Role of precipitates in commercial Al and Mg alloys

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Research and Advanced Engineering

Ford Motor Company

Outline

- Automotive interest in materials modeling
  - Cost- and time-effective
  - Fuel economy → Lightweight Al and Mg alloys
- Precipitates

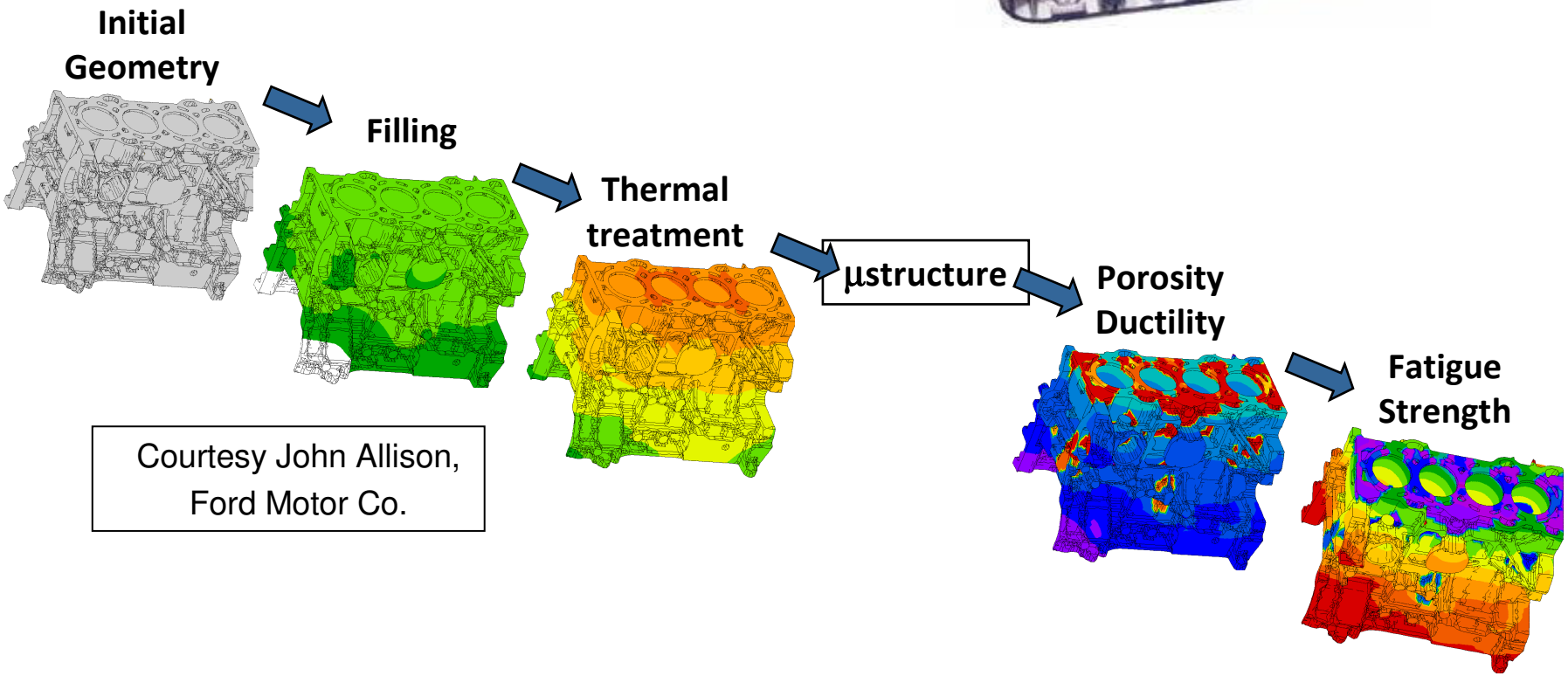
  Yield strength, ductility, thermal fatigue behavior
- From atomistic simulations to macro materials properties

  Integrated Computational Materials Engineering (ICME)
- Example: Mg-Al alloys & $Mg_{17}Al_{12}$ precipitates
  - Interfacial energy
  - Elastic properties

Simulations of cast Al alloys

Virtual Al Castings suite of programs

- Powertrain
- Improve time to market
- Improve quality
- Reduce cost



Courtesy John Allison, Ford Motor Co.

Wrought & cast alloys

2004 aluminum-bodied Jaguar XJ

Al alloys

- Al 5xxx and 6xxx series – body applications
  - Stamped and paint-baked
- Extrusions

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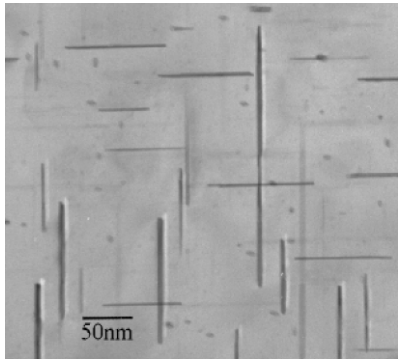
Mg Alloys – Virtual Mg Casting programs

- Lightweight body structures
- Replacing some Al with Mg
- Mg extrusions

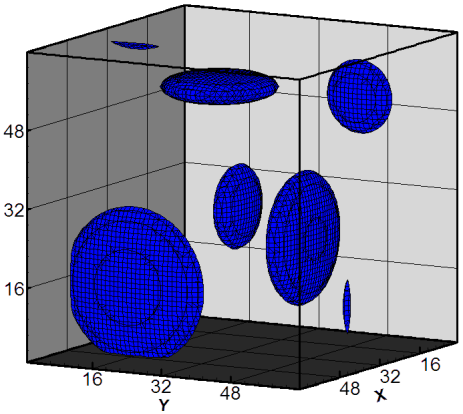
- Cost
- "Inferior" properties compared to steel
- Alloying technology & manufacturing not as mature

Strengthening precipitate orientations

Al-Cu (2xxx, 3xx)
θ'-Al_2Cu

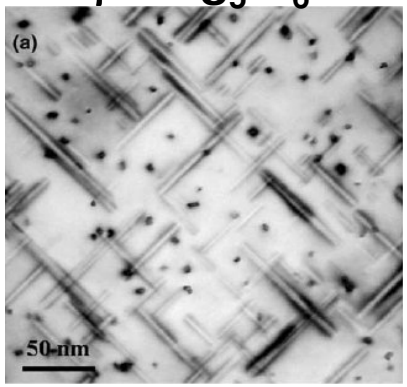


Ford Motor Co.

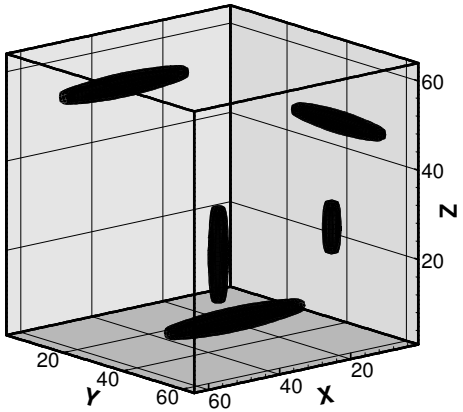


Ford phase-field prediction
Courtesy: Mei Li, Ford Motor Co.

Al-Mg-Si (6xxx)
β''-Mg_5Si_6

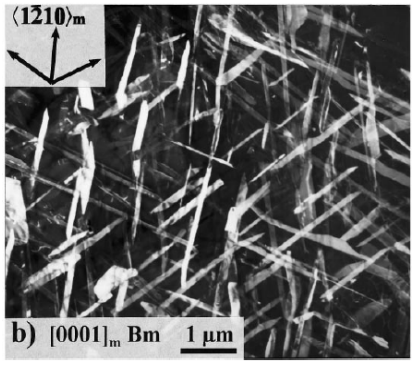


Tsao, Scripta Mater., 2005, 53, 1241.

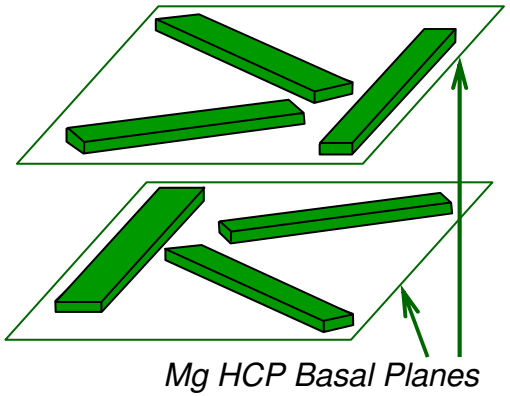


Ford phase-field prediction
Courtesy: Mei Li, Ford Motor Co.

Mg-Al-Zn (AZ91)
β-$Mg_{17}Al_{12}$



Celotto, Acta Mater., 2000, 48, 1775.



Mg HCP Basal Planes

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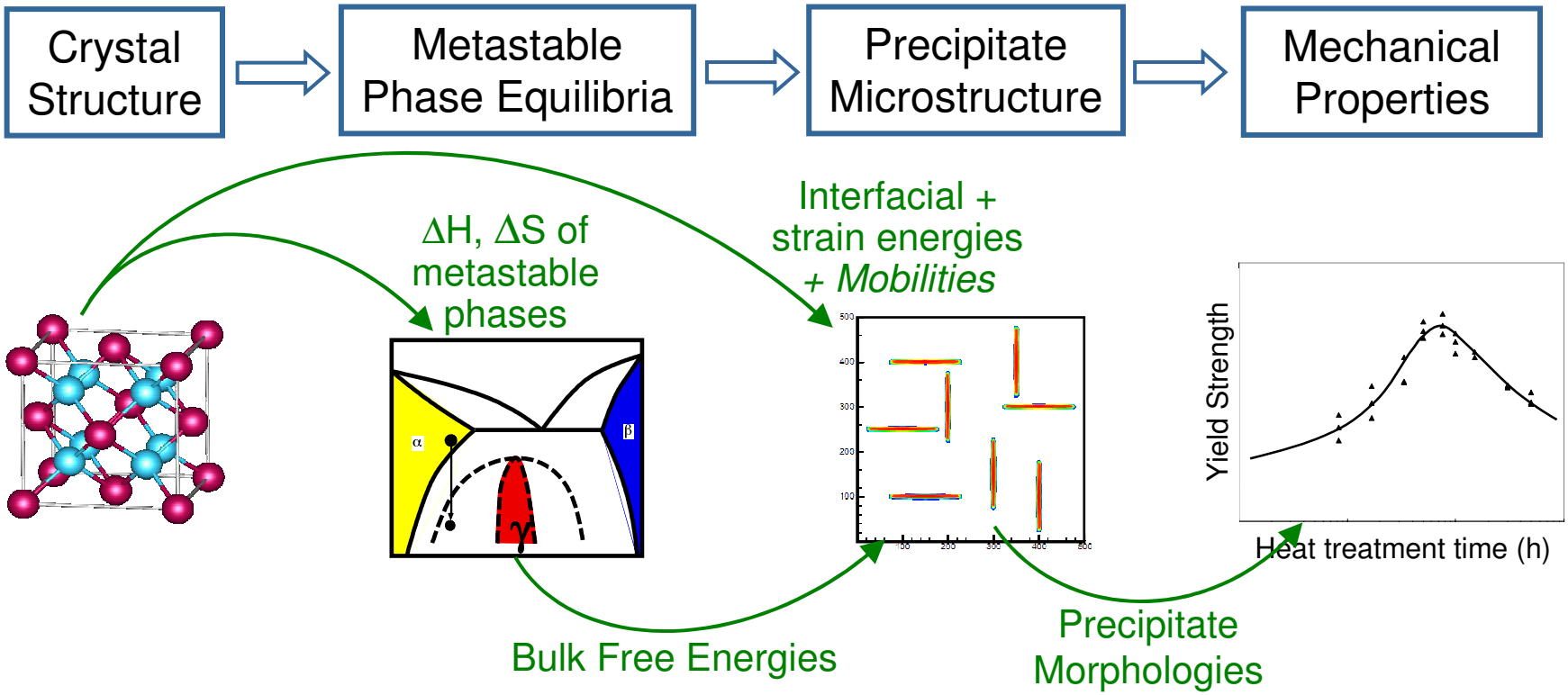
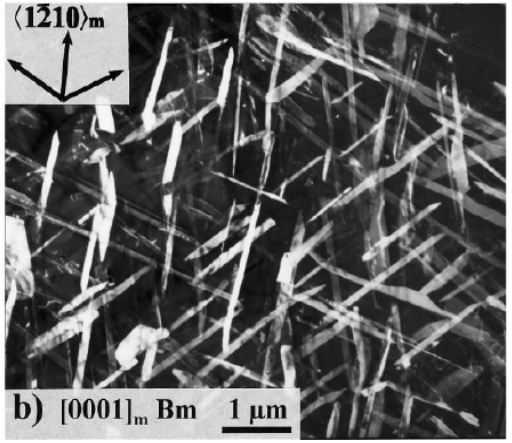
Integrated Comput. Materials Engineering



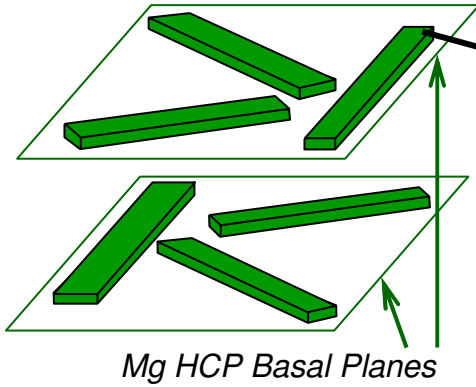
Atomistic simulations in Mg alloys

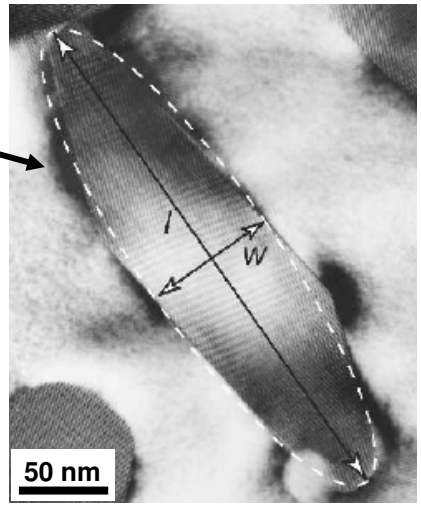
Mg ICME:

- High-strength Mg alloys – Mg-Al alloys
- Strengthened by platelet β-$Mg_{17}Al_{12}$ precipitates in Mg matrix



Celotto, Acta Mater. 48 (2000) 1775.





Hutchinson, Metall. & Mat. Trans. 36A (2005) 2093.

- Optimize growth of β precipitates (phase-field model)

  interface energies, strain energies, lattice parameters & elastic constants

- Promote growth of precipitates in **non**-basal planes (with Prof. Chris Wolverton, Northwestern University)

AZ91 alloy – Input for phase-field model

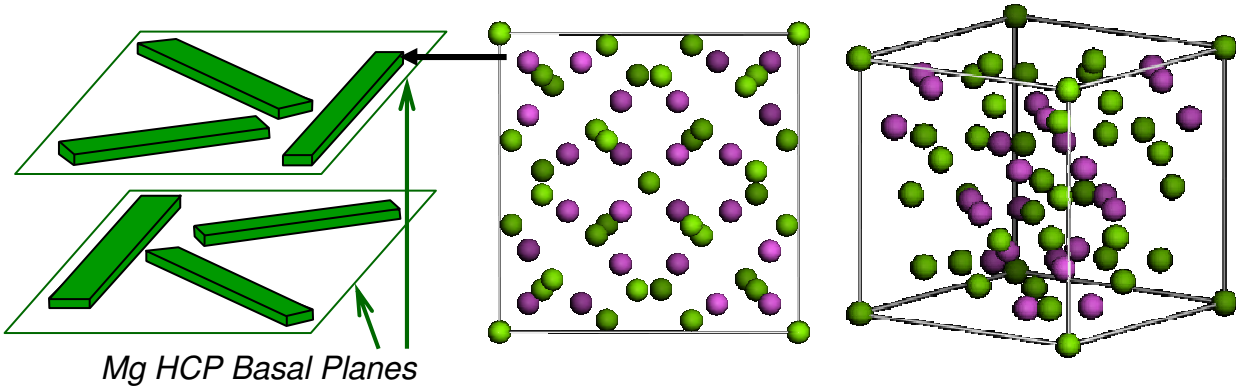
- Crystal structure:

  β-$Mg_{17}Al_{12}$:

  BCC, $I\bar{4}3m$

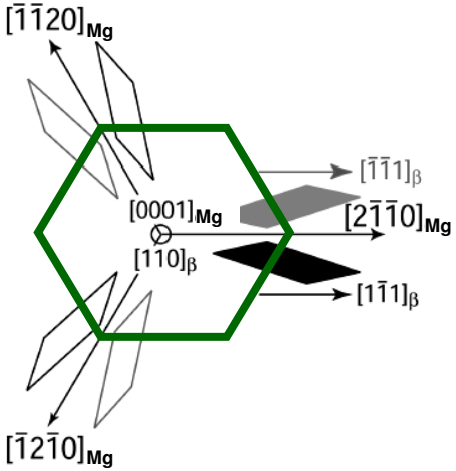
  a=1.056 nm

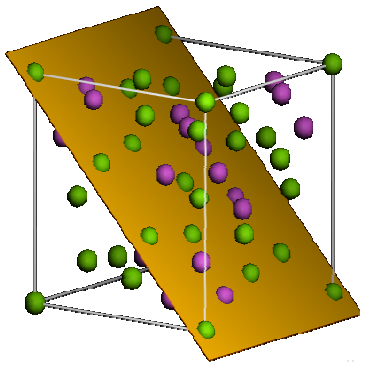
  58 atoms

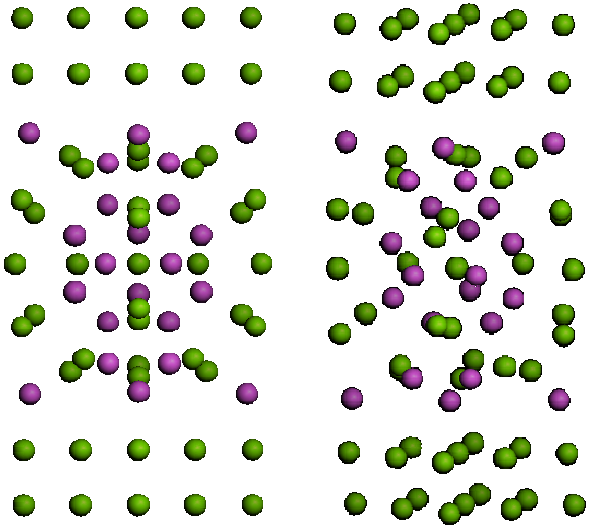


- Habit planes and orientation relationships:

$(0001)_{Mg} \parallel (110)_{\beta}$, $[1\text{-}210]_{Mg} \parallel [1\text{-}11]_{\beta}$







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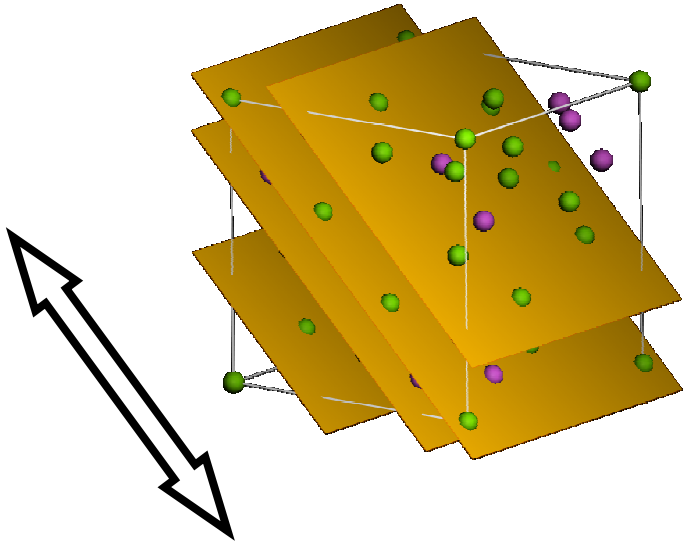
Mg-alloy β phase

- Termination of β:

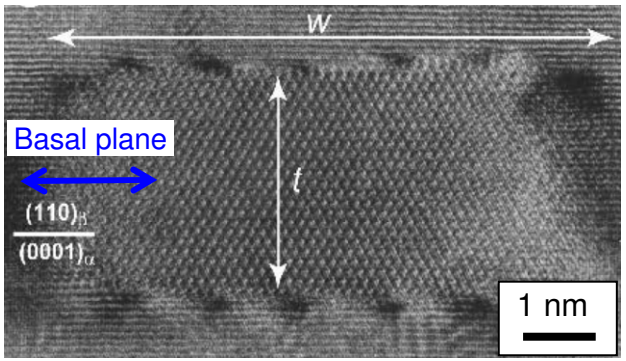


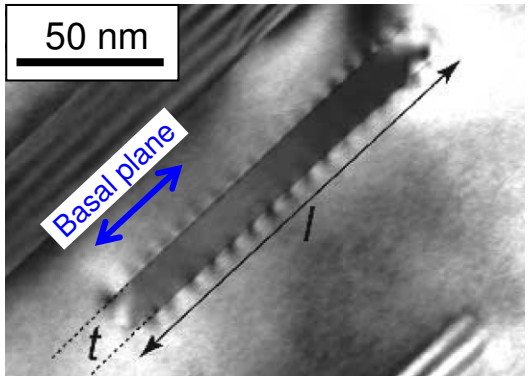
- Fitting BCC to HCP:

  Matrix: **HCP**, $P6_3/mmc$,
  a=0.321 nm, c=0.521 nm

- Coherency? … misfit dislocations?:

  Periodic strain contrast: semi-coh interface, punctuated by dislocations





Hutchinson et al., Metall. Mat. Trans., 36A (2005).

Conclusions

- Great automotive interest in materials modeling
  - Cast and wrought
  - Al, Mg, … steel
- Precipitates
  - Interface energy, elastic energy, …
- Atomistic simulations are needed
  - Integrated Computational Materials Engineering
  - Phase-field model
    - Gibbs Energy
    - Diffusion constant

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