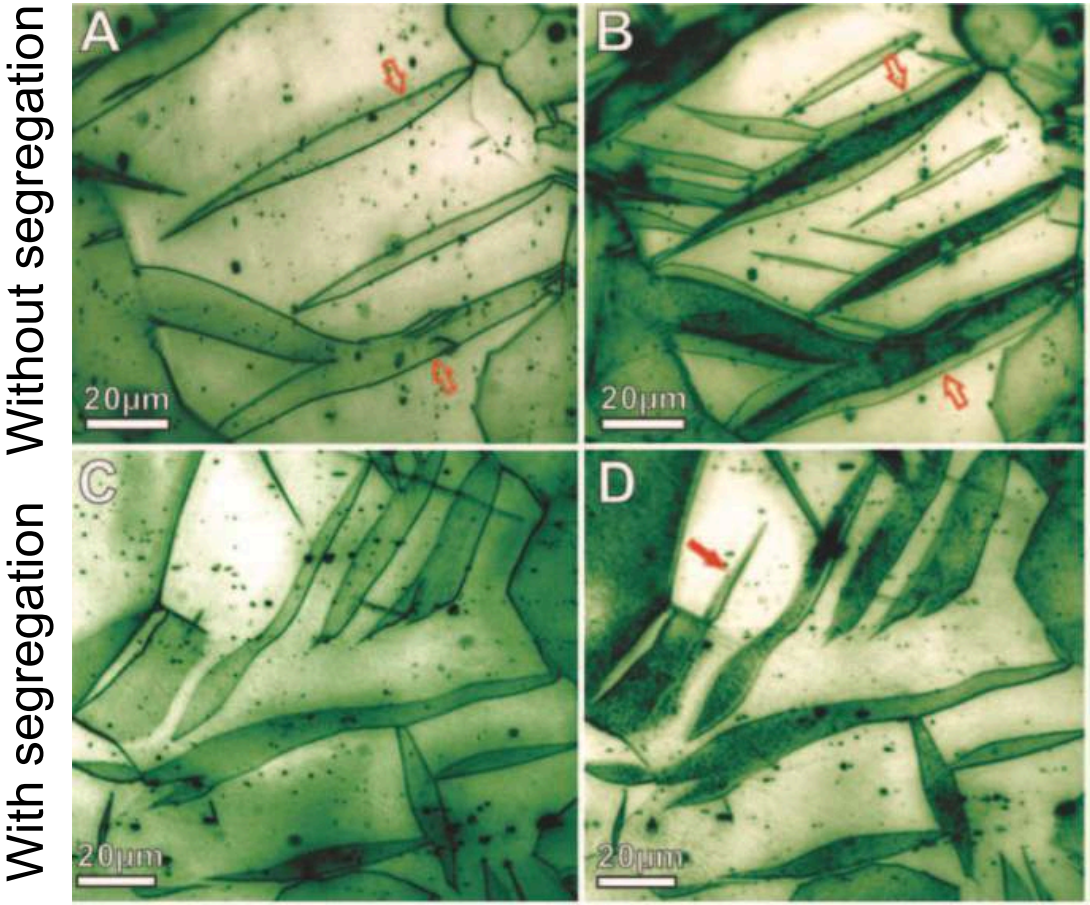


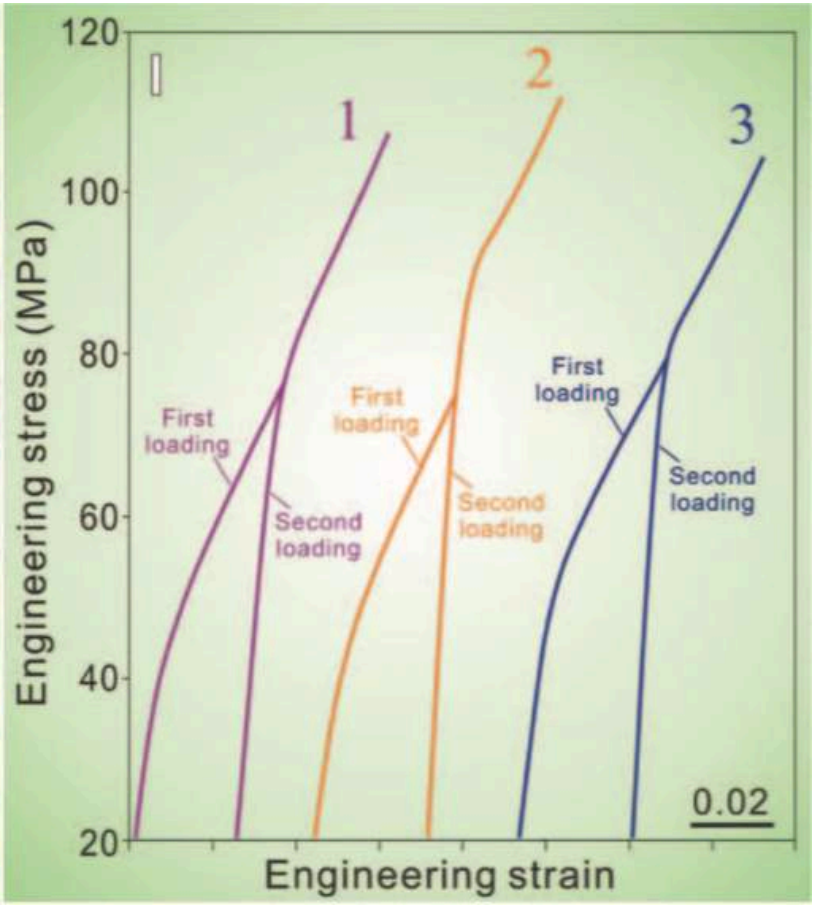


Strengthening Confirmed in Experiments

TB thermal stability

Mechanical Strengthening



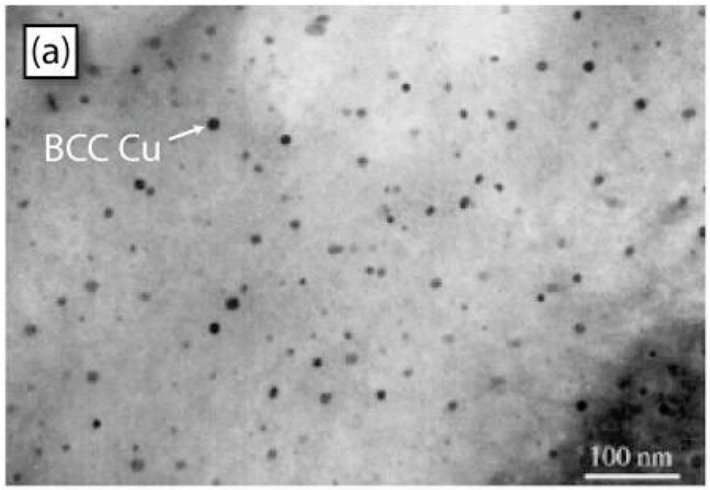


Mechanical properties of precipitates in Fe-Cu

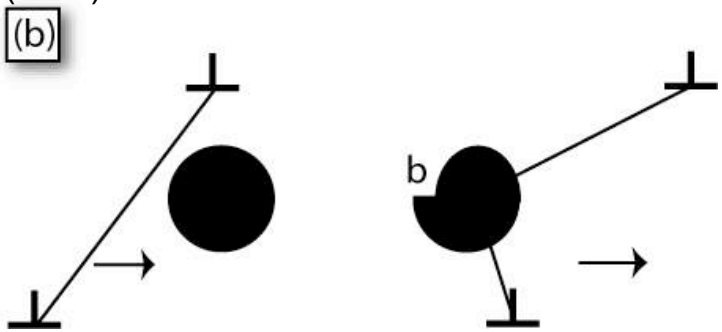
– Elastic modulus of metastable nanoscale precipitates (DFT)

– Nano-precipitates enhance macroscale mechanical properties of alloy (micromechanics model)

Fe-Cu BCC Alloy: Precipitate Hardening

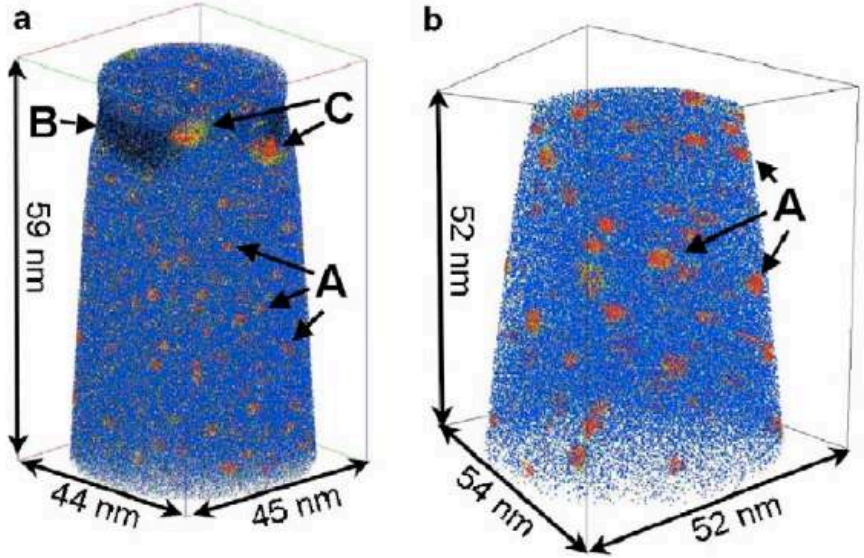


A. Deschamps et al. ISIJ International (2001)



Strength enhancement: 150-200 MPa

Precipitates: **BCC solid solution** with ~50% Cu



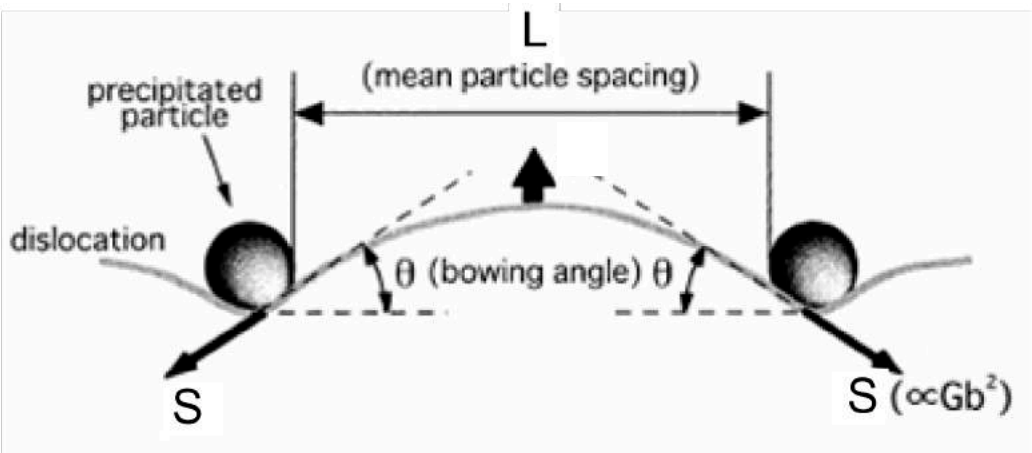
Isheim et. al., Script. Mater. 55, 35 (2006)

How to understand the strengthening?

Precipitate Strengthening in Alloys

- Alloys with Precipitates
  - Strength increase

$$\Delta\tau = \Delta\tau(f, r_p, \Delta a, \Delta\mu ...)$$



  - Precipitation from a supersaturated solid solution

Nucleation and growth ← Free energy difference $\Delta G = G_m - G_p$

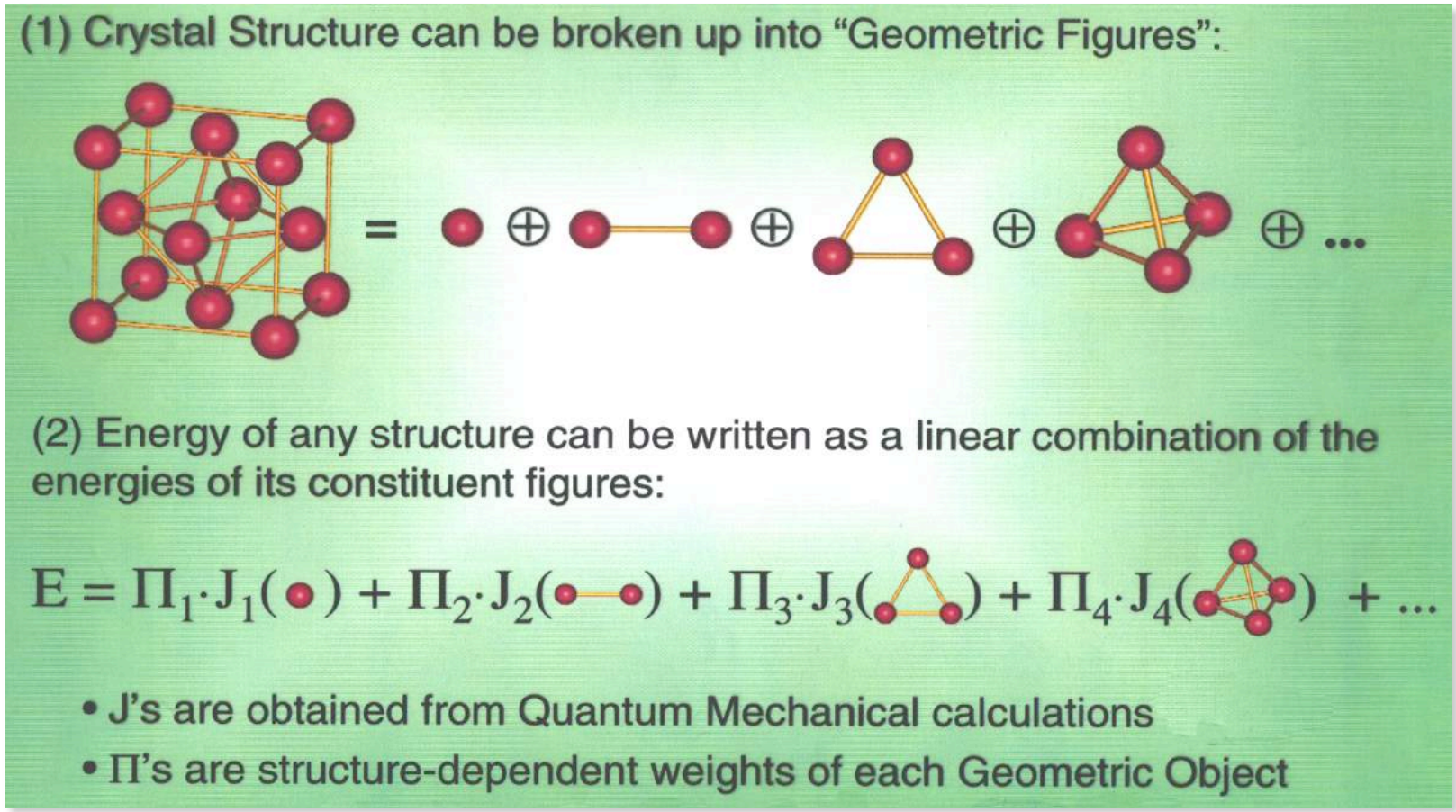
Nucleation and growth ← Interfacial free energy $\Delta\gamma$

  - Challenges in experiments
    - Small size: ~ 1-10 nm
    - Coherent precipitates are often meta-stable

How to calculate thermodynamic and mechanical properties?

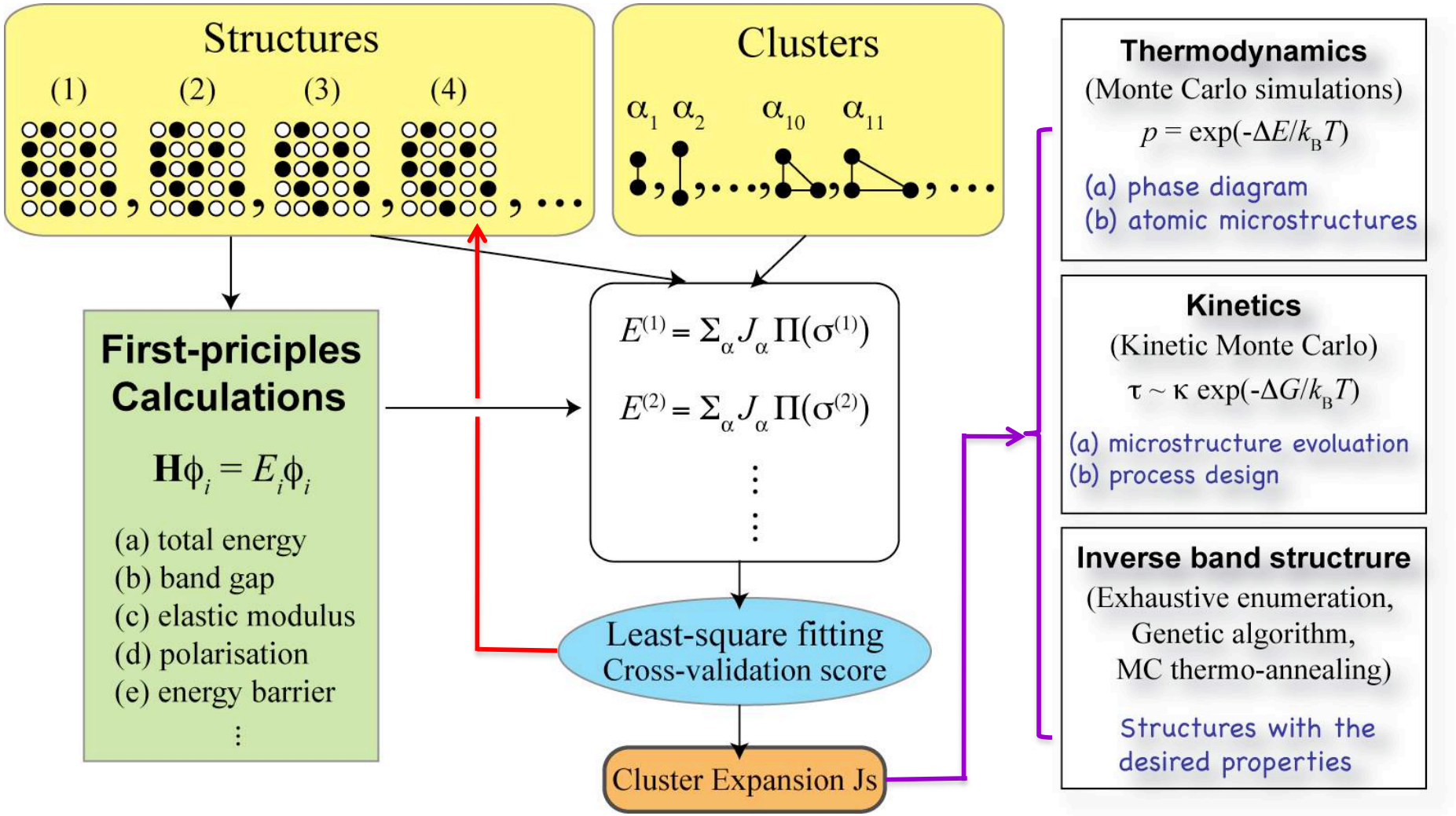
Core of Our Tool Kit

- **Cluster expansion**
  - An extension of the well-known Ising model.
  - An efficient & accurate approach to address the huge configurational space.



Sanchez, et.al., Physica A 1984; D.de Fontaine, solid state phys. 1994; Laks, et.al., PRB 1992

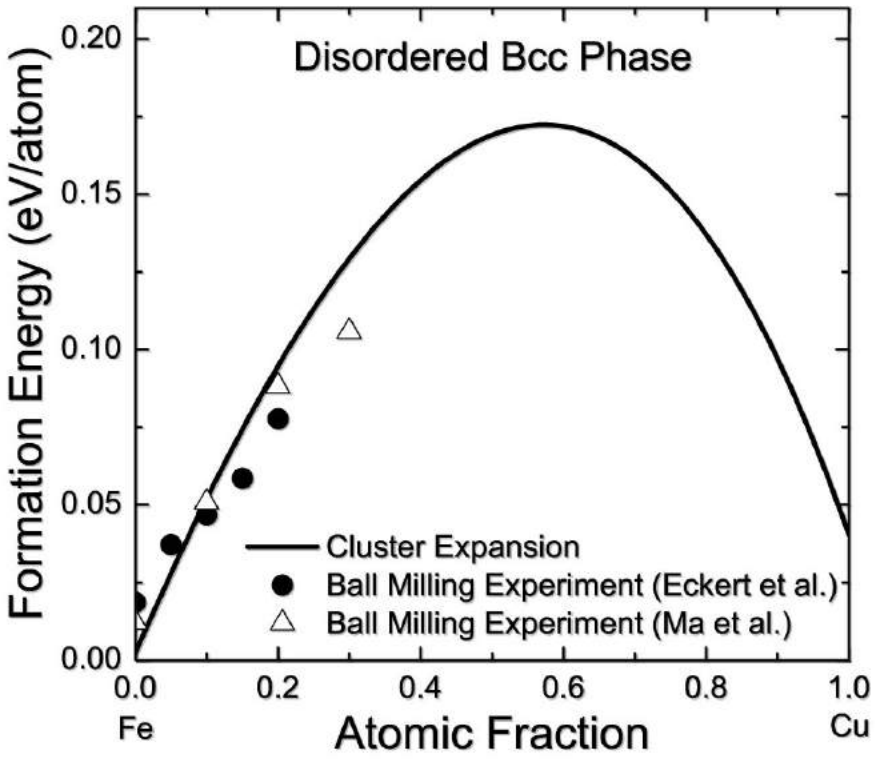
Flow Chart of Our Software Package



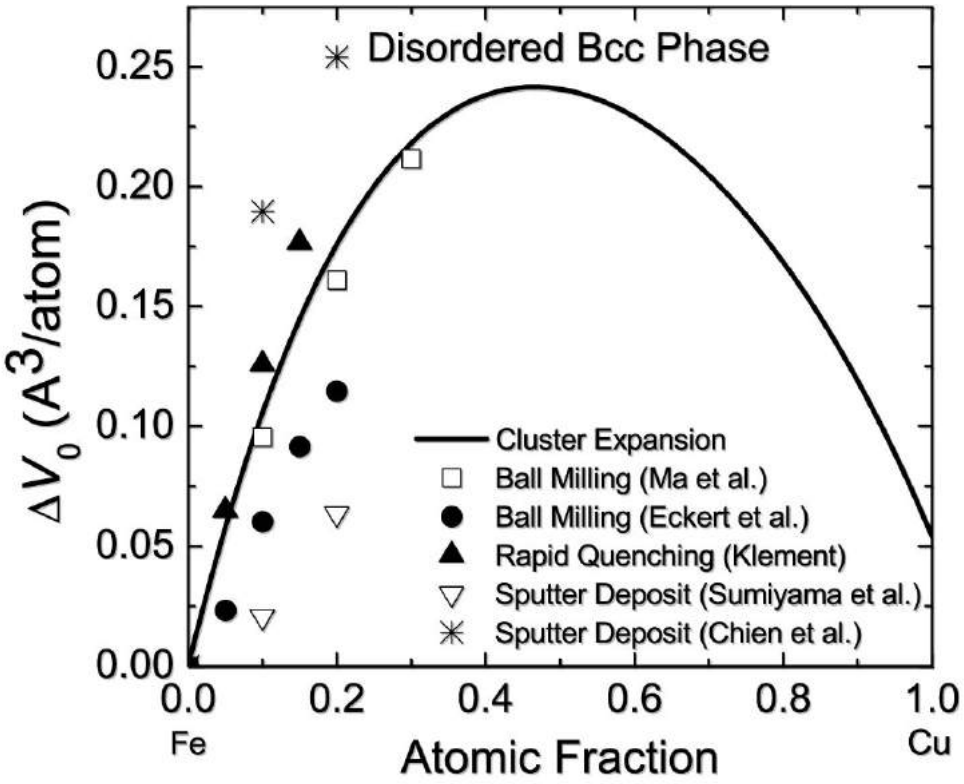
Formation Energy ΔE and Volume ΔV_0

$$\Delta E = E(\mathrm{Fe}_x\mathrm{Cu}_{1-x}) - xE(\mathrm{Fe\ Bcc}) - (1-x)E(\mathrm{Cu\ Fcc})$$
$$\Delta V_0 = V_0(\mathrm{Fe}_x\mathrm{Cu}_{1-x}) - xV_0(\mathrm{Fe\ Bcc}) - (1-x)V_0(\mathrm{Cu\ Fcc})$$

CV=0.013eV/atom

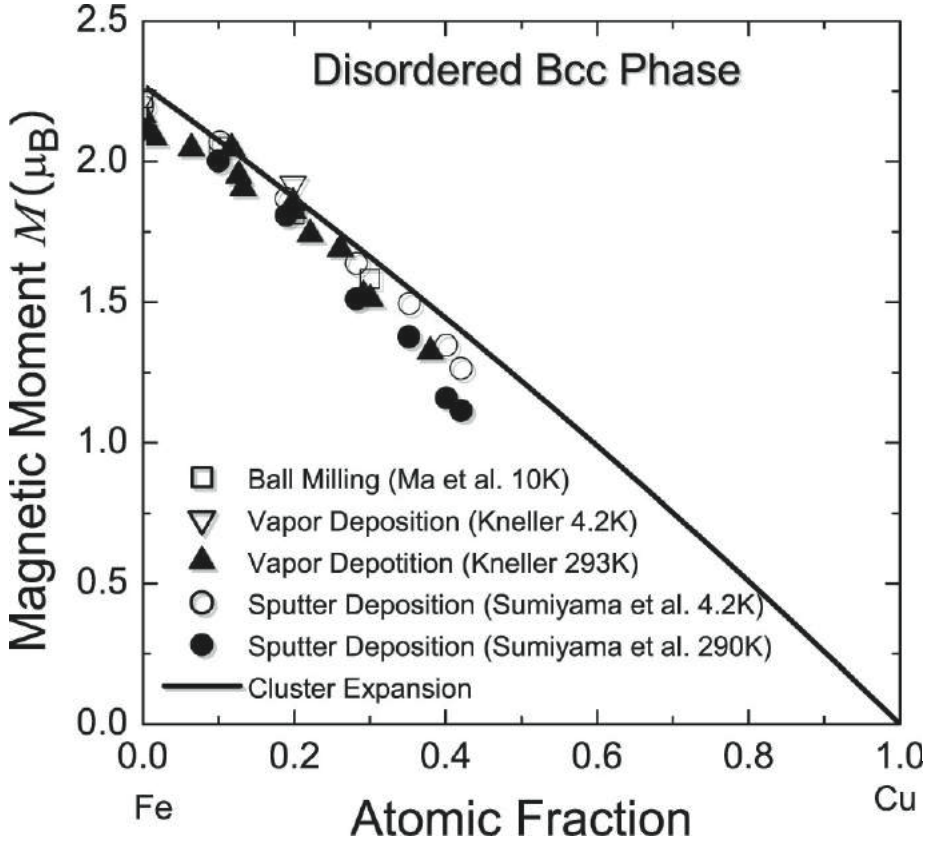


CV~0.010A^3

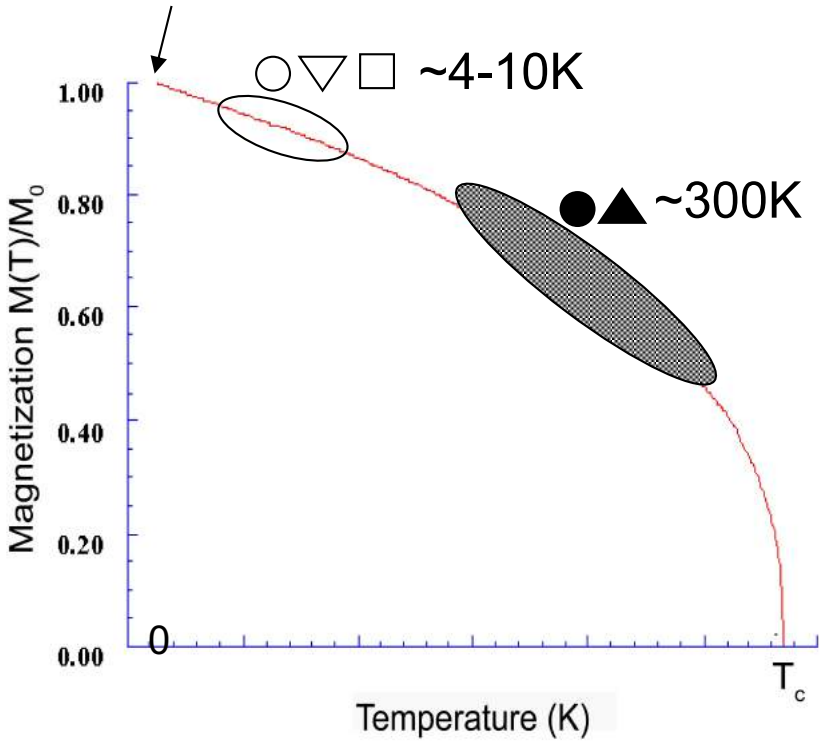


Magnetic Moment

CV = 0.085μ_B



First-Principles calculations



First-Principle calculations agrees with low temperature (4.2K) measurements.

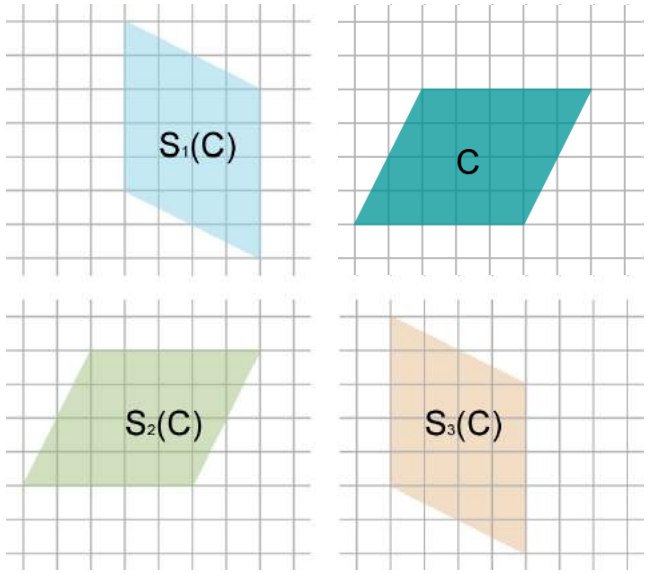
Method: CE for Elastic Constant Tensor

- Cluster expansion for full elasticity tensor $C(\sigma)$
  - Too many components (at most 21 for triclinic symmetry)
  - No parent lattice symmetry→ too many ECIs to fit

- Cluster expansion for *symmetrized* elasticity tensor $\bar{\mathbf{C}}(\boldsymbol{\sigma})$

$$\bar{\mathbf{C}}(\boldsymbol{\sigma}) = \sum_{i=1}^{n} S_i(\mathbf{C}(\boldsymbol{\sigma}))/n$$

S_i: point group of parent lattice
$S_i(C(\sigma))$: $C(\sigma)$ under symmetry operation

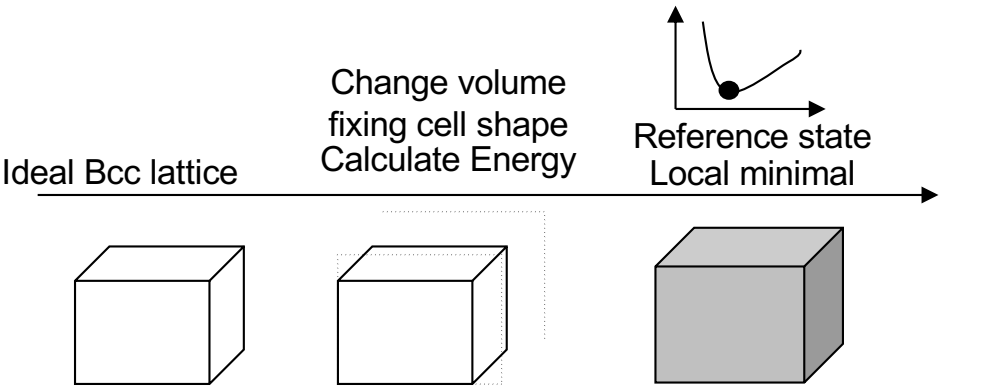
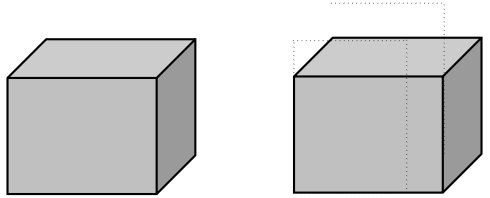
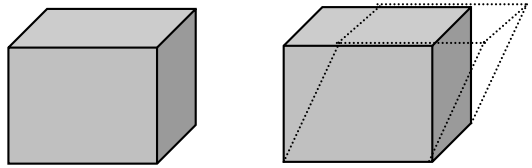


$$\bar{\mathbf{C}} = \frac{S_1(\mathbf{C}) + S_2(\mathbf{C}) + S_3(\mathbf{C}) + \mathbf{C}}{4}$$

- Only three independent components
- Share parent lattice symmetry
- Disordered Bcc Phase: $\bar{\mathbf{C}} = \mathbf{C}$

New method to calculate elastic constants for a disordered phase

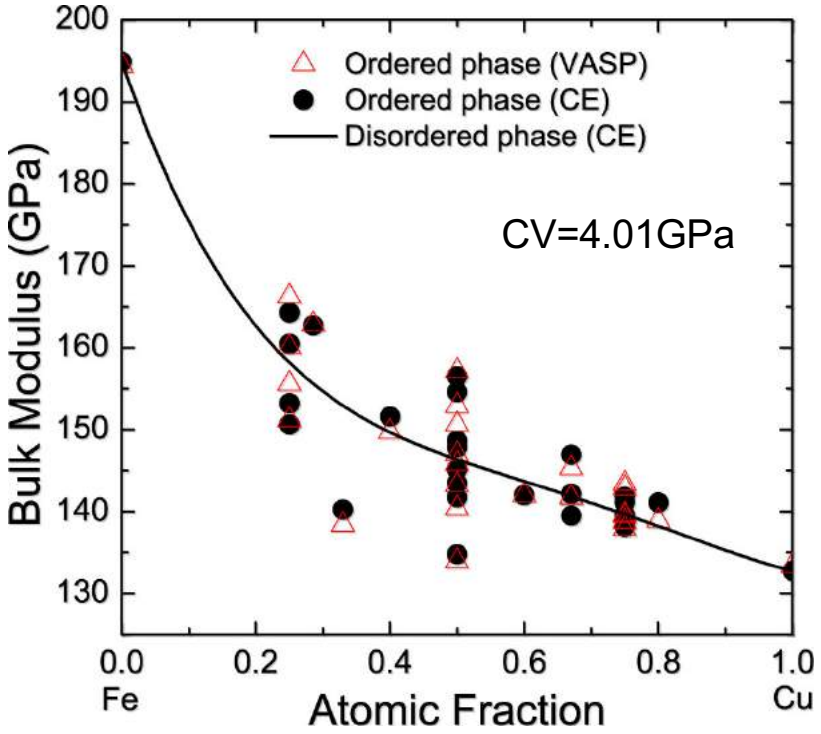
First-Principles Computations for Elastic constants

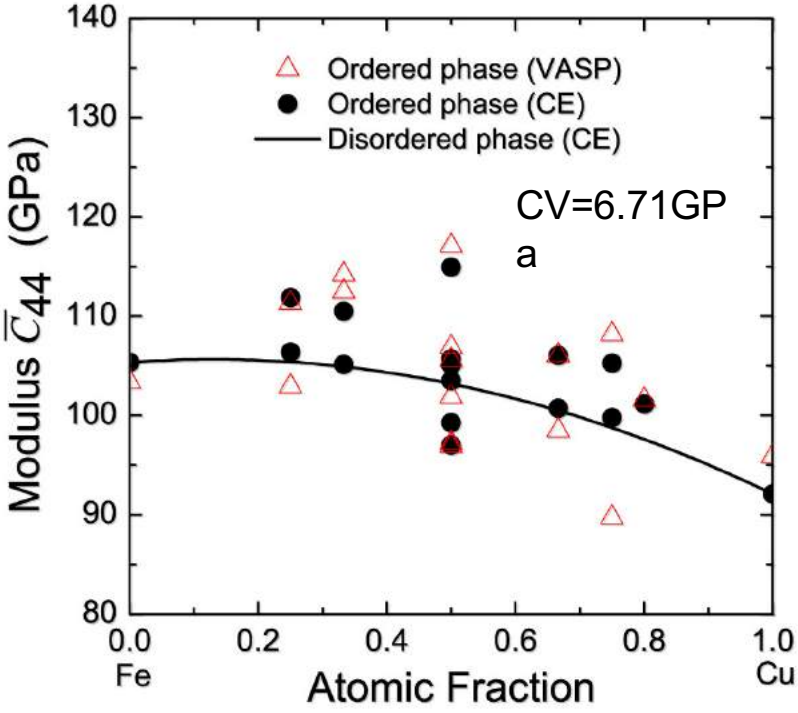
1	Ideal Bcc lattice → Change volume fixing cell shape Calculate Energy → Reference state Local minimal 	Energy: E_0 Bulk modulus: B Volume: V_0 Mean Magnetic moment: M_0
2	Reference state → $\varepsilon_x=\varepsilon_y=-\varepsilon_z/2$ Calculate Energy → $C_z'=1/3\ \partial^2E/\partial\varepsilon_z^2$ 	$\overline{C}' = \frac{C_x' + C_y' + C_z'}{3}$
3	Reference state → ε_{12} Calculate Stress → $C_{44}=1/2\ \Delta\sigma_{12}/\varepsilon_{12}$ 	$\overline{C}_{44} = \frac{C_{xy} + C_{yz} + C_{xz}}{3}$

DFT + CE to Predict Elastic Modulus

- CEs for *symmetrized* elastic tensor
  - ✧Three components: B, C', and C_{44}

$$\bar{\mathbf{C}}(\sigma) = \frac{1}{n}\sum_{i=1}^{n} \mathbf{S}_i \bullet \mathbf{C}(\sigma)$$

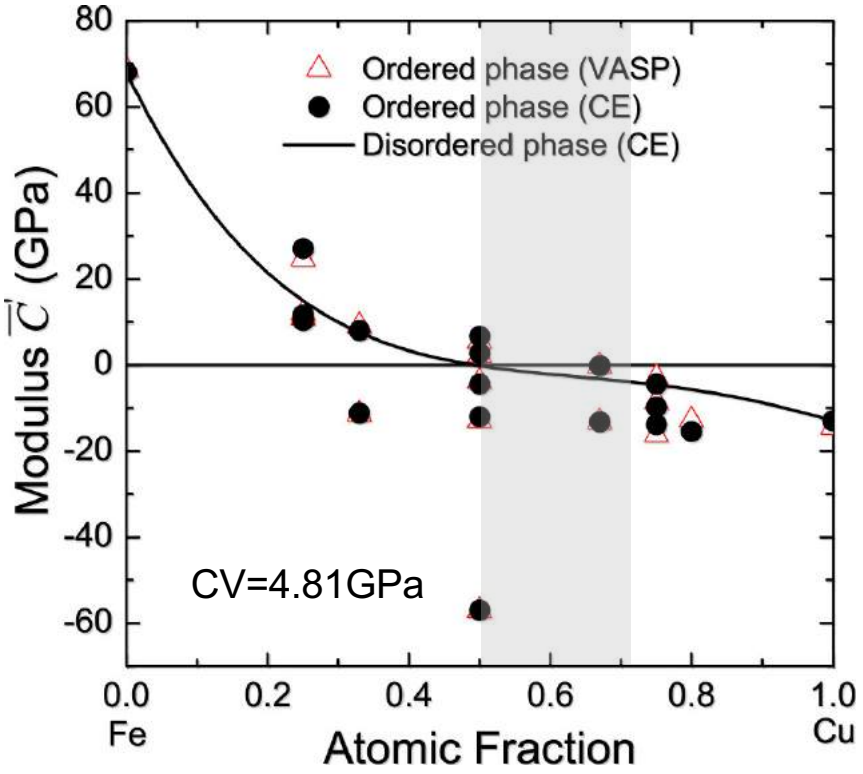


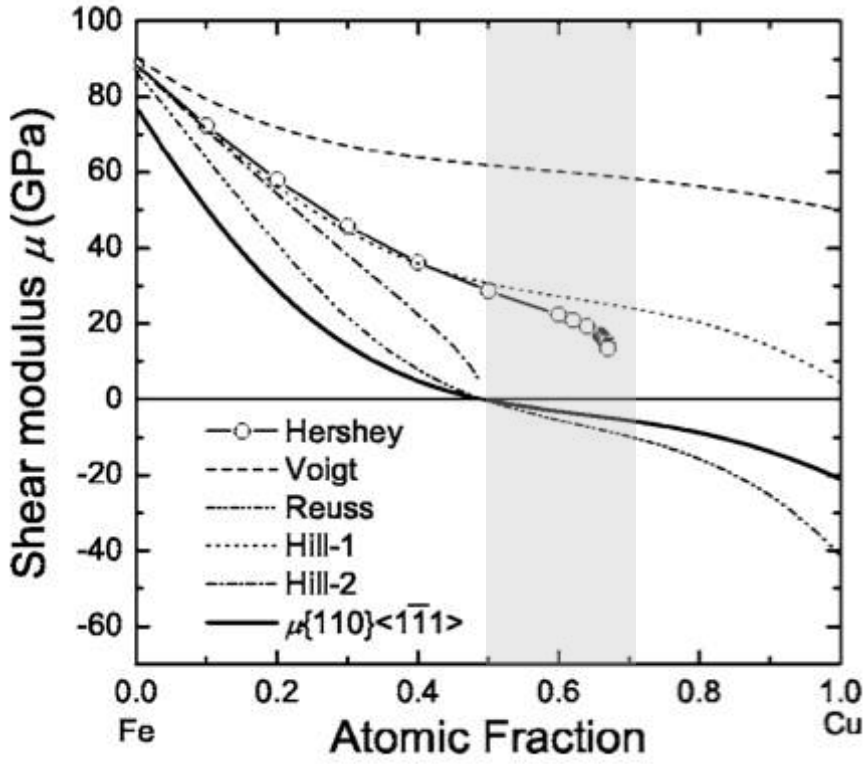


DFT + CE to Predict Elastic Modulus

- CEs for *symmetrized* elastic tensor
  - ✧Three components: B, C', and C_{44}

$$\mu_{\{110\}<1\bar{1}1>} = \frac{3C_{44}C'}{C' + 2C_{44}}$$





Theoretical Model for Strengthening Effect

f ~ 0.014[a,b], r ~ 2.5nm, b ~ 0.25nm[b], r_c ~ 1.75b[c]

μ_m ~ 77.1GPa, μ_p ~ 0.09GPa

- Russell-Brown model

$$\Delta\tau = \frac{\mu_m b}{L}\left[1-\left(\frac{E_1}{E_2}\right)^2\right]^{3/4}, \quad \arcsin\left(\frac{E_1}{E_2}\right) \geq 50^o$$

$$\frac{E_1}{E_2} = \frac{\mu_p \log\frac{r}{r_c}}{\mu_m \log\frac{R}{r_c}} + \frac{\log\frac{R}{r}}{\log\frac{R}{r_c}}$$

Δτ ~ 278MPa

- Nembach model

(E. Nembach, Particle Strengthening of Metals and Alloys, John Wiley & Sons Inc. 1997)

$$\Delta\tau = \frac{\alpha_1^{3/2}}{(2S\pi\omega_q)^{1/2}} \mid \mu_p - \mu_m \mid^{3/2} \frac{r^{(3\beta_1/2-1)} f^{1/2}}{b^{(3\beta_1/2-2)}}$$

Δτ ~ 180MPa

Experiments: ~ 150-200 MPa

Shear modulus mismatch contribute a significant part of hardening.

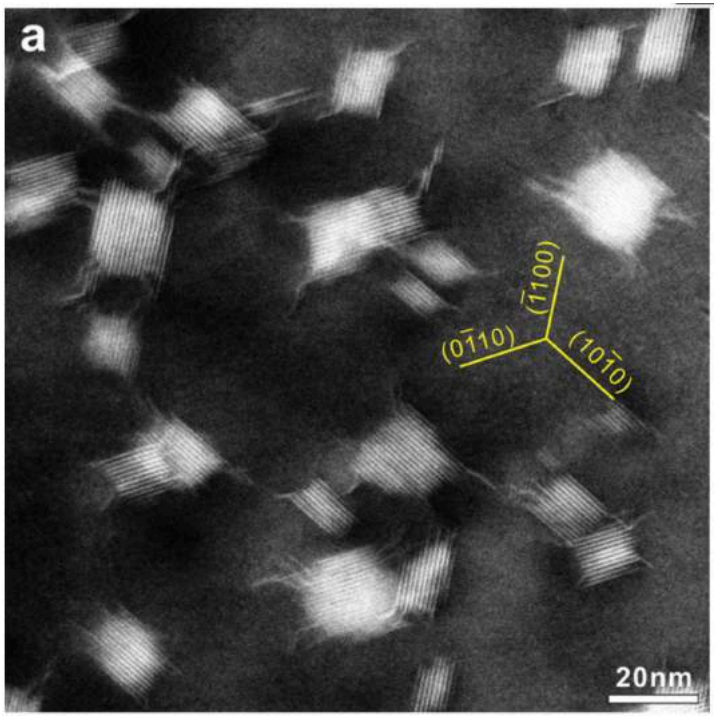
(a) D. Isheim et al., Surf. Interface Anal. 36, 569(2004) (b) M.E. Fine et al., Scripta Mater. 53, 115(2005)
(c) W. Xu et al., PRB 54, 6941(1996)

Precipitate strengthening in Mg and Al alloys

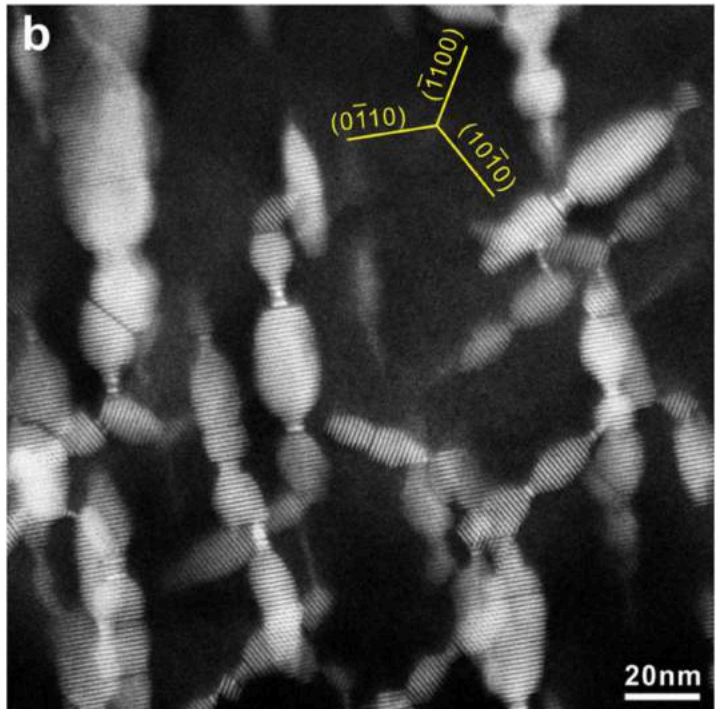
- Elastic modulus, elastic mismatch strain, and interface energy of precipitates (DFT)
- Growth of precipitates: competition between strain energy and interface energy (phase field)
- Precipitate strengthening: precipitate-dislocation interaction (phase field)

Background

- Mg-based alloys containing rare earth metal (RE) receive intensive interests in aerospace industry.
- The β' phase (Mg_7RE) is key strengthening precipitate in Mg-Y and Mg-Gd.



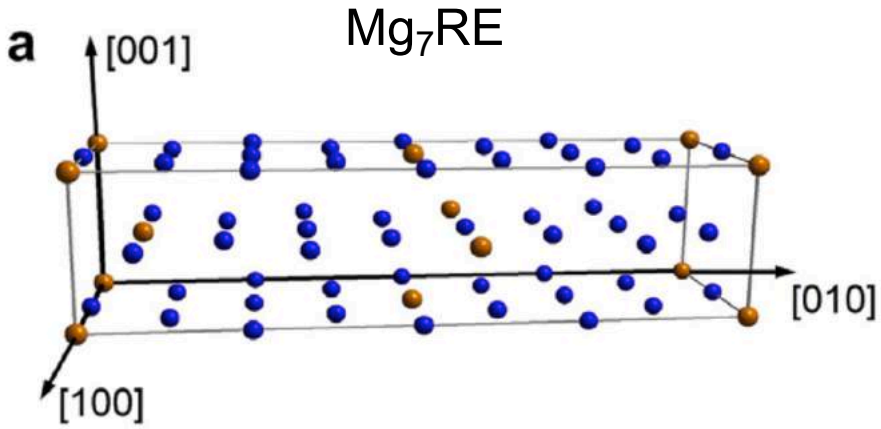
Equiaxed shape in Mg-Y



truncated lenticular shape in the Mg–Gd

Liu, et al., Acta Mater. 61, 453 (2013)

Lattice constant of β' phase



Mg_7RE

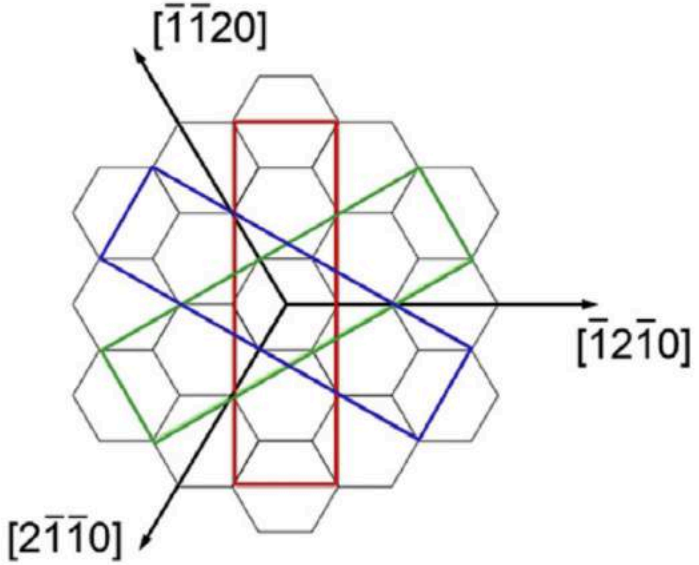
- Crystal structure from Nishijima et al.
- DFT calculations using VASP (PBE)

- For lattice coherence to Mg matrix,

$$a \sim 2a_{\mathrm{Mg}},\ b \sim 4\sqrt{3}a_{\mathrm{Mg}} \text{ and } c = c_{\mathrm{Mg}}$$

- Expansion in *a* and *b*, contraction in *c*

Orientation variants of Mg_7RE to Mg

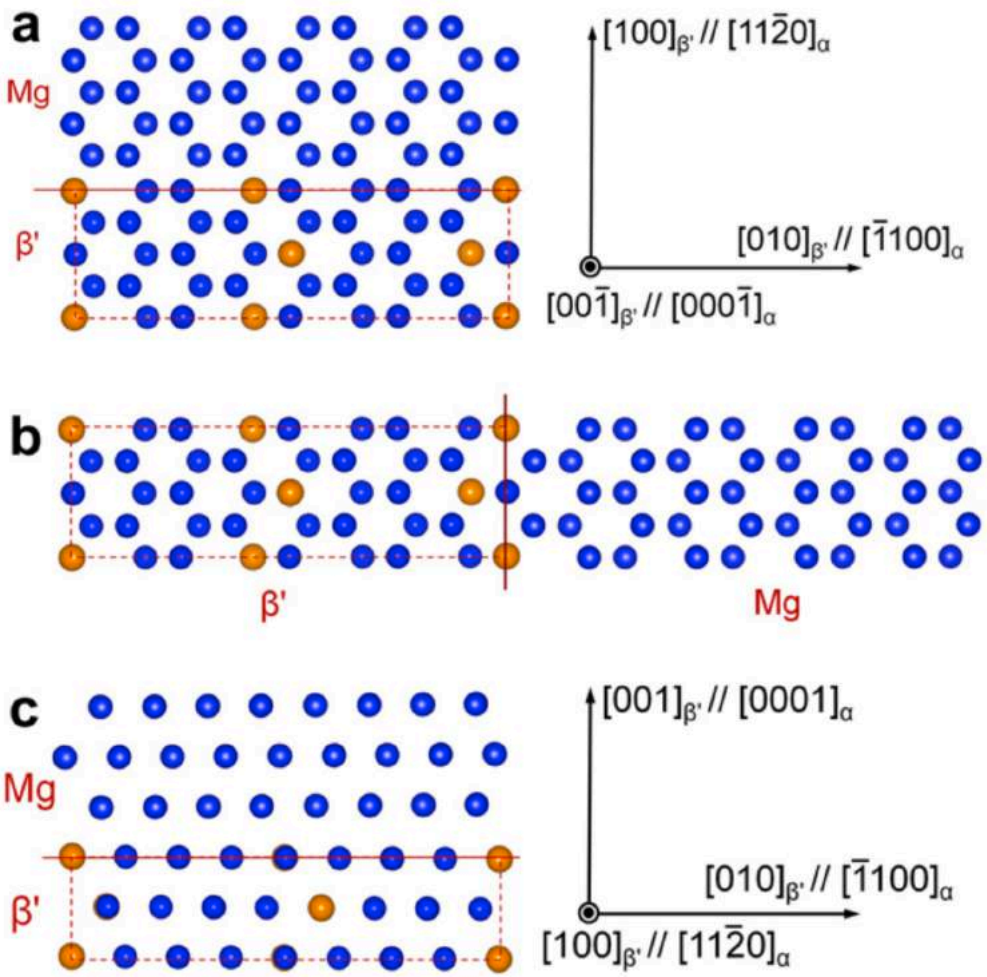


	a (nm)	*b* (nm)	*c* (nm)
β′-Mg_7Y	0.6596	2.2623	0.5176
β′-Mg_7Gd	0.6618	2.2574	0.5172
Mg	0.3200		0.5200

Liu et al., Acta Mat. 61, 453 (2013)

Interface energy of β' phase in Mg

$(100)_{\beta'}$ $(010)_{\beta'}$ and $(001)_{\beta'}$ interfaces



- Slab model for interfaces
- DFT calculations using VASP + PBE

Mg/β_0-Mg_7Y: 30.16 J/m^2
Mg/β_0-Mg_7Gd: 27.54 J/m^2

Mg/β_0-Mg_7Y: 4.39 J/m^2
Mg/β_0-Mg_7Gd: 3.67 J/m^2

Mg/β_0-Mg_7Y: 27.76 J/m^2
Mg/β_0-Mg_7Gd: 25.52 J/m^2

Phase field model

- Cahn-Hillard and Allen-Cahn equations for conc. and structure order parameters.

$$\frac{1}{V_m^2}\cdot\frac{\partial x_{RE}}{\partial t}=\nabla\cdot\left\{M\cdot\nabla\cdot\frac{\delta E_{tot}}{\delta x_{RE}}\right\}+\xi_x(\mathbf{r},\mathrm{t})$$

$$\frac{\partial\eta_i(\mathbf{r},t)}{\partial t}=-L\cdot\left\{\frac{\delta E_{tot}}{\delta\eta_i}\right\}+\xi_\eta(\mathbf{r},\mathrm{t})$$

- Total free energy includes chemical, strain, and interface energies.

$$E_{tot}=\int_V\left(f(x_{RE},\{\eta_1,\eta_2,\eta_3\})+\frac{\kappa_{RE}}{2}(\nabla x_{\mathrm{Y}})^2+\frac{1}{2}\sum_{p=1}^{3}\alpha_{ij}(p)\nabla_i\eta_p\nabla_j\eta_p\right)dV+E^{el}$$

Chemical free energy

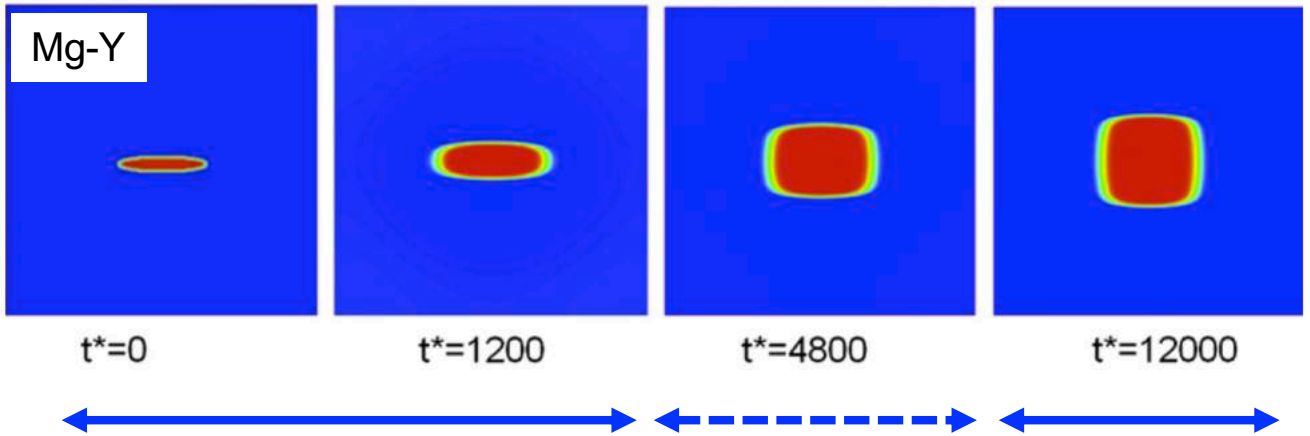
Interface free energy

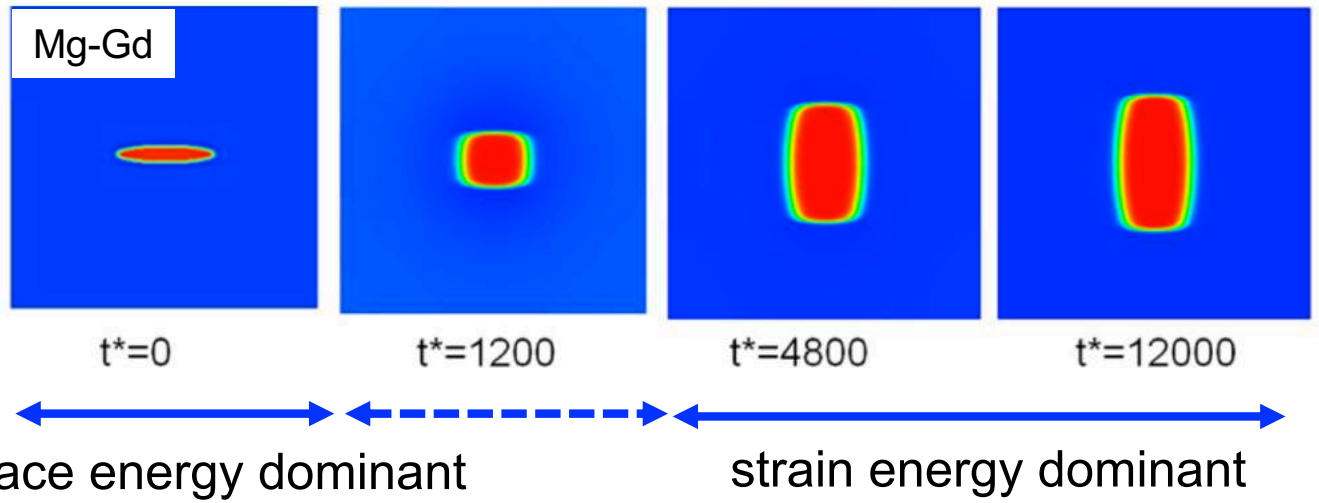
Strain energy

- Chemical free energy from CALPHAD database.
- Strain energy modelled by Khachaturyan's micro-elasticity theory using parameter from DFT calculations.
- Interface energy results are from DFT calculations.

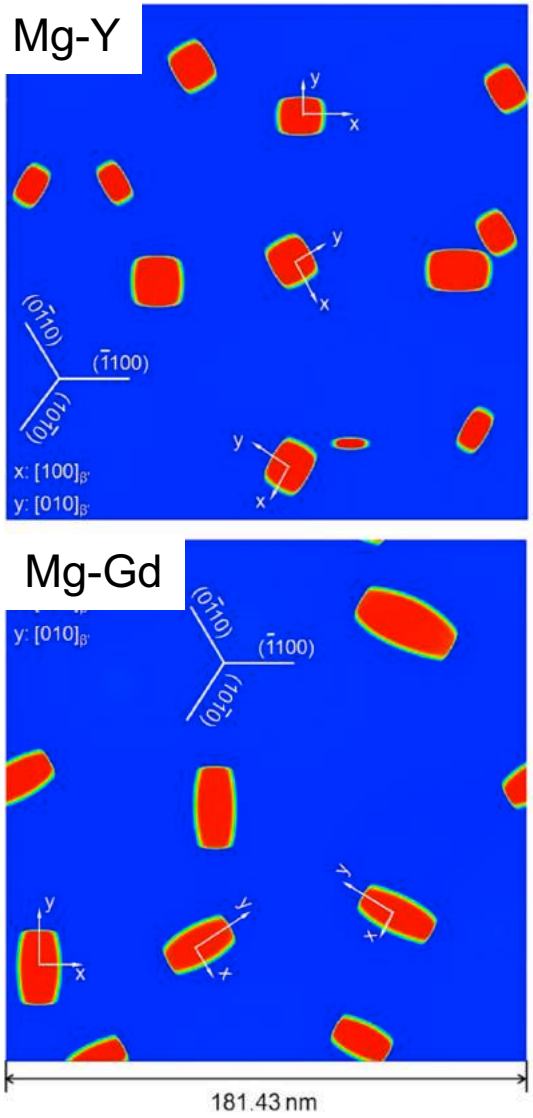
Evolution of microstructure from phase field

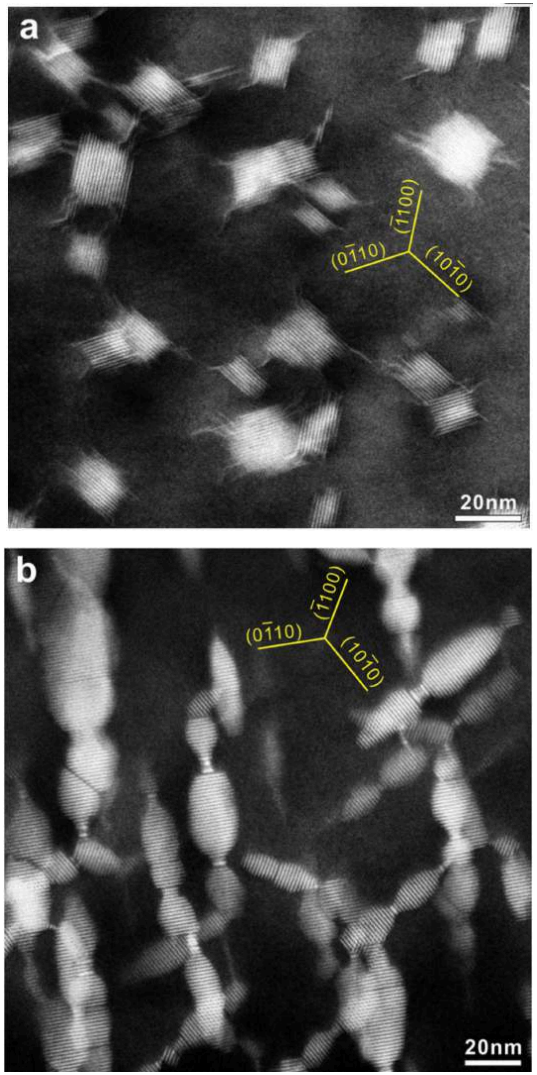
- Precipitate shape changes depending on precipitate size

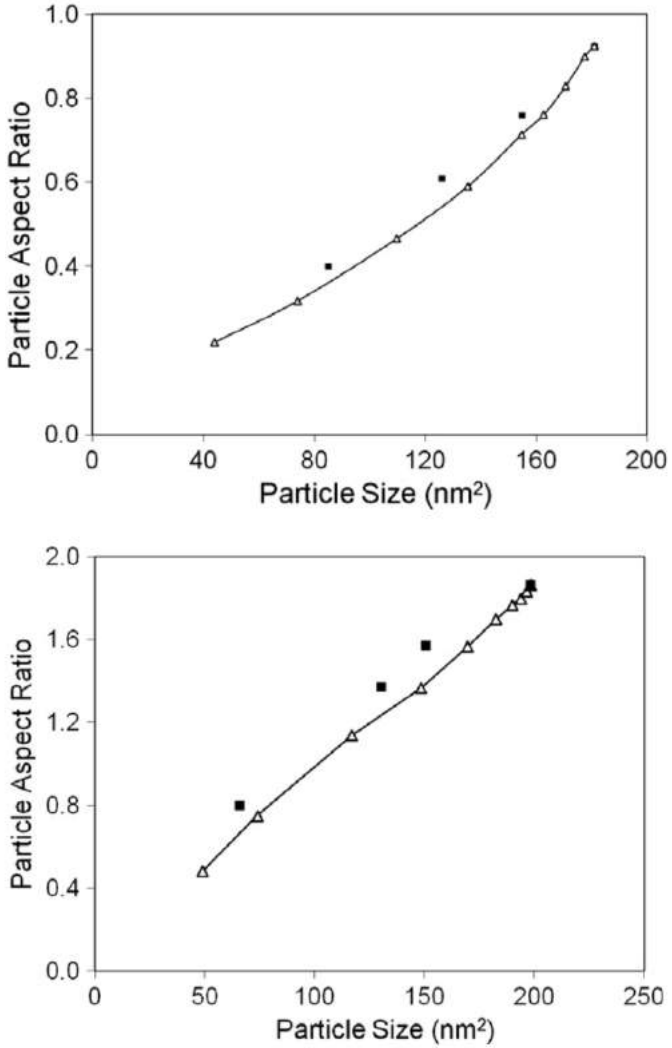




Comparison with experiments

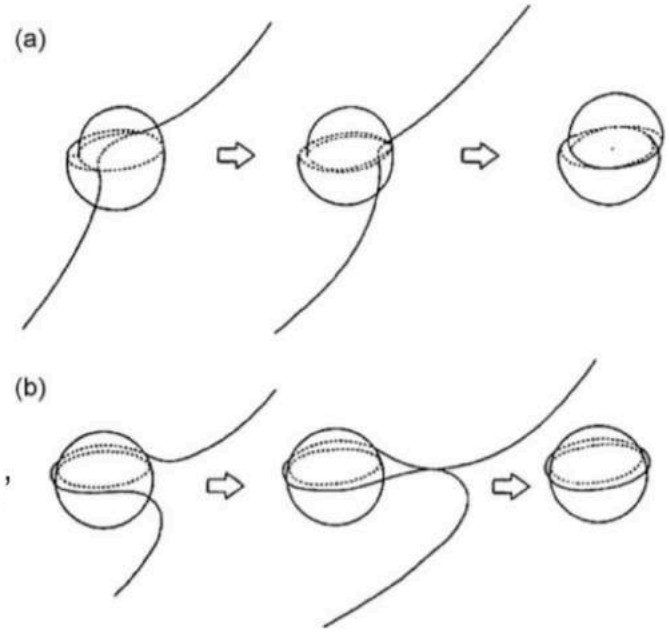


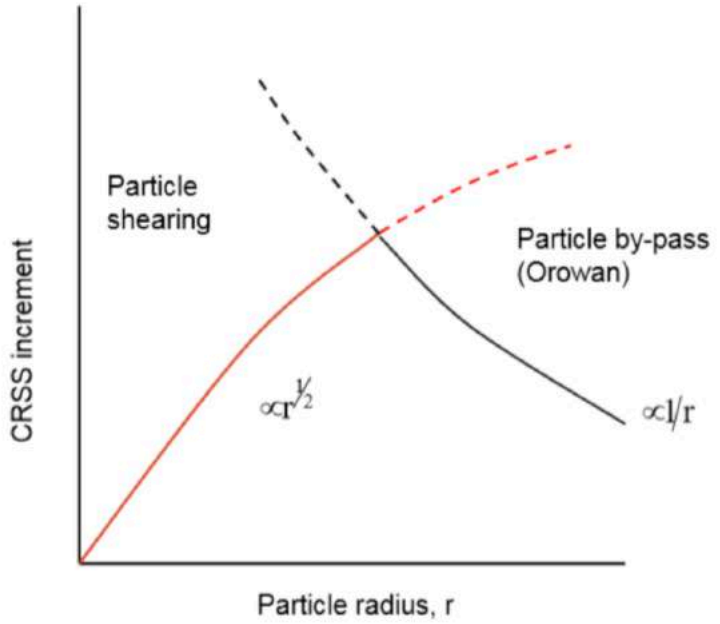




Strengthening from precipitates

- Precipitates can hinder the motion of dislocations in alloys and thus enhance yield strength (CRSS).
- Two types of precipitates, shearable and non-shearable.



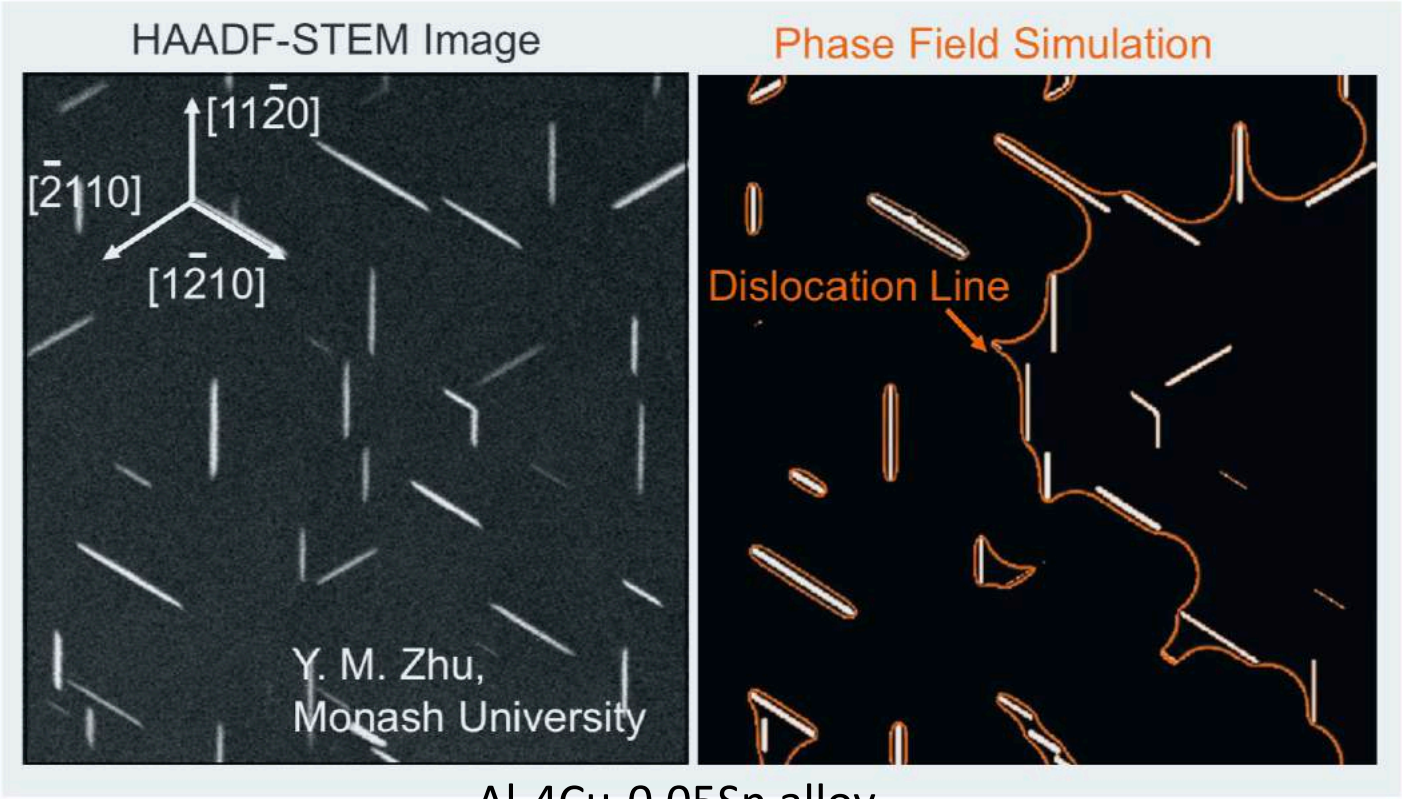


Which mechanism will operate in a given alloy?
How to quantitatively determine the CRSS increasement?

J. W. Martin, Precipitate hardening (1998)

Application of phase field method in precipitate strengthening

Key idea: calculating the minimum stress for a gliding dislocation passing through the precipitate forest

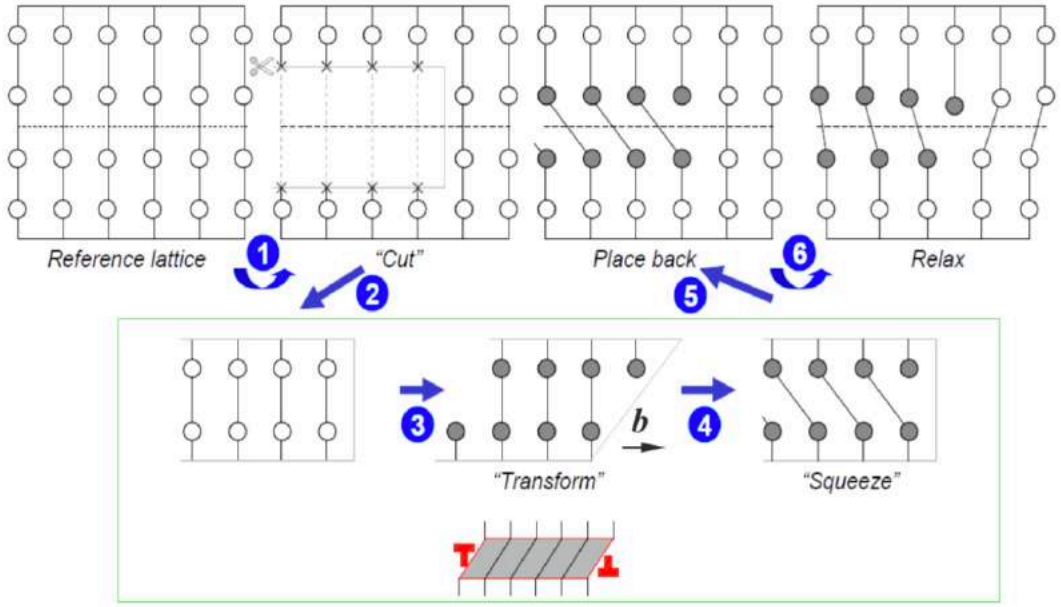


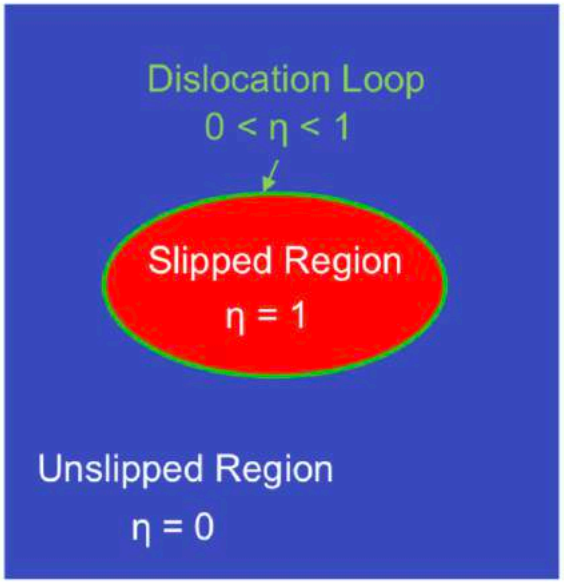
Al-4Cu-0.05Sn alloy

Advantages: No need to track the position of dislocation line at each time step.

Phase field – dislocation model

The description of a dislocation loop in phase field model is based on the **equivalence** between the atomic lattices around **a dislocation loop** and around **a sheared plate of one atomic layer thick** (the shear amount equal to the Burgers vector b)





Eigen-strain of a slip system:

Burgers vector — Slip plane normal

$$\varepsilon_{ij}^{dis} = \frac{\mathbf{b} \otimes \mathbf{n}}{2d} = \frac{b_i n_j + b_j n_i}{2d}$$

Inter-planar distance of the slip plane (thickness of the sheared plate)

Phase field – dislocation model

Evolution equation

$$\frac{\partial \eta}{\partial t} = -L\frac{\delta E}{\partial \eta} \rightarrow E = \int \mathrm{d}^3 r \left[E^c + \frac{\kappa_\eta}{2}(\nabla\eta)^2\right] + E^{elas}$$

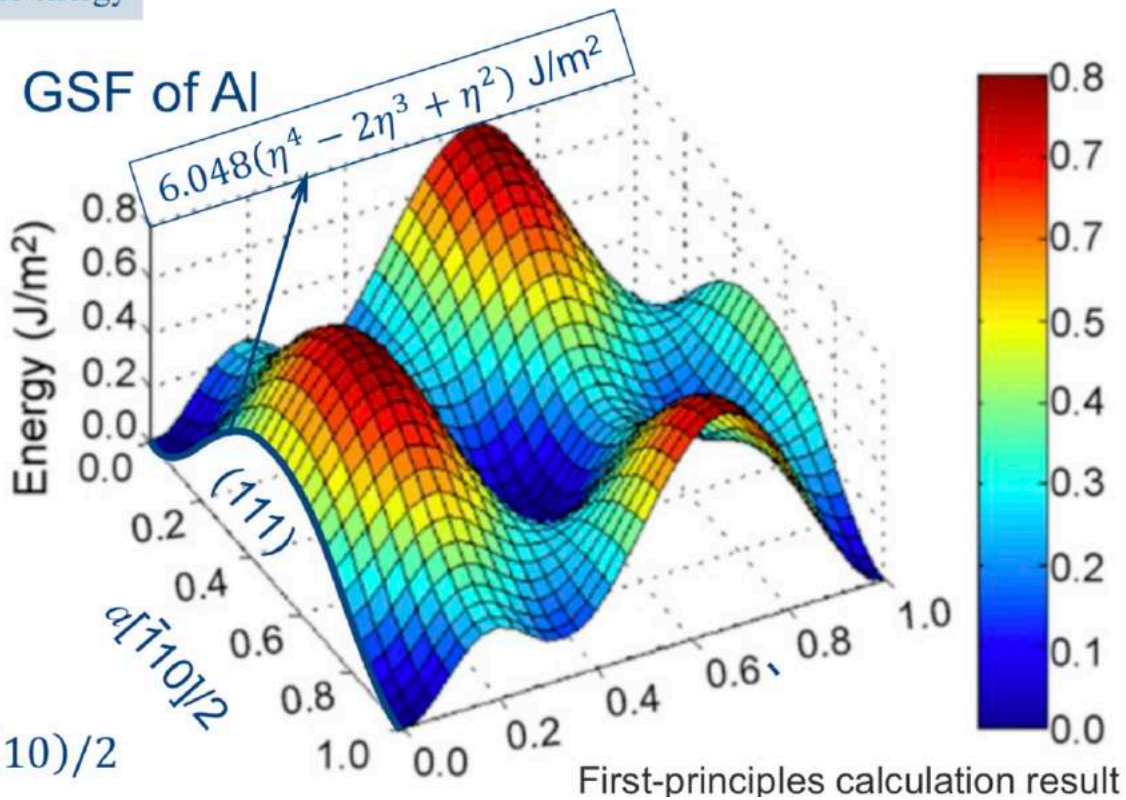
E^{elas} → Strain energy

E^c → Crystalline energy

Crystalline energy

- Often obtained from the atomistic calculations of the generalized stacking fault energy (GSF)
- For simplicity, if only one slip system is considered, we only need to use a proper function to fit the GSF data along this slip direction

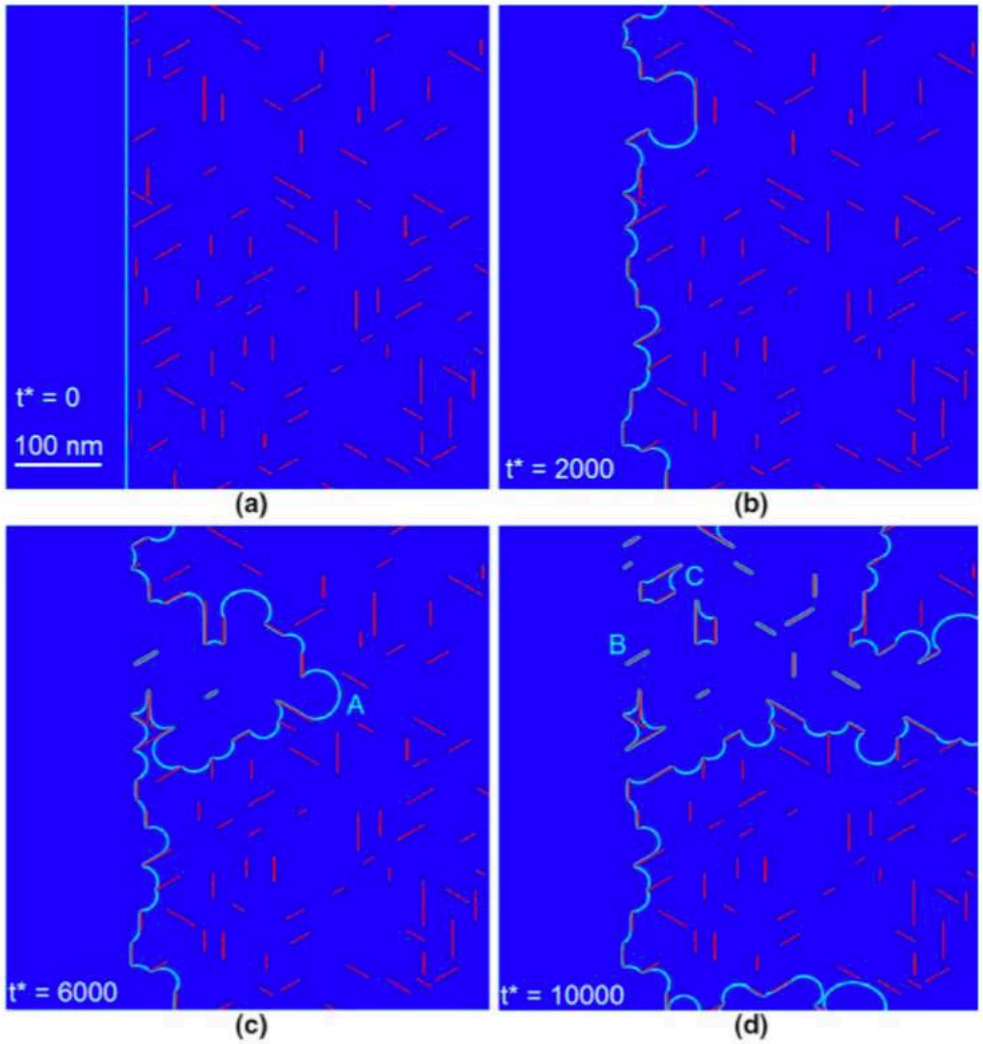
e.g. $\langle\bar{1}10\rangle(111)$ system, $\boldsymbol{b} = (\bar{1}10)/2$



Liu et al. MMTA 46A, 3287 (2015)

Results

Al-4Cu-0.05Sn alloy



- At each aging condition, ten samples following TEM experiments.
- Non-shearable mechanism works in this alloy.
- The simulated CRSS increase agree with experiments very well.

Table II. Simulated ΔCRSS (MPa) Values of Samples Aged at 473 K (200 °C)

	Aging Time (h)			
Group	0.5	3	48	168
1	63.60	92.98	64.31	38.50
2	73.36	93.53	64.90	52.53
3	67.03	88.09	61.95	43.39
4	68.09	87.54	67.85	44.37
5	60.16	88.63	56.64	49.92
6	60.69	94.44	54.87	48.94
7	74.42	87.54	60.18	45.02
8	73.89	87.77	57.82	39.80
9	74.42	88.09	69.62	43.71
10	70.42	86.08	67.85	47.31
$\overline{\Delta\tau}$	68.60	89.46	62.60	45.34
Standard deviation	5.60	3.00	5.13	4.33
Experimental data	70	84	60	47

Conclusion

- Multiscale mechanics is an essential part of ICME for metallic alloy design.
- Multiscale mechanics is critical for microstructures as well as the mechanical properties of metallic alloys.
- Integrating computational tools and models can quantitatively predict how the hierarchy of microstructures affects the mechanical properties of the alloys.
  - DFT for twin boundary segregation in MgGdZn
  - DFT + Micromechanics for precipitate strengthening in Fe-Cu
  - DFT + Phase field for precipitate growth and strengthening in some Mg and Al alloys.

Thank you!

Questions?

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