The Materials Genome Initiative and Lightweight Materials

Will Joost
Lightweight Materials
Vehicle Technologies Office
Transportation accounts for ~28% of U.S. energy consumption

Energy Information Administration (www.eia.gov)
~93% of transportation energy is from petroleum

~70% of petroleum is used in transportation

Energy Information Administration (www.eia.gov)
Transportation Energy Consumption by Mode - 2011

On-highway consumption: \( \sim 11.2 \text{ mbpd} \)

U.S. domestic production: \( \sim 5.7 \text{ mbpd} \)

Non-Highway:
- Military and Other: 5%
- Air: 9%
- Busses: 1%

Highway:
- Light Duty Vehicles: 60%
- Comm. and Heavy Duty Trucks: 19%
- Marine: 4%
- Rail: 2%

Energy Information Administration (www.eia.gov)
Vehicle Weight Reduction

**Conventional ICE**

- 6%-8% improvement in fuel economy for 10% reduction in weight

**Hybrid/Electric Vehicles**

- Improvement in range, battery cost, and/or efficiency

**Commercial/Heavy Duty**

- 13% improvement in freight efficiency for 6% reduction in weight
Lightweight Automotive Materials

**Magnesium Alloys**
- When it “works” → 40-70% weight reduction
- Otherwise → **Cost (~$3-10/ lb-saved)**
  - Lack of domestic supply, unstable pricing
  - Challenging corrosion behavior
  - Inadequate strength, stiffness, and ductility
  - Difficult to model deformation behavior

**Aluminum Alloys**
- When it “works” → 25-55% weight reduction
- Otherwise → **Cost (~$2-8/ lb-saved)**
  - Insufficient strength in conventional automotive alloys
  - Limited room temperature formability in conventional automotive alloys
  - Difficult to join/integrate to incumbent steel structures

**Advanced High Strength Steel**
- 15-25% weight reduction
  - Inadequate structure/properties understanding to propose steels with 3GAHSS properties
  - Insufficient post-processing technology/understanding
  - What other relevant properties should be considered? Hydrogen embrittlement, local fracture, etc.

**Carbon Fiber Composites**
- When it “works” → 30-65% weight reduction
- Otherwise → **Cost (~$5-15/ lb-saved)**
  - High cost of carbon fiber (processing, input material)
  - Joining techniques not easily implemented for vehicles
  - Difficult to efficiently model across many relevant length scales

Choi et. al., Acta Mat. 57 (2009) 2592-2604
Integrated Computational Materials Engineering (ICME)
Materials Genome Initiative (MGI)

**ICME:** A growing discipline in materials science and engineering

Replace and/or augment conventional experimental techniques with computational and/or high throughput techniques for generating parameters in engineering analysis

**MGI:** White House Office of Science and Technology Policy (OSTP) Initiative

Advance and integrate experimental tools, computation tools, and data to reduce the time from discovery to deployment for new materials
Deformation Modeling and Vehicle Design

Customer Requirements
Acceptable Cost, Good Crash Performance, Reliability and Durability, Fun to Drive, Low NVH, Exceptional Fit and Finish, etc...

Crash/Global Performance Modeling

Stamping/Manufacturing Modeling

Friction Law

Yield Law

Hardening Law

Failure Law


http://mml.postech.ac.kr/

A.S. Khan et al., Int. J. Plast. 26, 1432-1441, 2010


Purely Experimental

- Fixed set of materials (alloy, temper, supplier, etc.)
- Measure, measure, measure
- Calculate/fit to the best available constitutive equations
ICME and Vehicle Weight Reduction

Combined Computational/Experimental

- **Variable set of materials**
  - Alloy chemistry
  - Processing-structure
  - Within scope of selected models

- **Simulate fine-scale behavior, homogenize to higher level models**

- **Experimental input/validation where appropriate**

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**First Principles**


**Crystal/Grain Deformation**


**Microstructure Performance**


**Yield/Hardening**

1 = \((G + H)\sigma_1^2 - 2H\sigma_1\sigma_2 + (F + H)\sigma_2^2 + 2N\sigma_{12}^2\)

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**Failure/Fracture**

Magnesium Intensive Vehicle Front End

45% weight reduction
57% part consolidation

Develop, combine, and demonstrate Mg technology necessary to support implementation in large structural systems

DOE funding: $3M
USAMP, Industry Cost Share: $3M
Canadian/Chinese Activity: $6M
4 Years: FY12 – FY15
ICME for Mg Front End

Can we use ICME to quickly determine the (fatigue) behavior of various process – alloy – microstructure combinations? Can we accelerate the development of FEA material cards?

Process Modeling

Fatigue Life Modeling

Precipitation Modeling
Can we use ICME/MGI to develop 3rd Generation Advanced High Strength Steel?

- Identify steels exceeding 800MPa/1200MPa/30% and 1200MPa/1500MPa/25% (Tensile/Ultimate/Elongation)
- Reduce weight of a 4 component body assembly by >35% against a production baseline
- Reduce weight of a 4 component body assembly at a cost of less than $3.18 per pound saved

**Higher strength** – reduce gauge in strength limited components

**Greater Ductility** – enable room temperature forming

**Greater Ductility** – enable high modulus geometry in stiffness limited components
ICME for AHSS Project Structure

First Principles
- Crystal/Grain Deformation
- Microstructure Performance
- Yield/Hardening

Fine-scale Measurement
- Bulk Measurement

Failure/Fracture

ICME for AHSS Project Vision

• Produce a new steel using integrated models and experimentation across many length scales
  – Predict novel alloy chemistry and microstructure to meet challenging targets
  – Connect fundamental materials science to bulk simulations and validate against large system demonstrations

• Educate communities
  – Demonstrate the value of an ICME approach
  – Connect the best-and-brightest to fundamental metallurgy research

DOE funding: $6M
Industry Cost Share: ~$2.5M
4 Years: FY13 – FY16
Traditional models used by industry to predict component and system level performance and cost
Mass Reduction, Vehicles, and Energy:


EERE Vehicle Technologies Program Resources:

• Annual Reports
  http://www1.eere.energy.gov/vehiclesandfuels/resources/fcvt_reports.html

• Annual Review Presentations
  http://www1.eere.energy.gov/vehiclesandfuels/resources/proceedings/index.html

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