U.S. DEPARTMENT OF ENERGY
Energy Efficiency & Renewable Energy

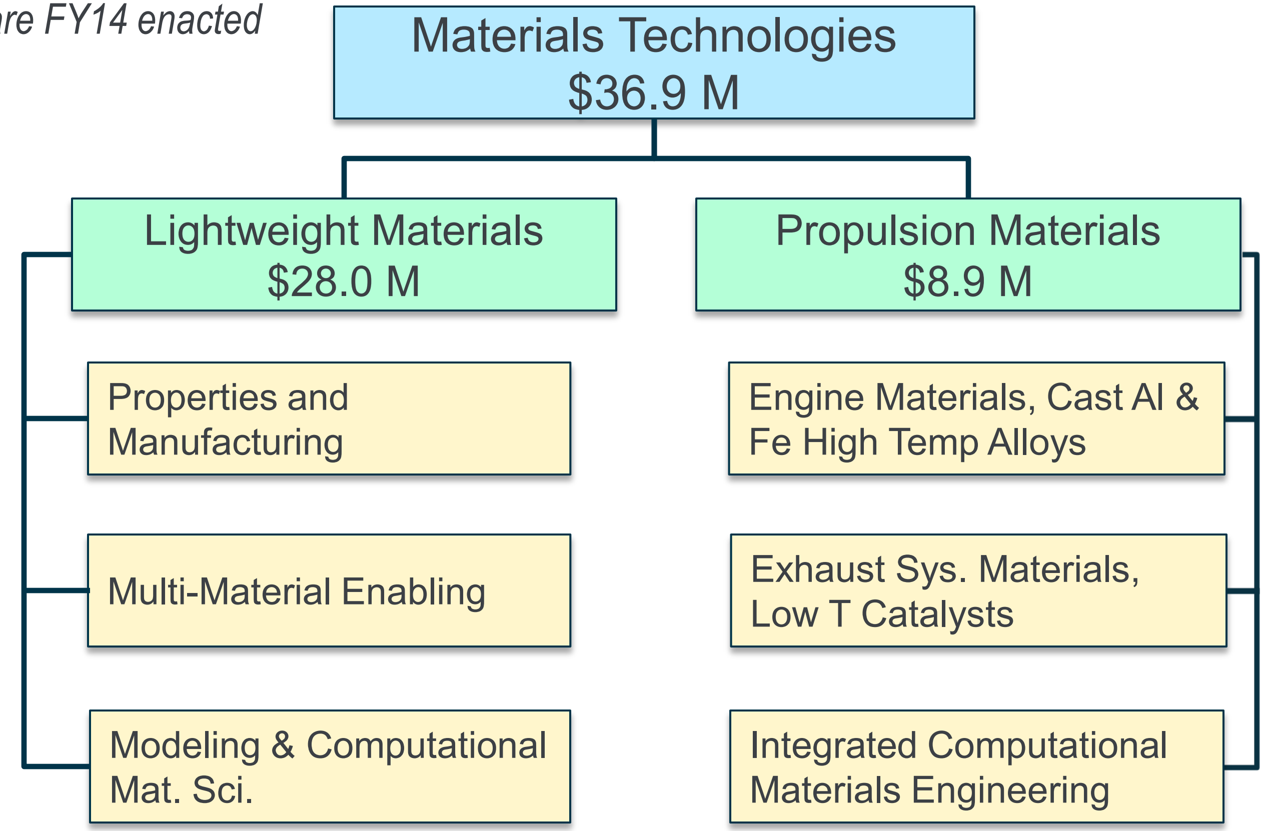
Vehicle Technologies Office

Materials Technologies

Ed Owens
Jerry Gibbs
Will Joost

Materials Technologies

Values are FY14 enacted



	Lightweight	Propulsion
FY13 Enacted	$27.5 M	$11.9 M
FY14 Enacted	$28.0 M	$ 8.9 M
FY15 Request	$47.0 M	$ 7.069 M

Materials Technology Gap Priorities

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Material	Mg	Carbon Fiber	CF composites	GF composites	AHSS	Al	Advanced Metals – (Ti, Ni)
Lack of Predictive Models	X	X	X	X	X	X	
Optimized Manuf. (lower cost)		X	X	X	X	X	X
Optimized Performance (lower cost, higher strengths, etc)	X	X		X	X		X
Design Tools		X		X			X
Raw material supply	X						X
Multi-material Joining			X			X	
Damage Detection			X				
Corrosion	X						

Workshop Propulsion Materials R&D Gaps and Targets

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Metric	2013	2050	Material Gaps
Powertrain Weight Reduction (ICE/HEV)	Baseline - LDV Baseline – HDV	40% lighter- LDV 20% lighter- HDV	Structure and Volumetric Efficiency (block, head, transmission; AL ,CF)
Power density	LDVs -2.7L 196 HP (73.4 HP/L) HD15L 475HP (32 HP/L)	LD 1.3L 196 HP (150 HP/L) LW-LD 0.7L 98 HP HD 9L 475HP (53 HP/L)	Structure and rotating components (crankshaft, pistons, connecting rods, gears; Steels +)
Energy Recovery	LDV <5% Turbocharged HD ~99% Turbocharged	LDV ~50% Turbo/ TEs/ Turbo-compounding HD~ 99%Turbo/TEs/ Rankine Cycle/Turbo-compounding	Turbochargers, Superchargers, Turbo-compounding, Rankine Cycle components, seals, fluid interactions
Exhaust Temperatures (Exhaust Valve to Turbo Inlet)	LDV - 800 °C HDV - 700 °C	1000 °C - LDV 900 °C - HDV	Valves (super alloys & Ceramics) E Manifolds, Turbochargers
Cylinder Peak Pressures	LDV ~ 50 bar HDV 190 bar	>103 bar - LDV gasoline >150 bar ATP-DI gasoline >260 bar – HDV	Structure and rotating components , gaskets, valves, friction
Engine Thermal Efficiency	LDV 30% e HDV 42% e	LDV 45% e, Stretch 55+% e HDV 55% e, Stretch 60% e	Control Heat Losses (Pistons, Cylinder wall, Cylinder head, exhaust manifold)

Vehicle Weight Reduction

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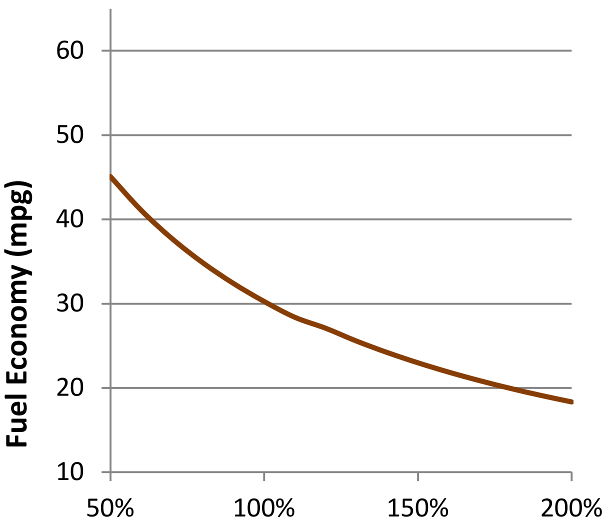
Conventional ICE

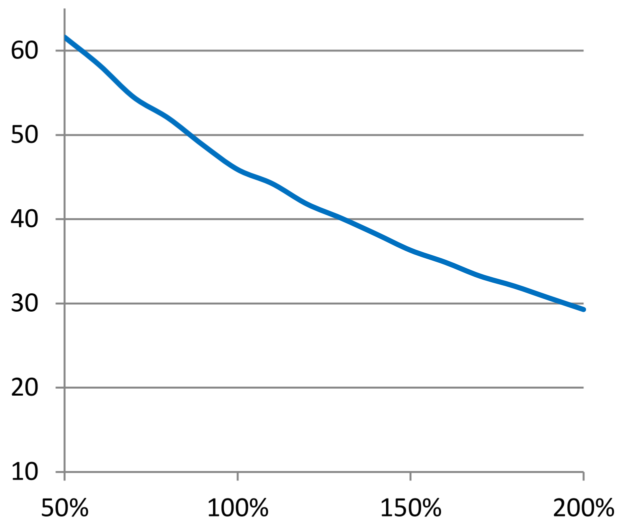


Percent of Baseline Vehicle Mass

NREL 2011

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

Hybrid/Electric Vehicles

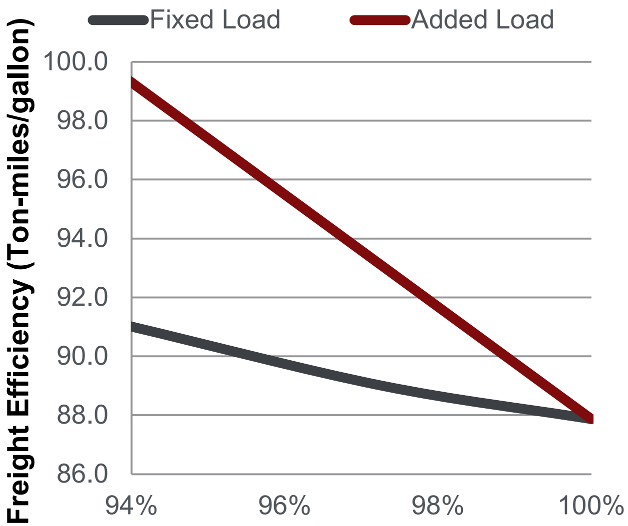


Percent of Baseline Vehicle Mass

NREL 2011

Improvement in range, battery cost, and/or efficiency

Commercial/Heavy Duty



Percent of Baseline Vehicle Mass Without Cargo

Ricardo Inc., 2009

13% improvement in freight efficiency for 6% reduction in weight

Trends in Vehicle Weight Reduction

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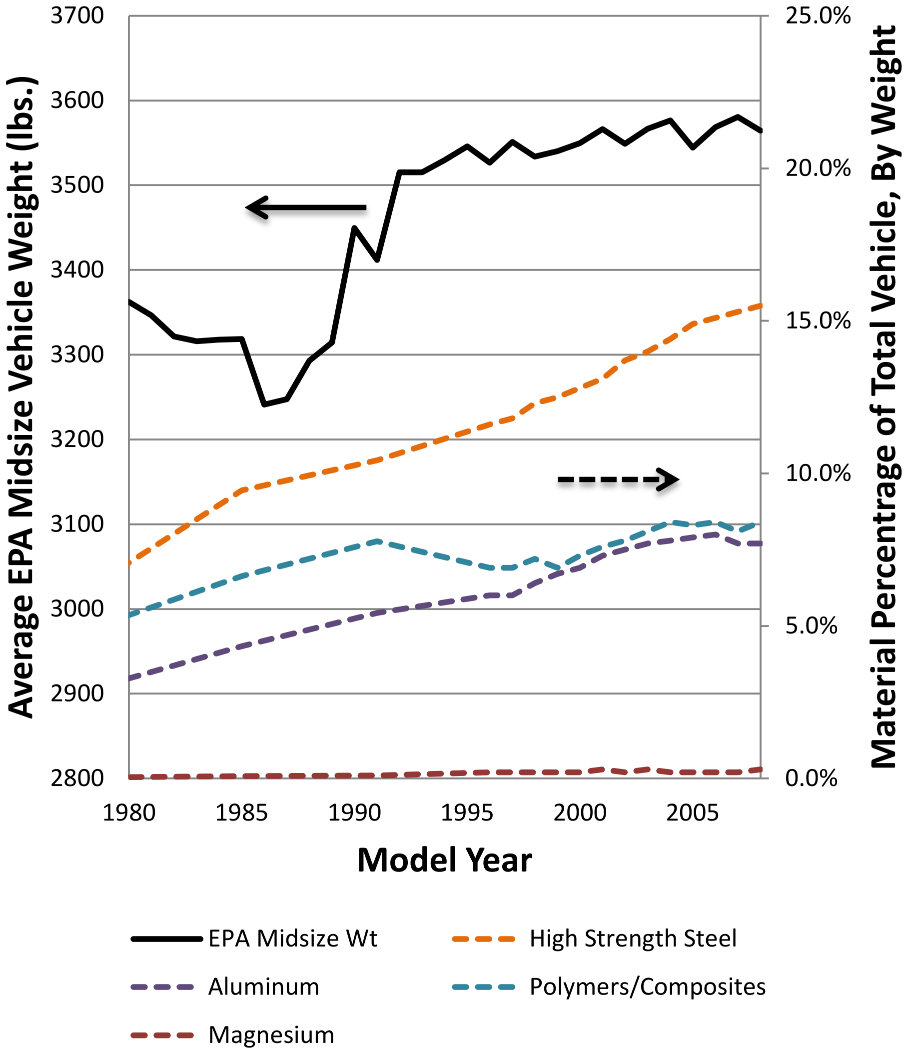
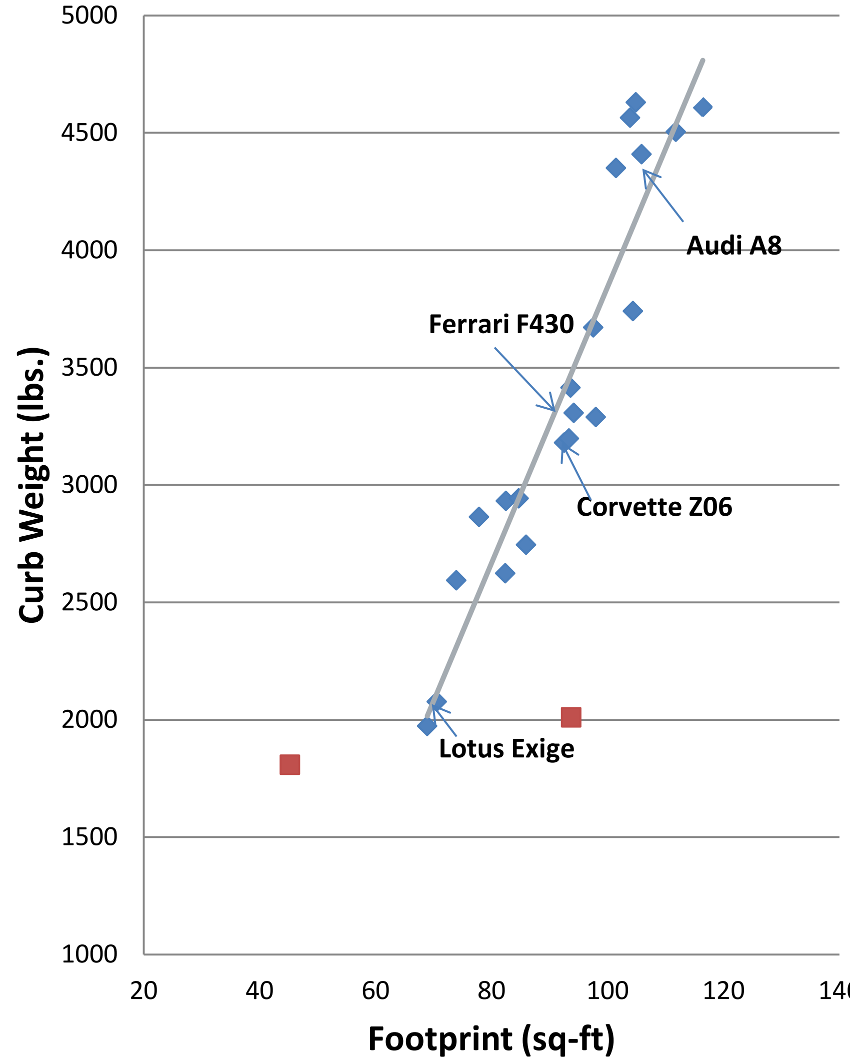
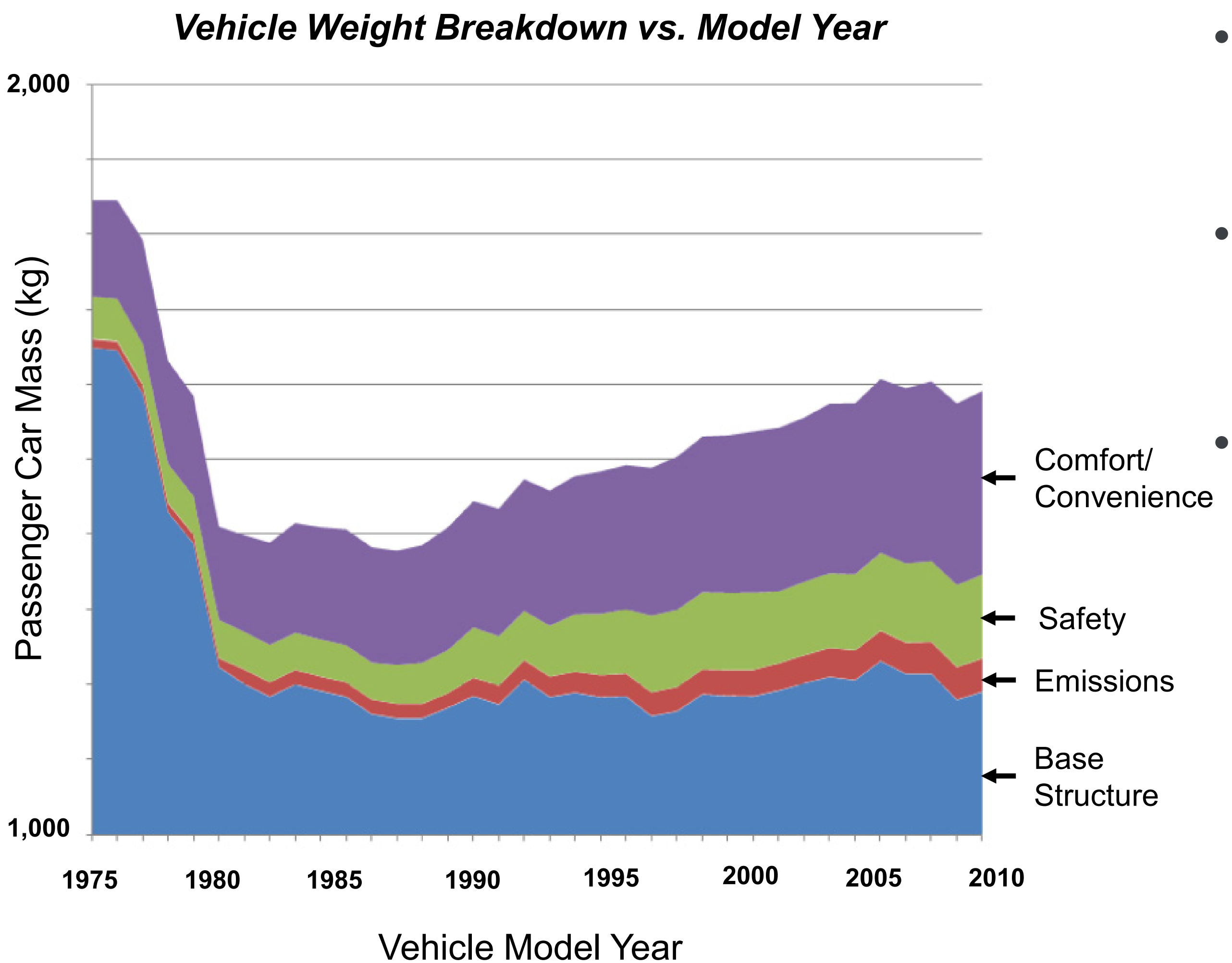
Average Vehicle Weight and Material Content



Vehicle Curb Weight vs. Footprint



Where's the Weight Reduction?



Stephen M. Zoepf "Automotive Features: Mass Impact and Deployment Characterization" MS Thesis, Massachusetts Institute of Technology, June 2011, page 36.

- Comfort, safety, and emissions control have all improved
- Base structure weight has decreased
- *System and component weight reduction has been applied to performance and comfort rather than total vehicle weight reduction*

Acceptable Cost – Societal View

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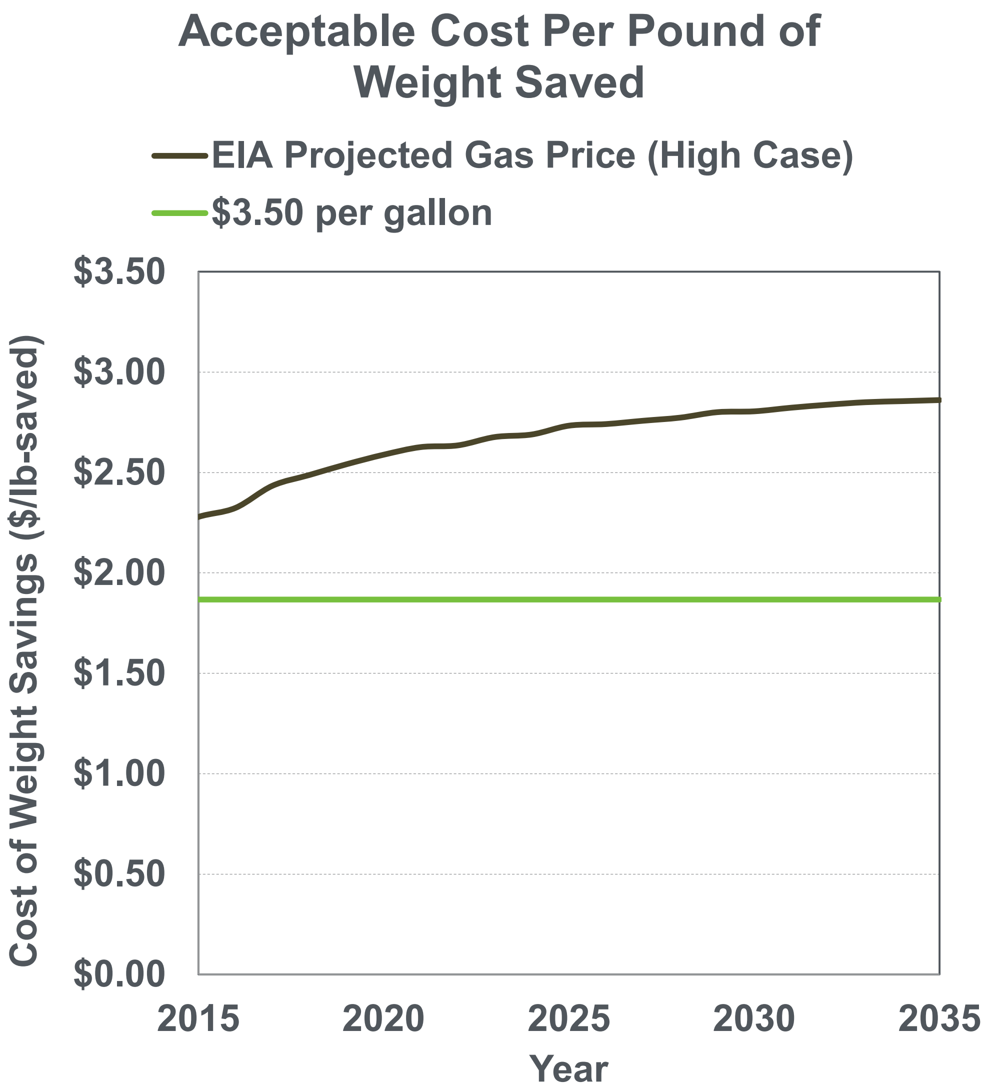
Societal view: Fuel efficiency improvement must pay back lightweighting cost over vehicle lifetime

- Model Input
  - Baseline weight: 3500 lbs.
  - Baseline FE: 28.4 mpg
  - VMT per year: 12,000 mi.
  - Vehicle life: 15 yr.
  - FE improvement per weight saved: 7%/10%
  - Fuel Price
    - $3.50/gal
    - EIA projection
  - Discount rate: 7%



Total Vehicle Weight Reduction Potential

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Sources of weight are from three categories:

Direct weight savings with lightweight materials

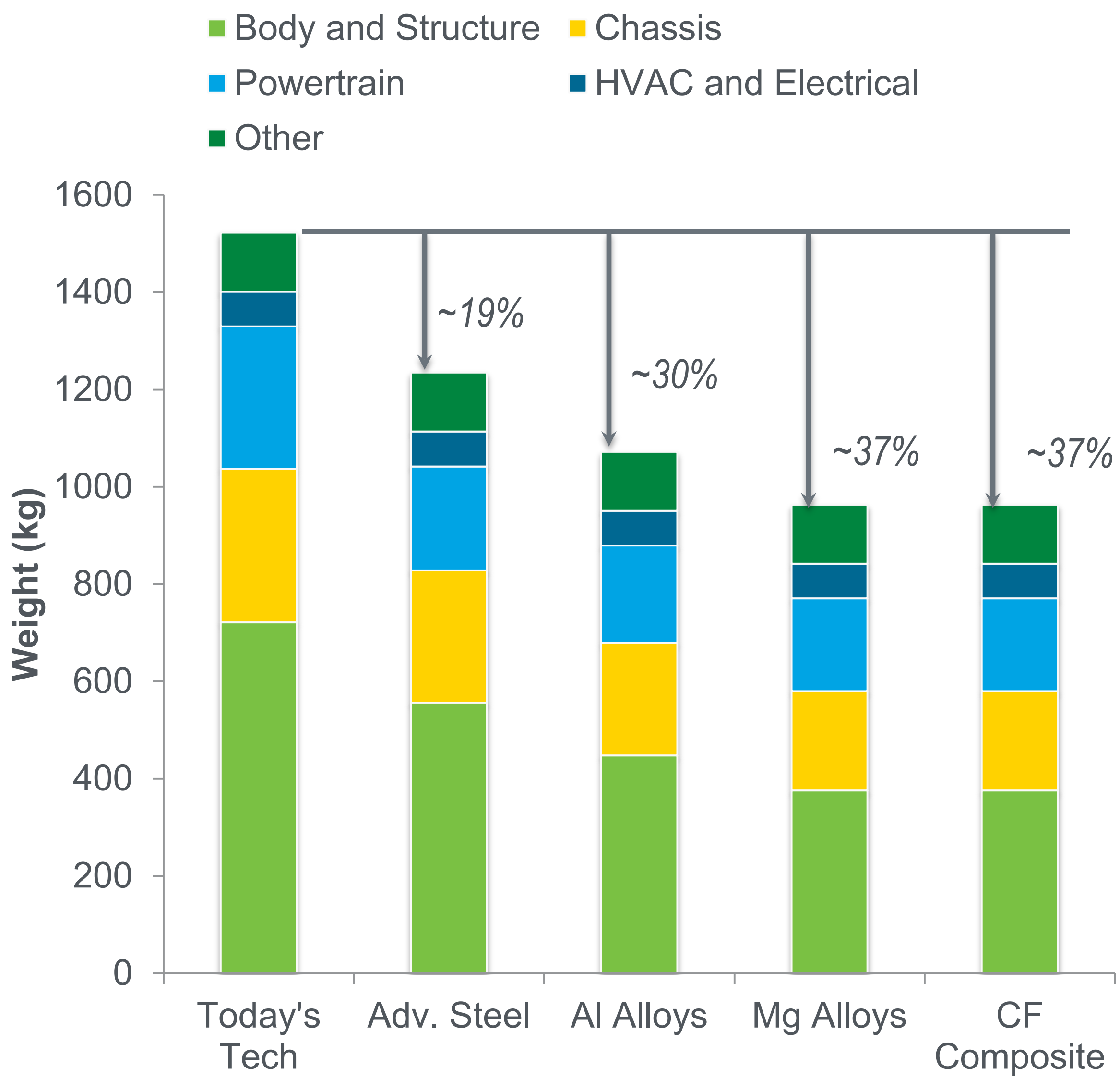
- *Body & Structure, parts of Chassis and Powertrain*

Indirect weight savings by reducing requirements

- *Lighter vehicle can use lighter brakes, lighter suspension, etc.*
- *"Mass Decompounding"*
- *Powertrain and Chassis*

No significant savings through lightweighting

- *Many systems are essentially a function of vehicle volume*
- *Windshield, wiring, head lights, HVAC, etc.*



Lightweight Materials Program

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Light- and Heavy-Duty Roadmaps

Properties and Manufacturing

- Reduce cost
  - raw materials
  - processing
- Improve
  - performance
  - manufacturability

Multi-material Enabling

- Enable structural joints between dissimilar materials
- Prevent corrosion in complex material systems
- Develop NDE techniques

Modeling and Simulation

- Accurately predict behavior
- Tools to optimize complex processes efficiently
- ICME: Developing new materials and processes

Demonstration, Validation, and Analysis

Properties and Manufacturing

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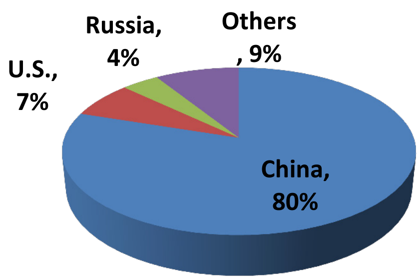
Magnesium Alloys

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)*

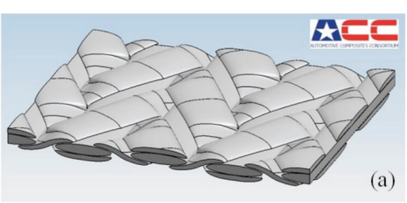
- Insufficient strength in conventional automotive alloys
- Limited room temperature formability in conventional automotive alloys
- Difficult to join/integrate to incumbent steel structures

Carbon Fiber Composites

When it "works" → 30-65% weight reduction

Otherwise → *Cost (~$5-15/ lb-saved)*

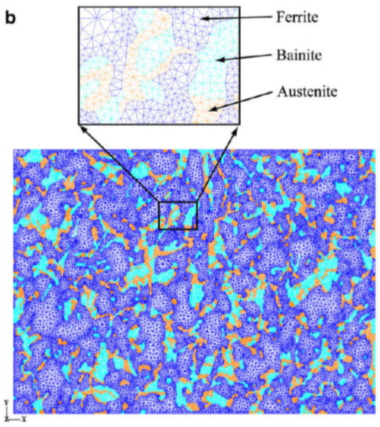
- High cost of carbon fiber (processing, input material)
- Joining techniques not easily implemented for vehicles
- Difficult to efficiently model across many relevant length scales



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.



Choi et. al., Acta Mat. **57** (2009) 2592-2604

Multi-material Enabling

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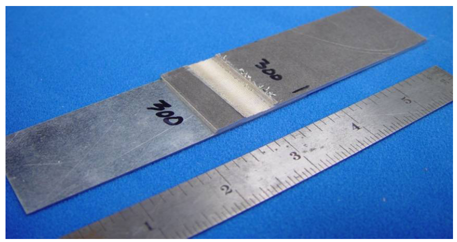
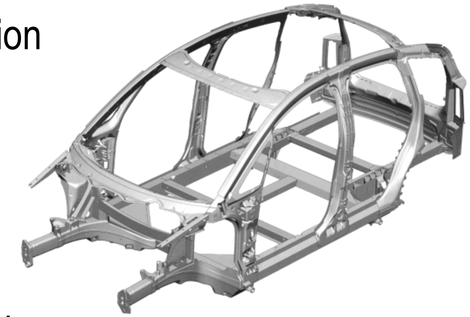
Magnesium Alloys

- Corrosion (galvanic and general)
- Difficulty Joining
  - Mg-Mg
  - Mg-X
  - Riveted Joints
- Questionable compatibility with existing paint/coating systems



Aluminum Alloys

- HAZ property deterioration
- Difficulty joining mixed grades
  - Joint integrity
  - Joint formability
- Difficulty recycling mixed grades



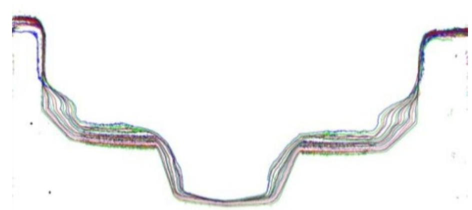
	Mg	Si	Cu	Zn
5182	4.0 - 5.0	< 0.2	< 0.15	< 0.25
6111	0.5 - 1.0	0.6 - 1.1	0.5 - 0.9	< 0.15
7075	2.1 - 2.9	< 0.4	1.2 - 2.0	5.1 - 6.1

Carbon Fiber Composites

- Corrosion and environmental degradation
- Some difficulty joining
- Questions regarding non-destructive evaluation

AHSS

- HAZ property deterioration
- Limited weld fatigue strength
- Tool wear, tool load, infrastructure



Modeling and Computational Materials Science

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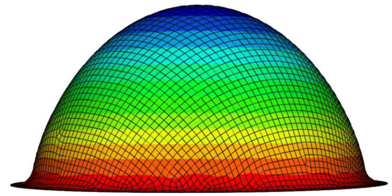
Magnesium Alloys

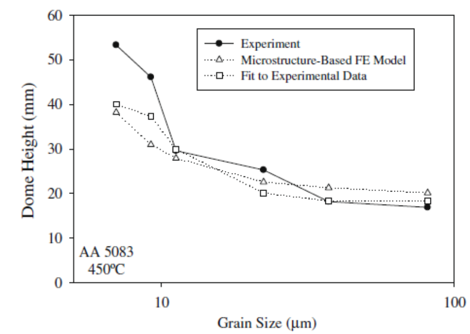
- Complicated deformation in HCP Mg alloys
  - Highly anisotropic plastic response
  - Profuse twinning
- Few established design rules for anisotropy
- Substantial gaps in basic metallurgical data

Q. Ma et al. *Scripta Mat.* **64** (2011) 813–816

Aluminum Alloys

- Basic metallurgical models are well established
- Substantial fundamental data is available
- Useful predictive models established for some conditions
- Truly predictive, multi-scale models are still lacking





P.E. Krajewski et al. *Acta Mat.* **58** (2010) 1074–1086

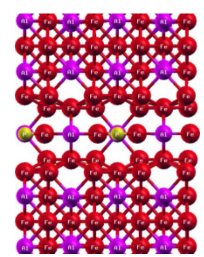
Carbon Fiber Composites

- Insufficient capability in modeling relationships between physical properties, mechanical properties, and ultimately behavior
- Lack of validated, public databases of CFC material properties
- Inadequate processing-structure predictive tools

AHSS

- General lack of understanding on structures, phases, and deformation mechanisms to achieve 3GAHSS properties
- Very complicated structures, phases, and deformation mechanisms likely

N.I. Medvedeva et al. Phys. Rev. B **81** (2010) 012105



Lightweight Materials – Properties and Manufacturability

Materials Technologies
$36.9 M

Lightweight Materials
$28.0 M

- Properties and Manufacturing
- Multi-Material Enabling
- Modeling & Computational Mat. Sci.

– Carbon fiber (CF)
  - **ORNL**: Carbon Fiber production process optimization using plasma oxidation
  - **ORNL**: Carbon Fiber Technology Center – prototyping and batch production facility
  - **Zoltek**: Low cost carbon fiber production using traditional and non-traditional starting materials

– Light Metals
  - **U. Michigan, PNNL, Ohio State U., Arizona State U., Mississippi State U., ORNL**: Building the Scientific Foundation for Advanced Magnesium Alloys
  - **INFINIUM**: Scale-Up of Low-Cost Zero-Emissions Magnesium by INFINIUM Electrolysis
  - **PNNL**: Processing an property improvements for aluminum and magnesium alloys, advanced steel microstructure development
  - **USAMP**: Mg Intensive Vehicle Front End R&D

Lightweight Materials – Multi-material Enabling

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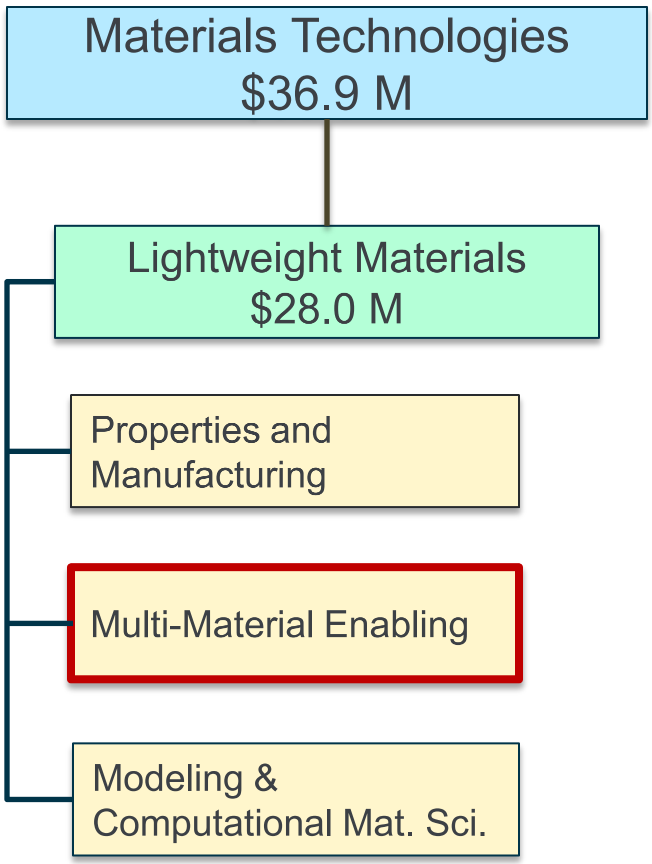

- Cross-cutting
  - **Vehma and Ford**: Multi-Materials Lightweight Vehicle
  - **IBIS** : Technical Cost Modeling of Lightweight Vehicles
  - **LBNL** : Safety Data and Analysis
- Light Metals
  - **Chrysler, Ohio State, Johns Hopkins, ORNL, Michigan State**: Breakthrough Concepts in Multi-material Joining
  - **ORNL:** Fundamentals of Mg corrosion in automotive-relevant environments
  - **ORNL**: Demonstrating techniques for AHSS and mixed material joining
  - **Ford**: Pulsed/Impact Joining of Al and Advanced Steels
  - **PNNL**: Demonstrating techniques for Al and Mg joining

Lightweight Materials – Modeling and Computational Materials Science

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Materials Technologies
$36.9 M

Lightweight Materials
$28.0 M

- Properties and Manufacturing
- Multi-Material Enabling
- Modeling & Computational Mat. Sci.

– Carbon fiber (CF) and carbon fiber composites (CFC)
  - **ORNL & PNNL**: CFC Predictive Engineering-Long Fiber Injection Moldings
  - **USAMP** : Validation of Front Bumper Crash Models of Polymer Composites

– Light Metals
  - **PNNL** : Mechanistic-based Ductility Predictions for Complex Mg Castings
  - **USAMP** : ICME Development of Advanced Steel for Lightweight Vehicles

Materials Technologies

Values are FY14 enacted

Materials Technologies
$36.9 M

- **Lightweight Materials $28.0 M**
  - Properties and Manufacturing
  - Multi-Material Enabling
  - Modeling & Computational Mat. Sci.
- **Propulsion Materials $8.9 M**
  - Engine Materials, Cast Al & Fe High Temp Alloys
  - Exhaust Sys. Materials, Low T Catalysts
  - Integrated Computational Materials Engineering

	Lightweight	Propulsion
FY13 Enacted	$27.5 M	$11.9 M
FY14 Enacted	$28.0 M	$ 8.9 M
FY15 Request	$47.0 M	$ 7.069 M

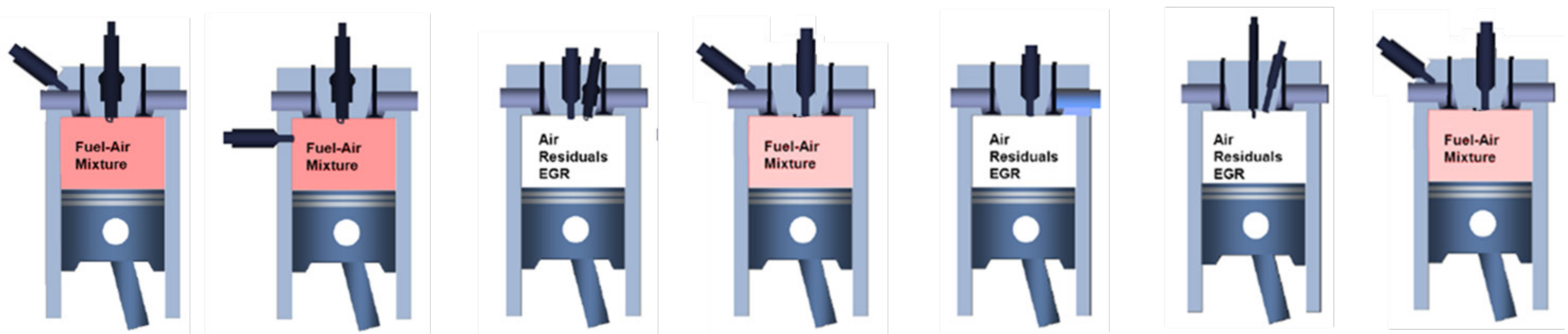
Propulsion Materials

- Targets powertrain materials requirements for future automotive and heavy-duty applications: engine, transmission, exhaust components, and targeted materials for electric powertrains.
- Addresses materials for high efficiency Internal Combustion Engines, powertrain materials interactions with new fuel compositions.
- Most (85%)Propulsion Materials projects utilize Integrated Computational Materials Engineering (ICME) to set performance targets and accelerate results in materials discovery, materials formulation, and materials processing techniques.
- Identifies gaps in existing ICME tools and develops new topics to expand the use of computational methods in materials development and materials engineering

Pathways to High Efficiency ICEs

Multiple high efficiency combustion pathways, each having unique thermal, peak pressure, and pressure rise rate parameters, result in a variety of engine design and materials challenges.

What are the components and materials that will limit designers ability to build reliable engines from the outcome of this combustion research?



PFI-SI Stoichiometric | GDI-Si | Stratified GDI-SI | HC-CI | GDI-CI | DI-CI Lean | Dual Fuel PFI-DI-CI

Materials Target Setting

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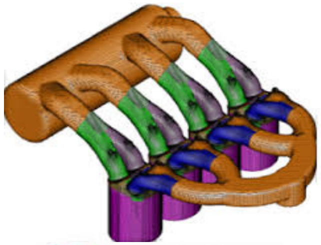
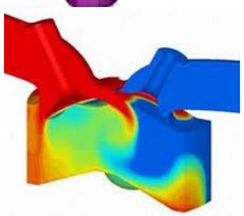
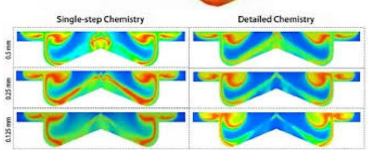
Advanced Combustion Models



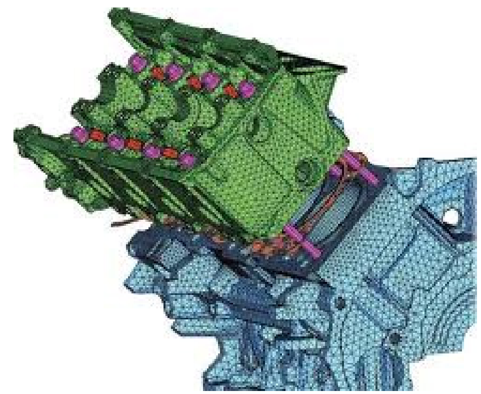




Temperature and pressure
Boundary conditions

Efficiency
improvement potential

Finite Element Baseline
Design Constraints



Prioritized
Components
and
Material
Property
Targets

Identify and prioritize the material improvements needed to enable high efficiency combustion systems, and <u>quantify the benefits</u>.

Propulsion Materials Program

**Light- and Heavy-Duty Roadmaps,
US Drive Low T Catalyst Workshop Report**

Engine Materials	Exhaust System Materials	Integrated Computational Materials Engineering

Improve Engine Efficiency
• Improved Materials
  • Strength
  • Durability
  • Operating T
  • Manufacturability
  • Lower Cost
	• Low Cost High Temp Alloys for Exhaust Manifolds, Turbocharger Housings and Turbines
	• Low Temp Catalyst Materials and ceramic substrates
		New materials and processes using multi-scale modeling
		• Modeling to create tailored materials
		• Predict behavior
		• Optimizing complex processes

Demonstration, Validation, and Analysis

Propulsion Materials–Internal Combustion Engine (ICE) materials

- Materials Technologies $36.9 M
  - Propulsion Materials $8.9 M
    - Engine Materials, Cast Al & Fe High Temp Alloys
    - Exhaust Sys. Materials, Low T Catalysts
    - Integrated Computational Materials Engineering
    - Materials for Hybrid and Electric Drive Systems

– Targets the Advanced Combustion Engine team stretch goals, 50%+ efficiency for heavy-duty and automotive engines

- **Lightweight Cast alloys for automotive engines and transmissions: GM; Ford; ORNL/Chrysler**: Lightweight high strength aluminum alloy development to replace A356 or A319 and enable higher operating temperatures and higher efficiency combustion regimes.
- **High performance Cast Ferrous Alloys for Heavy-duty Applications: Caterpillar**: High strength, low cost cast alloy development to provide performance superior to Compacted Graphite Iron, easily cast and machined, and at a cost similar to cast iron, enabling engines with higher peak cylinder pressures and increased efficiency.
- **High performance Cast Steels for Crankshafts: Caterpillar/GM**: High performance low cost cast steel providing performance similar to high cost forged steel units, enabling a low cost pathway to increased engine efficiency in automotive and heavy duty applications.

Propulsion Materials– Exhaust System Materials, Low T Catalysts

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Materials Technologies
$36.9 M

Propulsion Materials
$8.9 M

- Engine Materials, Cast Al & Fe High Temp Alloys
- Exhaust Sys. Materials, Low T Catalysts
- Integrated Computational Materials Engineering
- Materials for Hybrid and Electric Drive Systems

– Low Temperature Aftertreatment Catalyst Materials
  - **ORNL:** Evaluation of catalyst microstructures and
– Exhaust Aftertreatment Components
  - **ORNL/Ford**: Impacts of biofuels on component life and development of mitigation strategies
  - **ORNL**: Durability of diesel particulate filters

Propulsion Materials– Properties and Manufacturability

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- Materials Technologies $36.9 M
  - Propulsion Materials $8.9 M
    - Engine Materials, Cast Al & Fe High Temp Alloys
    - Exhaust Sys. Materials, Low T Catalysts
    - Integrated Computational Materials Engineering
    - Materials for Hybrid and Electric Drive Systems

– Integrated Computational Materials Engineering

- **ORNL**: Exploratory methods based on First Principals Calculations, Density Functional Theory, and Calculated Density of States to identify new materials compositions with tailored properties:
  - Thermoelectric Materials, 3 new compositions have been validated;
  - Non-rare earth magnetic materials, 2 new compositions have been validated;
  - Low Temperature Catalyst materials, 1 new low temperature catalyst have been validated for Oxides of Nitrogen
- Each Propulsion Materials FOA project includes a multi-scale ICME application, validation, and gap analysis component (two were included in the President's Materials Genome announcement).

Propulsion Materials– Materials for Hybrid and Electric Drive Systems

- Materials Technologies $36.9 M
  - Propulsion Materials $8.9 M
    - Engine Materials, Cast Al & Fe High Temp Alloys
    - Exhaust Sys. Materials, Low T Catalysts
    - Integrated Computational Materials Engineering
    - Materials for Hybrid and Electric Drive Systems

– Projects very limited in scope to address specific gaps in material properties, materials processing, or material joining

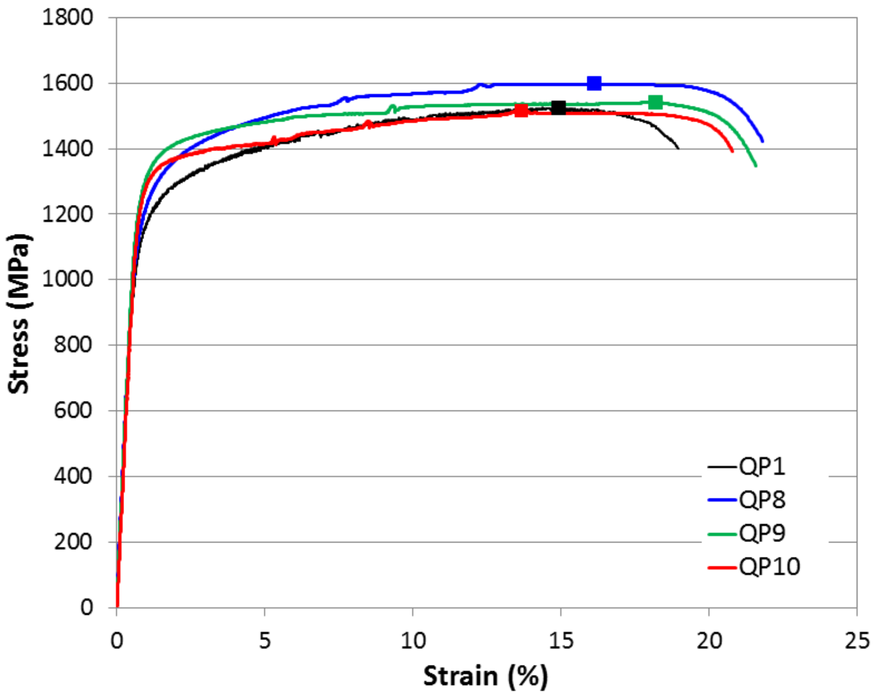
- **ORNL:** Enabling Materials for High Temperature Electronics: Organic materials not 200°C-capable
- **ORNL:** Enabling Materials for High Temperature Electronics: Solders not 200°C-capable
- **PNNL**: Novel Manufacturing Technologies for High Power Induction and Permanent Magnet Electric Motors

- Goal to rapidly transition results to the APEEM team

New non-rare earth magnetic materials are predicted within the ICME activity and validated by the APEEM team

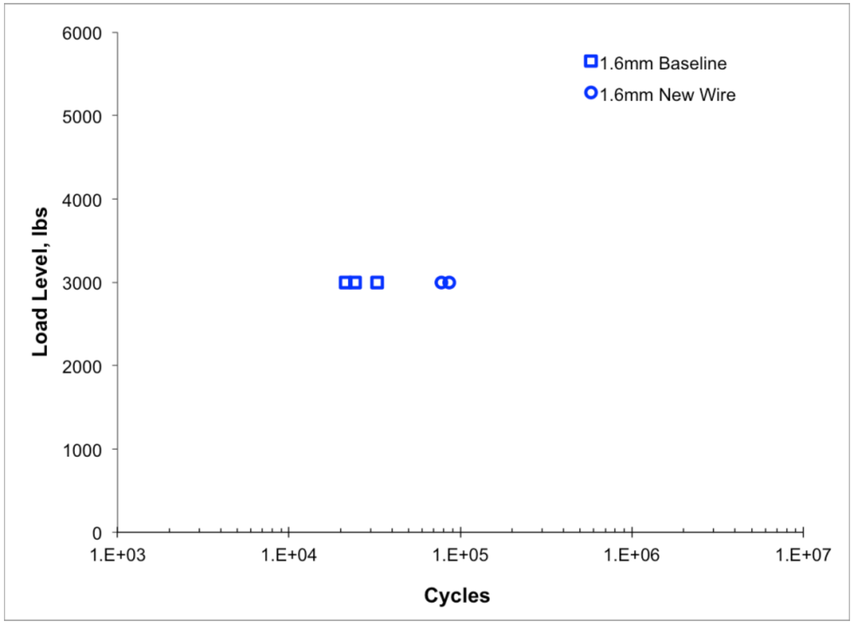
2013 Accomplishments

Developed a high-strength sheet steel with strength exceeding 1500 MPa while maintaining more than 20% elongation to failure



Pacific Northwest National Lab

Demonstrated proof-of-concept for improving weld fatigue life of advanced steels through the use of novel weld wire chemistry and processing



Oak Ridge National Lab

2013 Accomplishments

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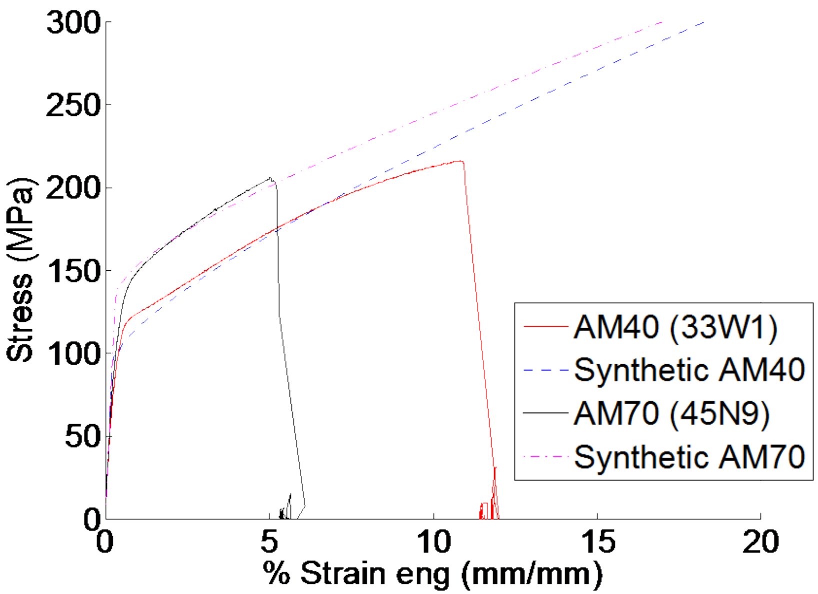
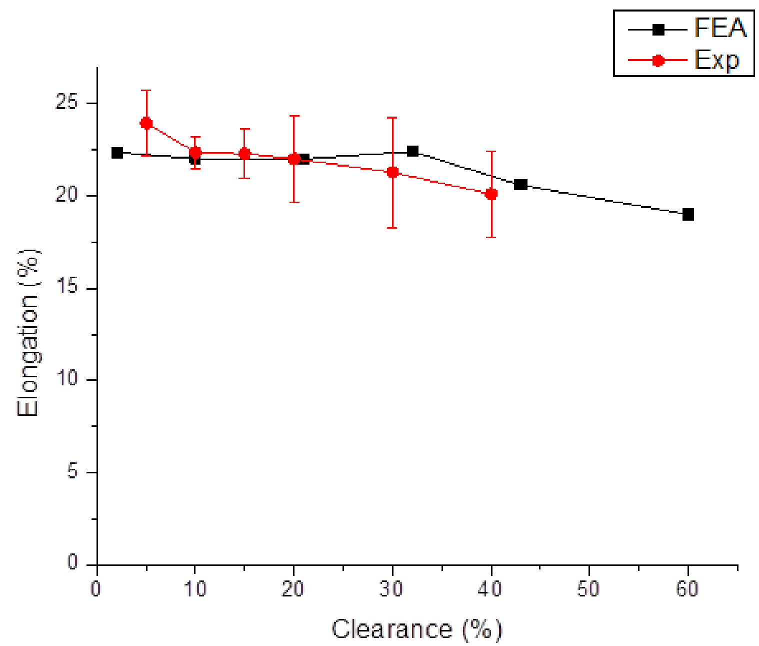
Demonstrated a polycrystal finite element-based model utilizing intrinsic and extrinsic factors to predict yield and hardening in Mg die castings to greater than 90% accuracy



Pacific Northwest National Lab

Produced and experimentally validated numerical model of formability in aluminum sheet as a function of edge condition that predicts elongation to failure with accuracy >90%



Pacific Northwest National Lab

2013 Accomplishments

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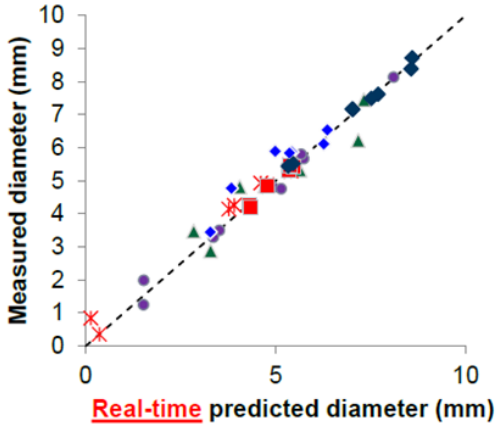
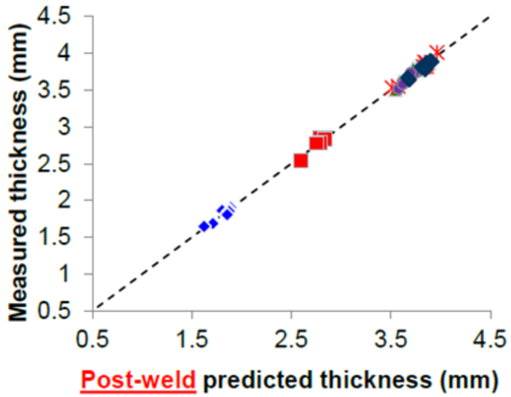
Developed and demonstrated robust, non-contact method for weld property measurements in real-world environments





Oak Ridge National Lab

Validated commercial scale process for manufacturing carbon fiber using precursors with 25% lignin

Zoltek

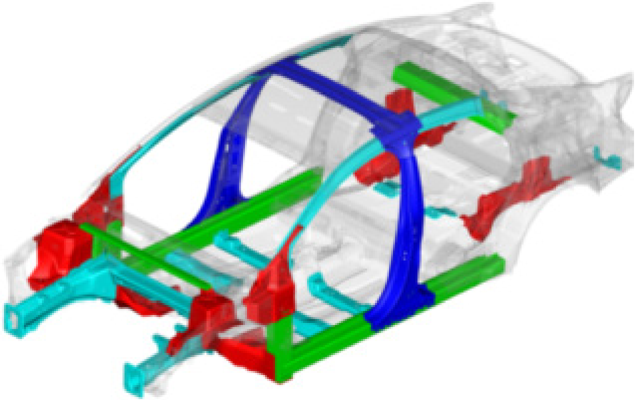
2013 Accomplishments

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Brought large-scale carbon fiber reactor online to support continued advancement of carbon fiber research

Oak Ridge National Lab

Completed design/CAE and significant portion of prototype construction of a multi-material, lightweight vehicle with >23% weight reduction compared to conventional vehicles



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