Materials for Energy Applications

Lawrence Berkeley National Laboratory
The Claremont Hotel, Berkeley CA
1 February, 2012

EXPLORE AND COLLABORATE

AMERICAN INDUSTRY AND AMERICA'S NATIONAL LABS

MATERIALS FOR ENERGY APPLICATIONS

The idea of this workshop (and a companion workshop on high performance computing to be held in Austin Texas) grew out of a brainstorming session we organized with several National Lab directors and industry representatives.

The Challenge: How can the National Labs (and universities!) help improve our economic and industrial competitiveness?

"The Evolving Structure of the American Economy and the Employment Challenge"

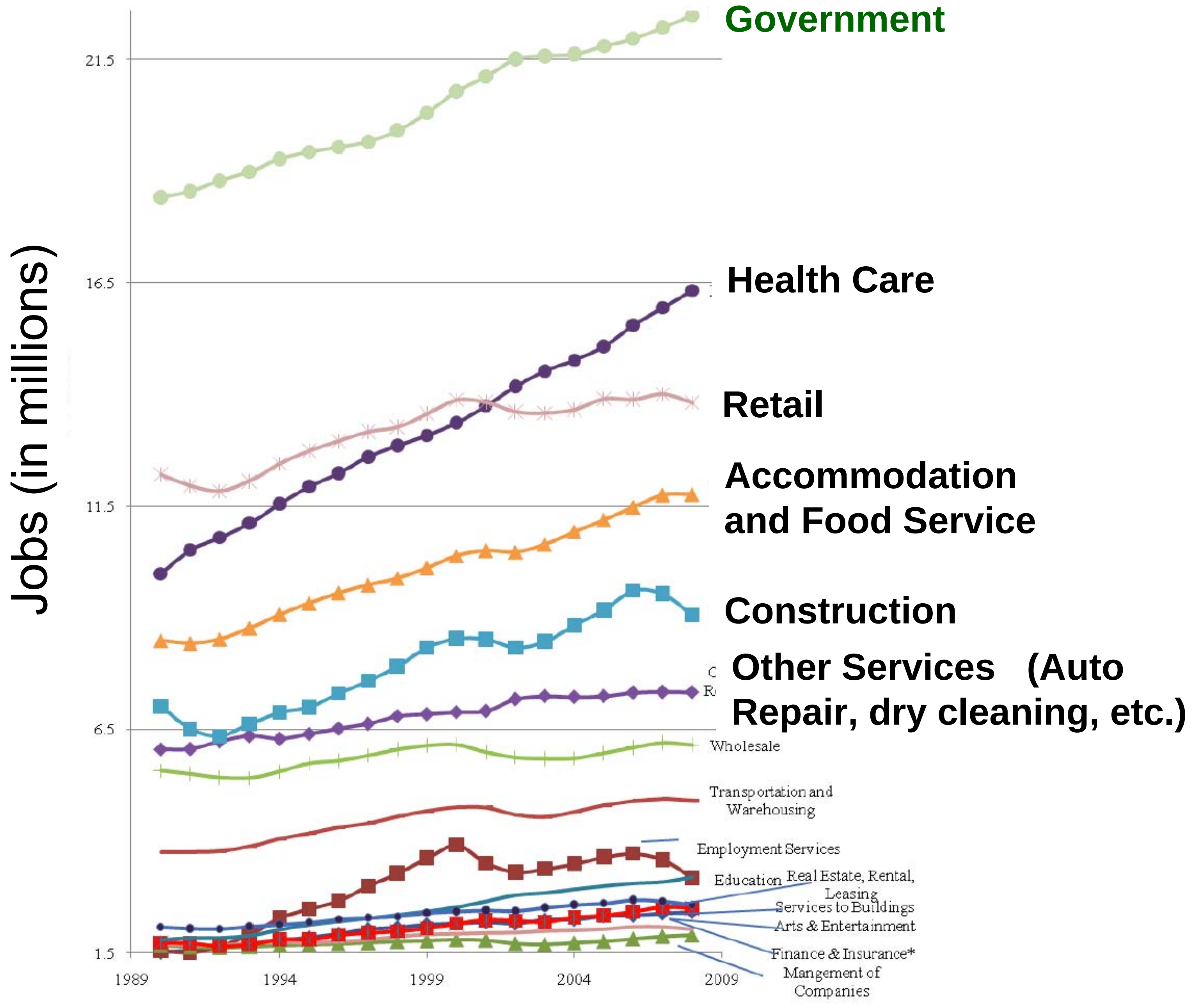
Michael Spence and Sandile Hlatshwayo
Working paper, Council on Foreign Relations (2011)

Tradable jobs: Goods and services that can be produced in one country and consumed in another. Airplanes, cars, electronics …

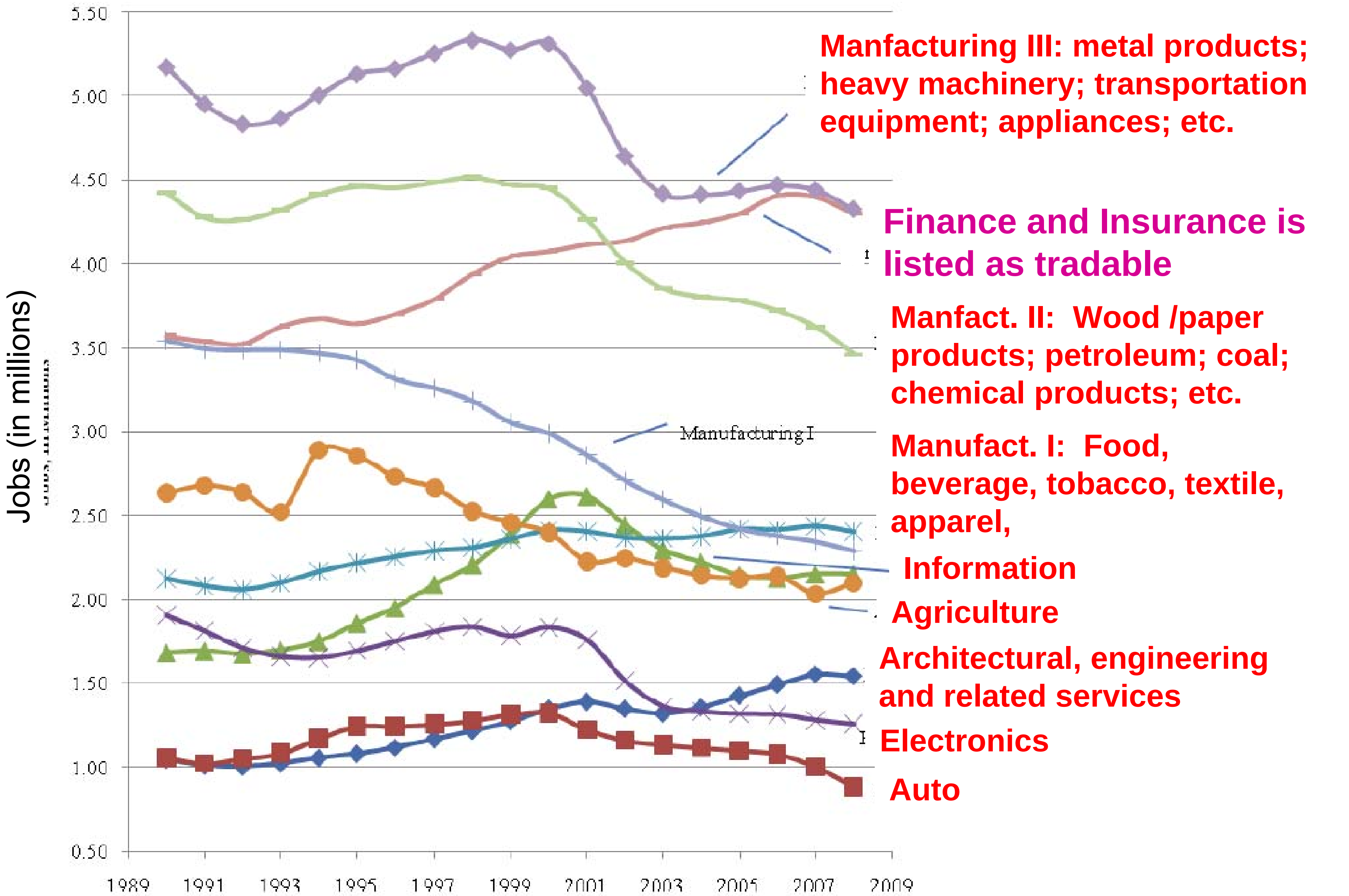
Non-Tradable jobs: Goods and services that ***have*** to be produced domestically. Government, healthcare, construction, much of legal services because of legal differences across countries.

From 1990 – 2008 employment grew by 27 million jobs. Almost all of it was in the non-tradable side. **There was negligible employment growth on the tradable side of the economy where we compete with other people.**

Major non-tradable Industry Jobs (1990 – 2008)



Tradable Industry Jobs (1990 – 2008)



What has the Department of Energy done to increase collaborations between the National Labs and industry?

- Created new funding mechanisms such as ARPA-E, Energy Innovation Hubs, Energy Frontier Research Centers (EFRCs).

- Appointed Karina Edmonds, DOE's first dedicated technology transfer officer. Reports to the Sec. of Energy.

- Patents, patent disclosures and industry collaborations are performance criteria of National Lab scientists and engineers.

Changed DOE technology transfer policies

- Streamlined CRADA agreements, reduced funds-in-house requirements.

- Lowered the cost of initial patent licensing for start-ups. (We are piloting a $1K Option Fee up to 3 patents)

- Added flexibility to IT licensing: exclusive patent licensing and *equity positions* in lieu royalties ***are*** permitted.

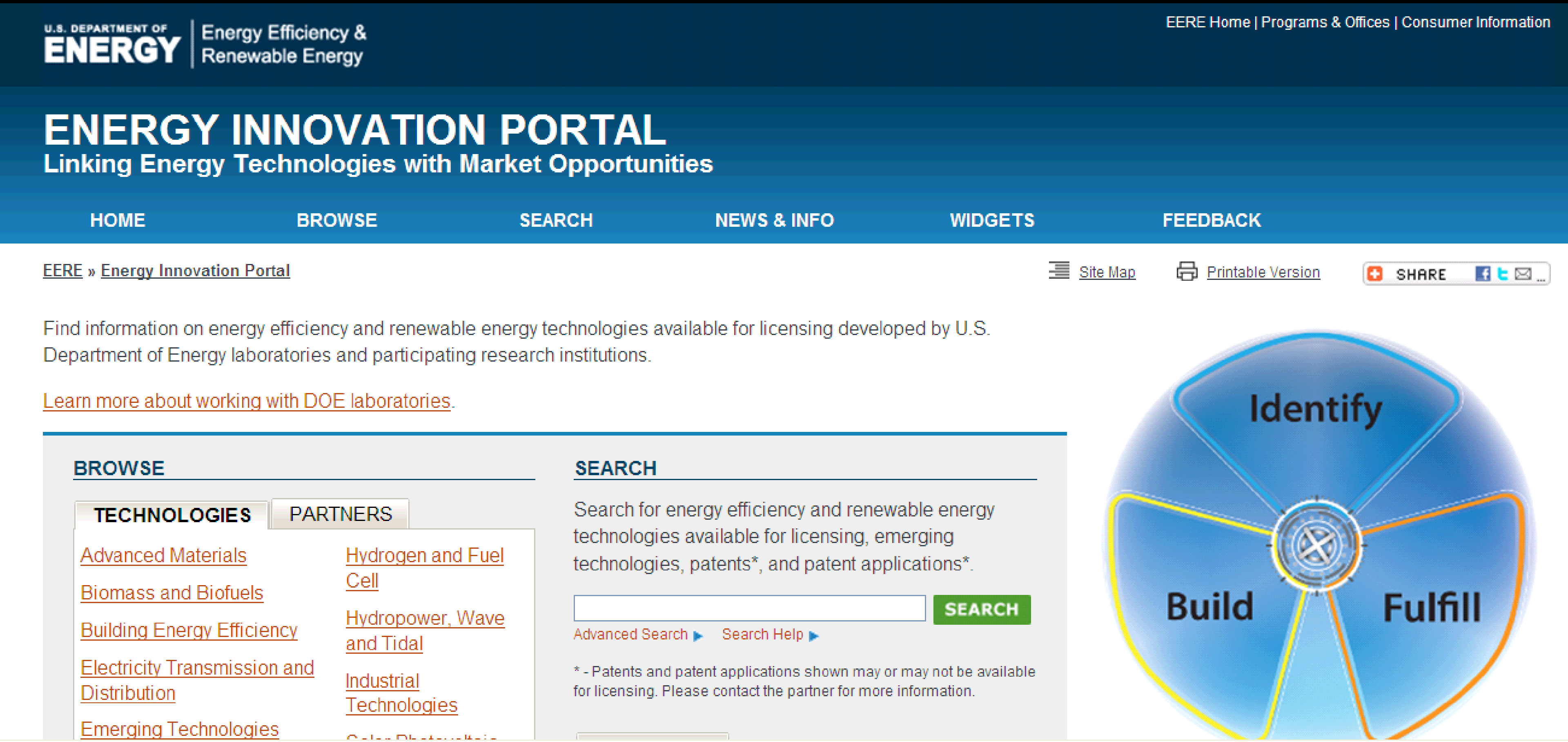
- Eliminated 'March-in-rights' for WFO agreements for Start-ups.

- Began America's Next Top Energy Innovator Awards

- DOE will soon implement ACT (Agreement for Commercializing Technology). Selected labs will have the ability to negotiate with industry on more industry standard terms (performance guarantee, flexibility in Indemnity clauses, modified government use rights)

Technology transfer opportunities in the DOE

http://techportal.eere.energy.gov/



Innovation in energy technologies and high technology manufacturing are intimately connected with materials science and industrial processing methods.

We can (and should) compete in those industries where discovery, invention and innovation are essential.

It's a competitive world out there.

Materials for Energy Applications

- High-strength, lightweight materials for transportation

- Materials for power electronics
  - Wide band gap semiconductors (SiC, ZnO, diamond, ...)
  - Hard and soft magnetic materials

- Photovoltaic materials and processes

- Energy storage materials

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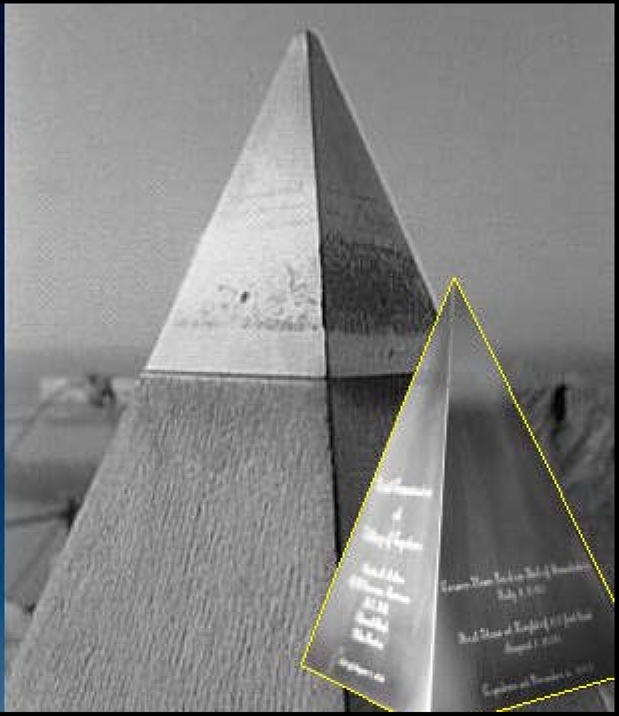
New materials and manufacturing methods can change the landscape of energy solutions

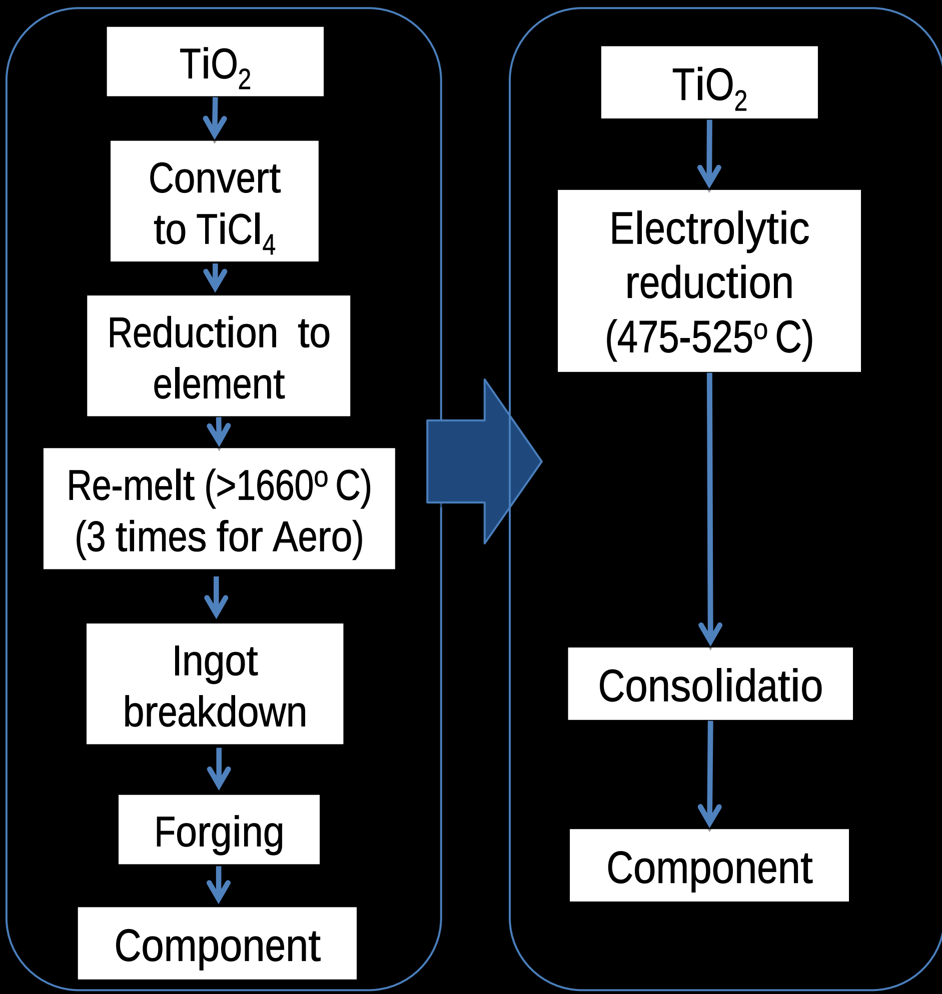


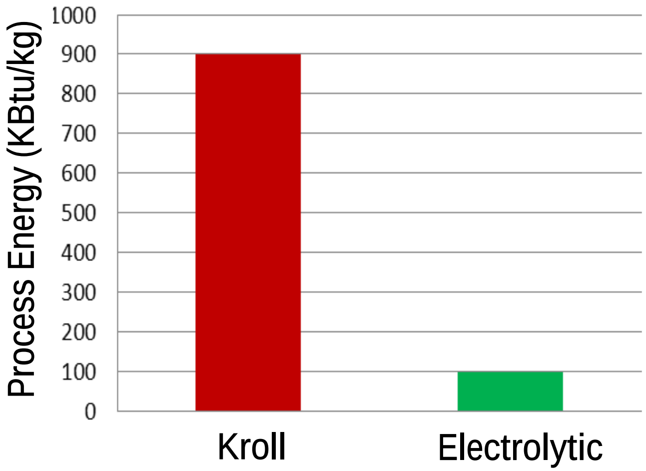
In 1884, the price of aluminum was $1/oz and the price of gold was $20/oz. The highest skilled craftsman working on the Washington Monument was paid $2/day.

Today's prices: Al = 6¢/ oz Au ~ $1776/oz.

Next Generation Processes Example: Titanium

Kroll (conventional) | **Electrolytic (next generation)**





- 9x reduction of process energy
- Potentially 5x savings
- Process product (titanium powder) permits new generation additive manufacturing

Airplanes have become much more energy efficient.

Boeing 707, designed after a military contract for the KC 135 tanker

The Boeing 787 uses only 30% of the fuel as the 707.

Out-of-the-Autoclave Composites

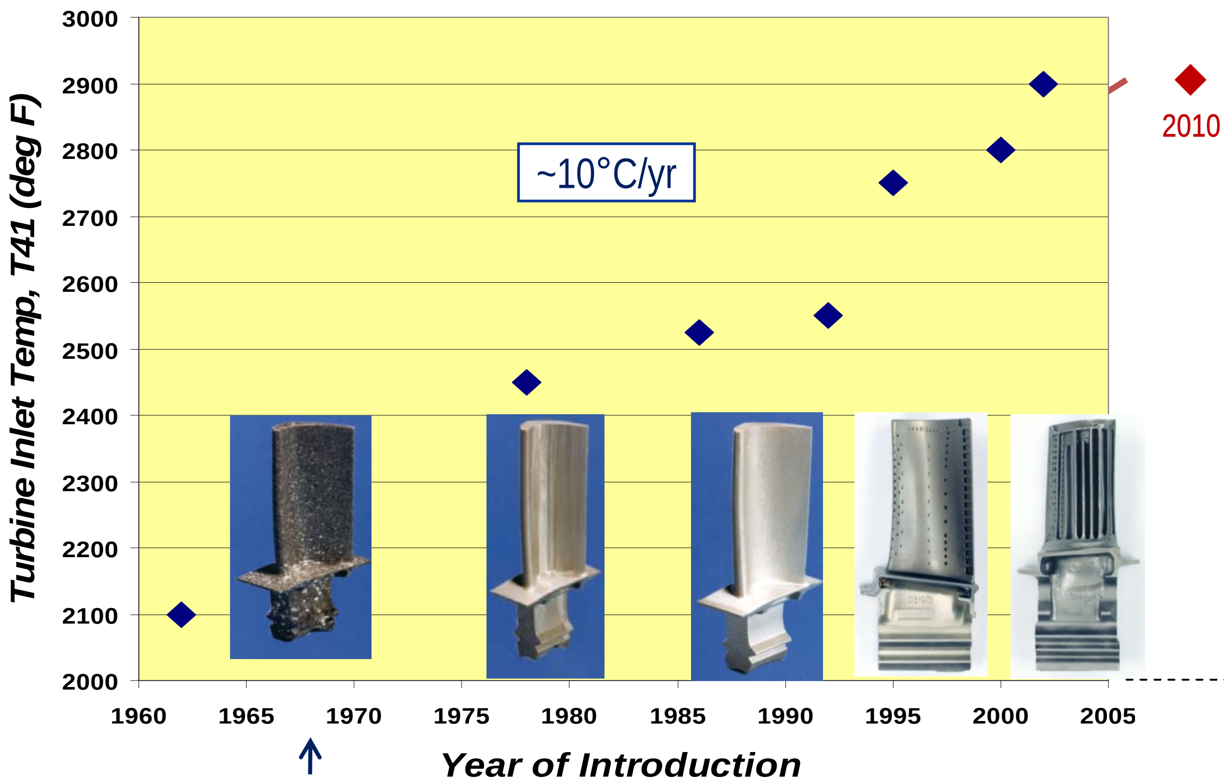
Autoclave (conventional)

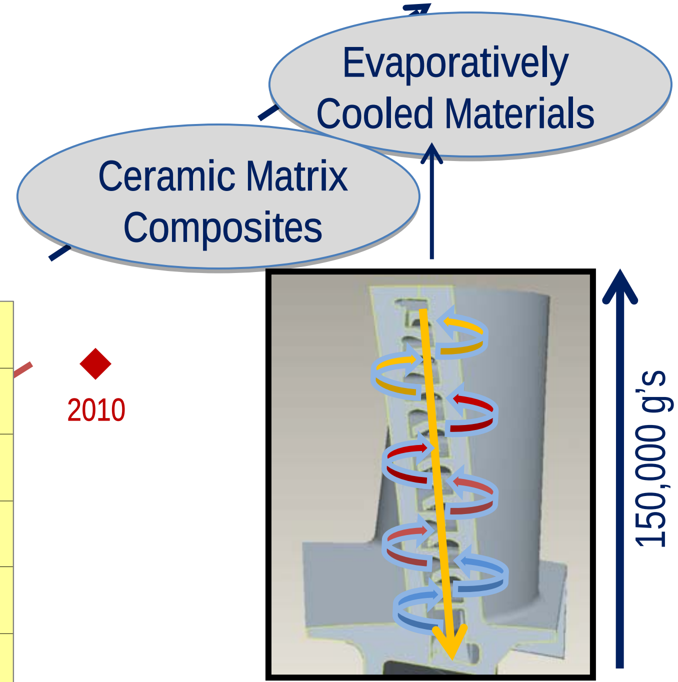
Out-of-the-Autoclave

The manufacturing of inexpensive carbon composites that can be molded as a thermo-plastic?

Jet engines have become 50% more efficient

Increase in turbine inlet temperature enabled by changes in SIZE and CONFIGURATION of nickel alloy STRUCTURE and NOT Chemistry





Equiaxed crystals

Oriented crystals

Single crystal

Single crystal tailored configuration

The Hundai Elantra, a 5 passenger mid-size 148 hp (1.8 liter engine) car weighs ~2700 lbs and is rated at 29 mpg city and 40 mpg highway.

The 2013 Chrysler Dodge Dart is 68% high-tensile strength steel. Preliminary tests with a 160-hp, 1.4 L turbo-charged engine with 184 ft-lbs. of torque is anticipated to have even better EPA ratings.

Joe Veltri, Chrysler vice president tries to sell me a Dart

Ford has a 1.2 L engine with 135 hp and is developing a 900 cc turbocharged engine with 127 hp!

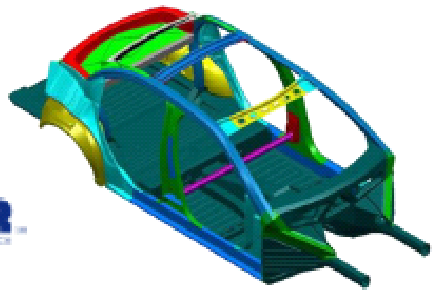
Auto/Steel Partnership

Evolution of Advanced High Strength Steels in Automotive Applications

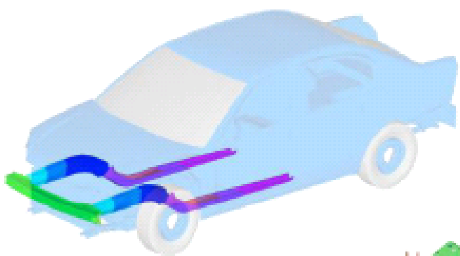
Jody N. Hall
General Motors Company
Chair, Joint Policy Council, Auto/Steel Partnership
May 18, 2011

The application of high strength steels in automobiles

Domestic (Auto/Steel Partnership) DOE-Funded Engineering Projects 22% to 32% Weight Reduction, 2002-2009

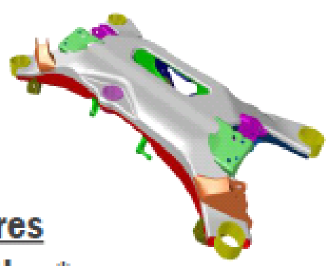


Future Generation Passenger Compartment
- 30% mass reduction *
- Improved crash performance
- At no additional cost

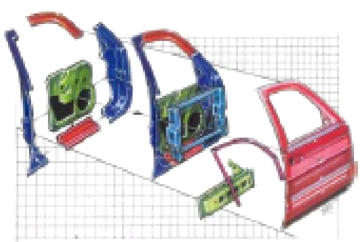


Lightweight Front-End Structures
- 32% mass reduction *
- At no additional cost

FreedomCAR Goals
50% mass reduction
same cost



Lightweight Rear Chassis
- 24% mass reduction*
- At no additional cost



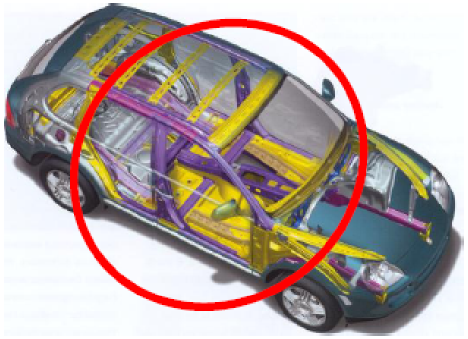
Lightweight Closures
- 22% mass reduction*
- At no additional cost

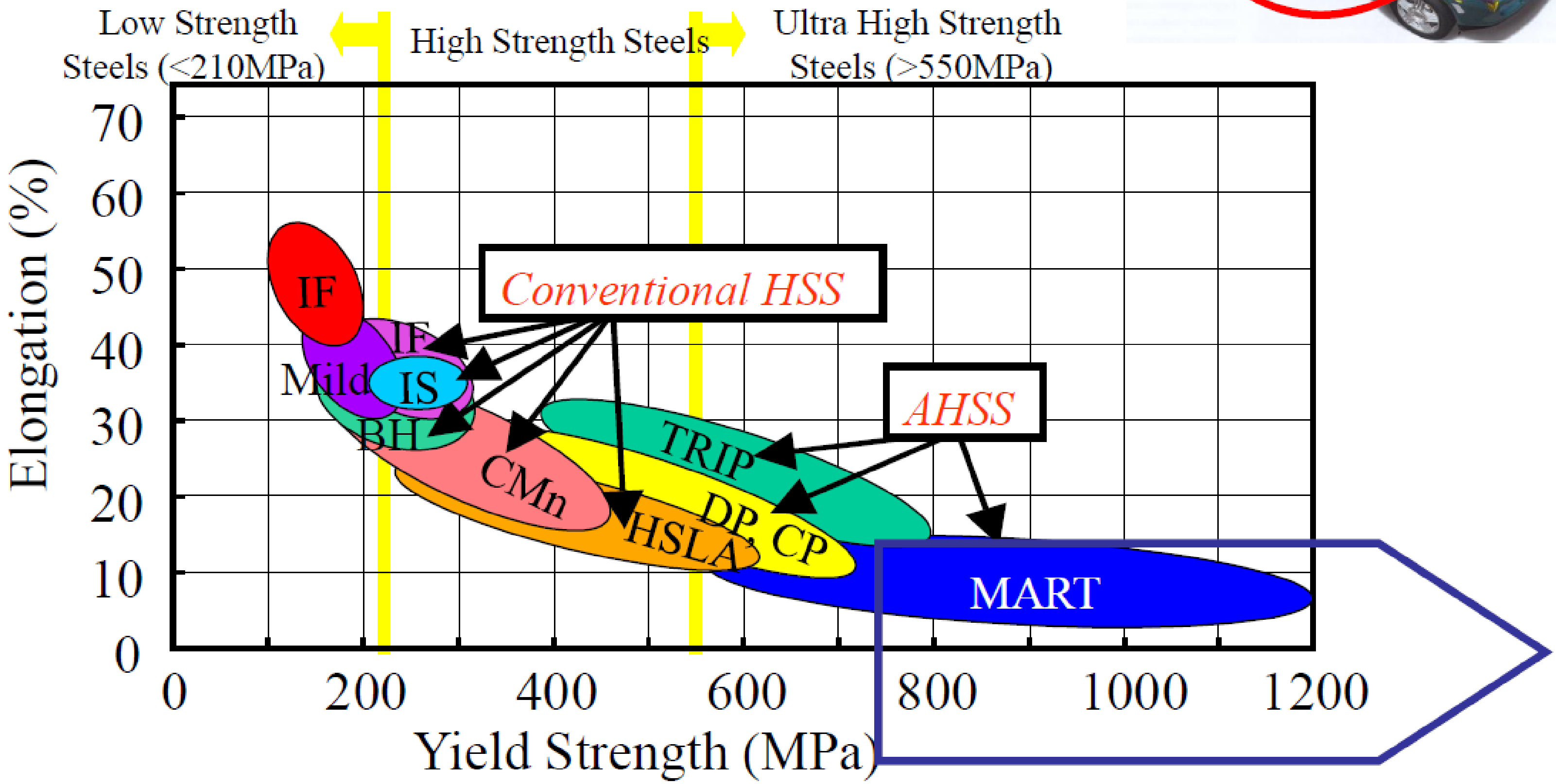
* Mass Reductions versus actual OEM donor vehicles

Safety

Steels for Passenger Compartment Zone

- Highest Strength
- Martensite, and Boron Steels Preferred

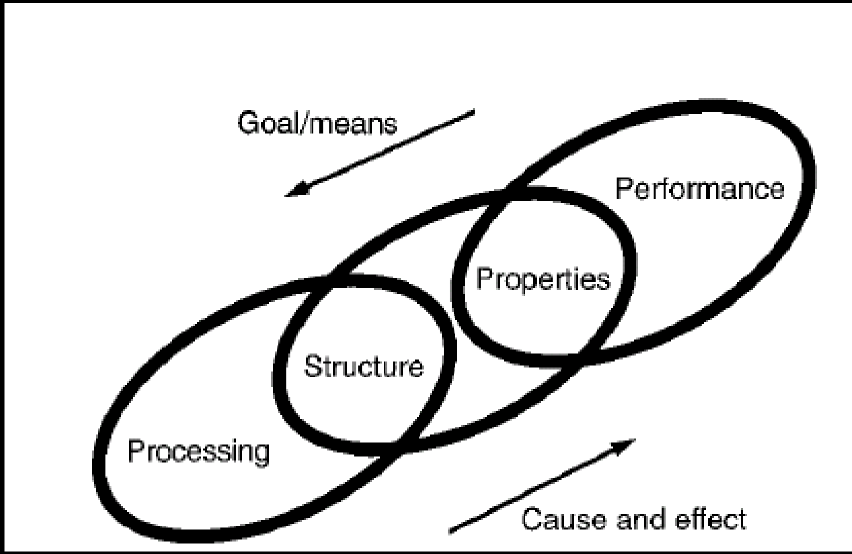




Computational Design of Hierarchically Structured Materials*

- There is a hierarchy of length scales from the atomic, nano, meso to more macro scales.

- It has been known for centuries that material properties are dependent on their processing pathway (history). Modern material science has recognized that this is due to a spectrum of characteristic relaxation times. The structures are essentially in non-equilibrium states.



1985; **Steel Research Group**

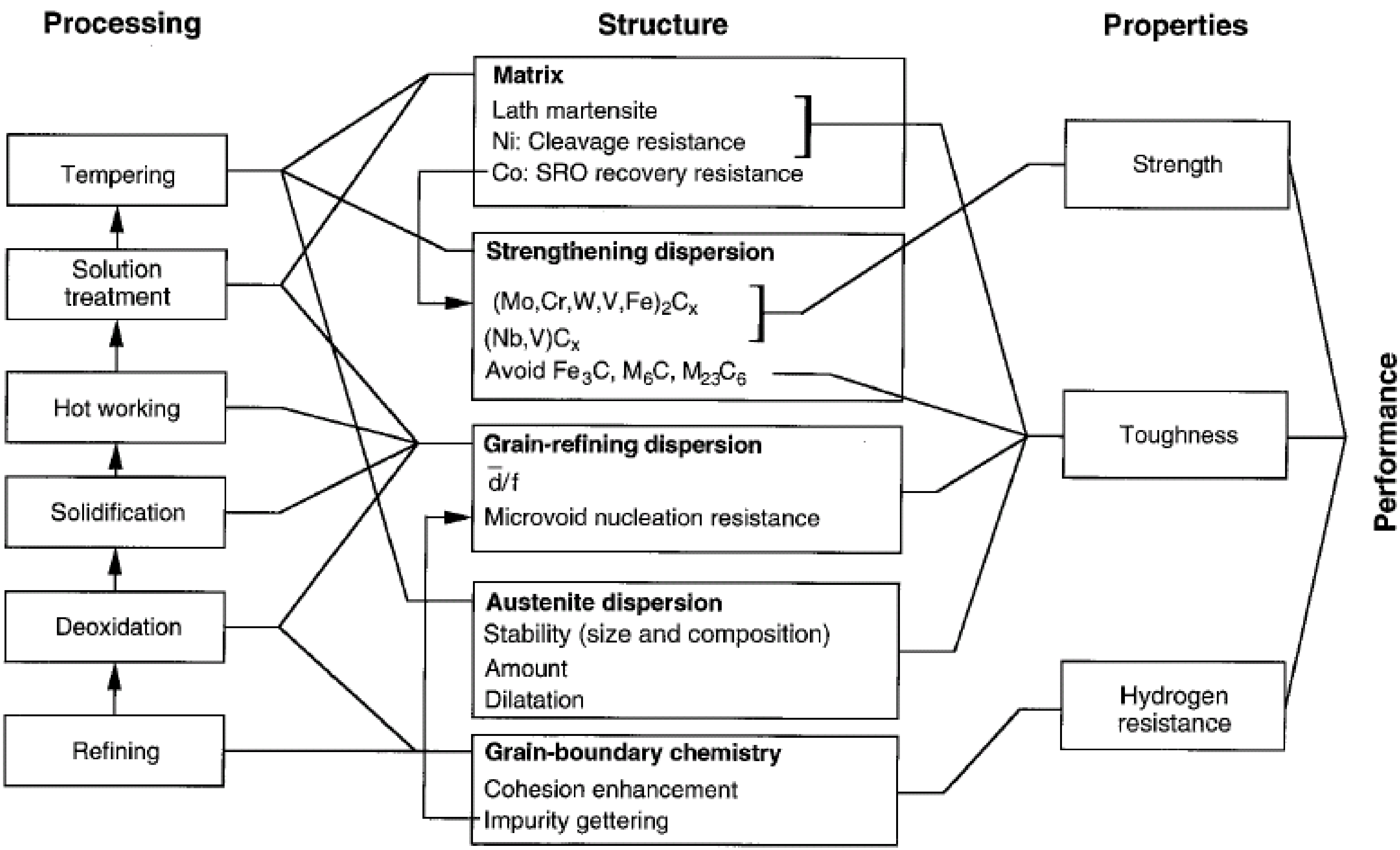
An international collaboration
Funded by the NSF with industrial, academic, and government labs for the science-based production of high performance steels.

* G. B. Olson, Science **277**, 1237 (1997)

Target materials:

- Ultra high-tensile strength martensitic alloy steels
- High-strength formable automotive sheet steels
- Ferritic super-alloys for power generation.

Relationships between processing, structure and properties of high-tensile strength martensitic steels



It was known that M_2C carbide strengthens steels due to its high modulus misfit with BCC Fe and its ability to precipitate coherently at the nano scale.

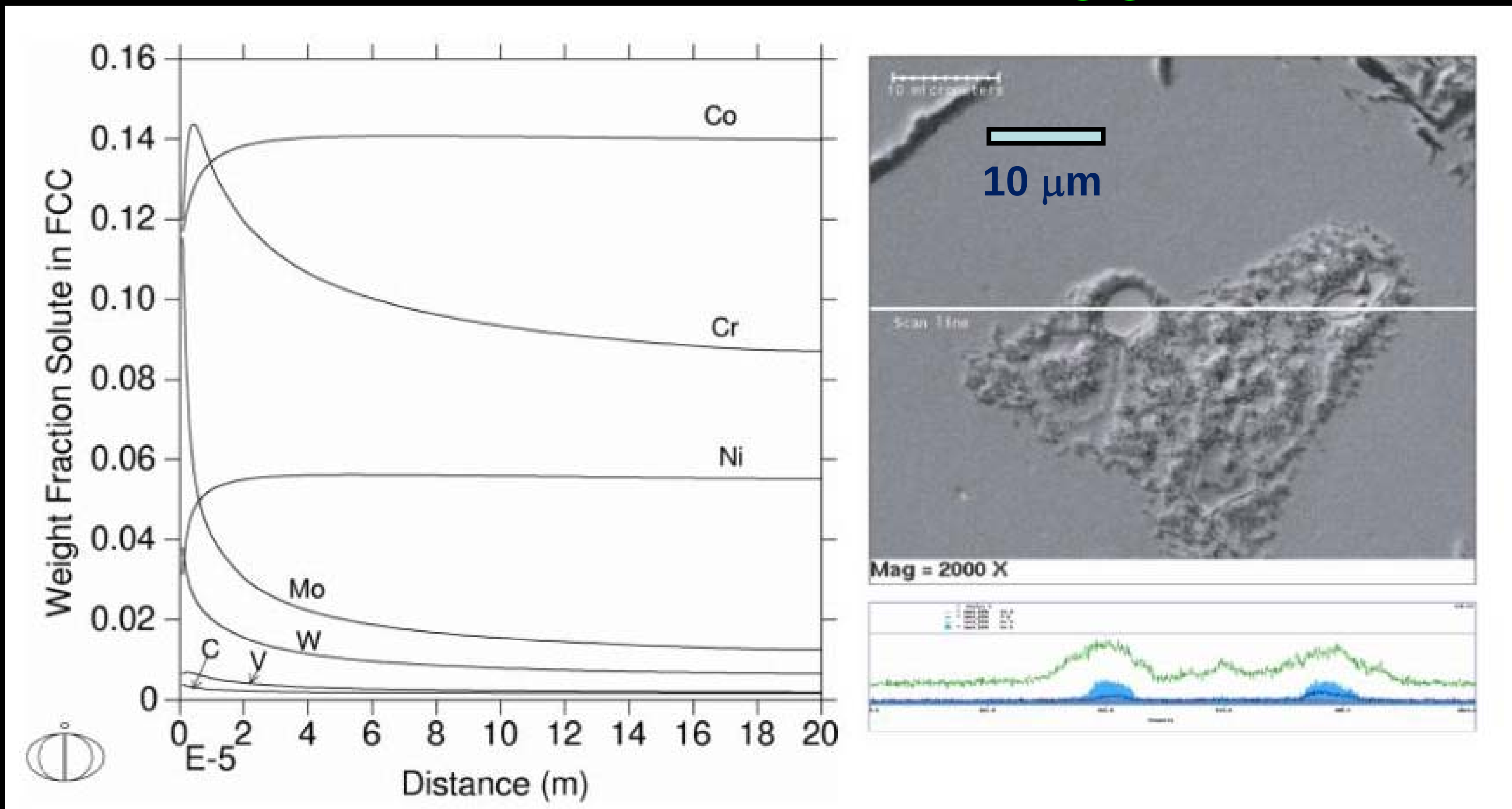
- Electron microscopy (TEM and analytical)
- X-ray scattering
- Neutron scattering
- Scanning probe microscopies

Computational design tools have been used to calculate interfacial boundary energies, precipitation rates, etc. Some quantum mechanical calculations are used to compute segregation energy differences.

We understand how structures change during the forming process, but don't yet have a fundamental understanding of how alloying or thermal treatments create those properties.

Computer simulations

Ferrium® S53 is the first flight certified, corrosion-resistant steel (used in landing gear).

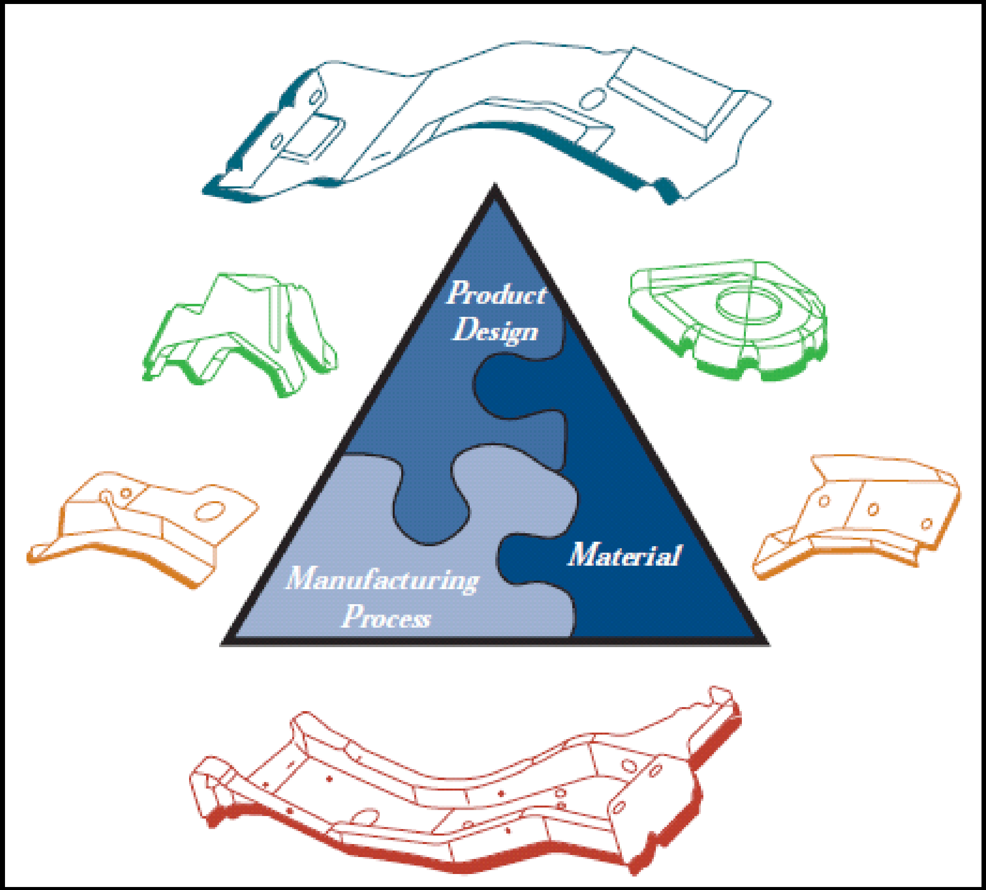


1D multi-component diffusion simulations of the solidification of impurity dendrite growth of ingot scale material and SEM confirmation.

High Strength Steel Stamping Design Manual

A/S P Auto/Steel Partnership

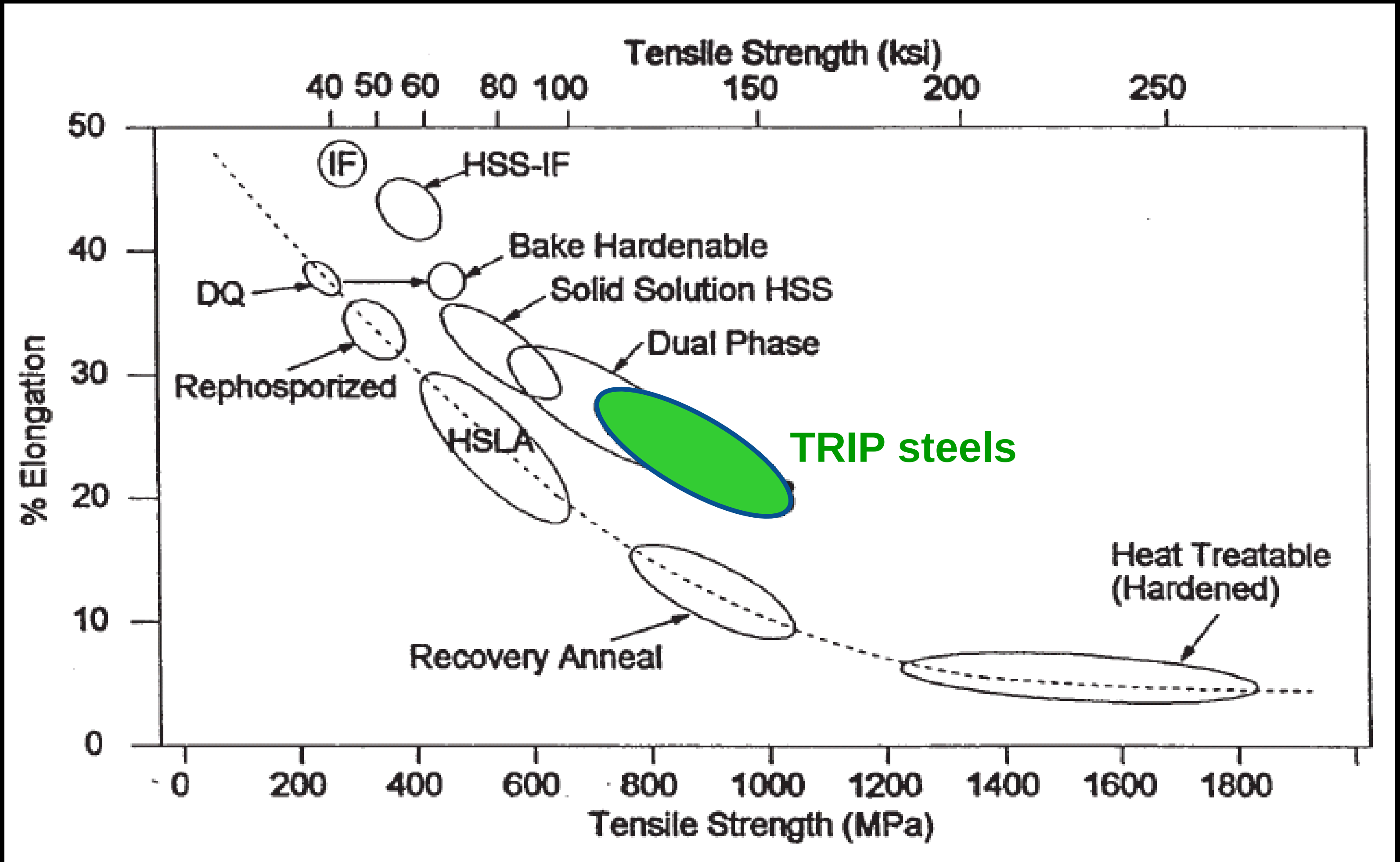
Celebrating 20 Years of Partnership Excellence



"It is important that the product designers work closely with the die process planners and the steel suppliers when parts are being designed to avoid improper material/part design/die process combinations.

"For structural parts such as rails and crossbars, spring-back on flanges will increase as compared to mild steel. The manufacturing process will therefore require over-bend of flanges to allow for spring-back compensation."

“Transformation Induced Plasticity Steels (TRIP): Trip steels have improved ductility by virtue of special alloying and thermal treatment, or annealing after rolling. The microstructure of TRIP steels contains residual austenite in a ferritic-bainitic matrix that transforms into martensite during forming. **Availability of these steels is currently very limited in the U.S.”**



The major high tensile strength steel manufacturers in the world

ArcelorMittal

Indian-based company

Severstal

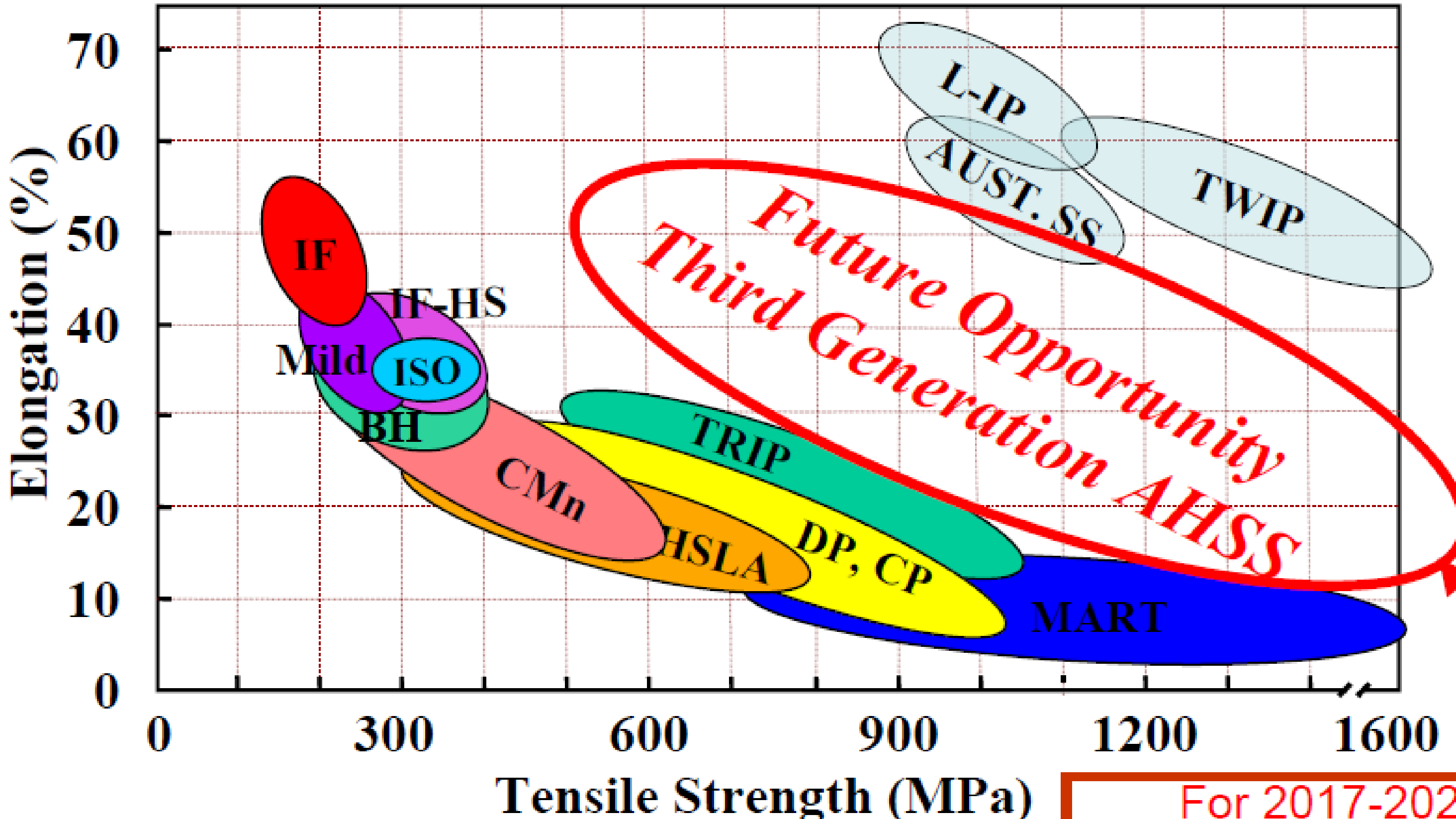
Russian-based

ThyssenKrupp

German-based

3rd Generation of AHSS

...we are researching a new generation of steels for the future.



For 2017-2025, new formable AHSS grades will enable more steel mass reduction

Carbon composite thermoplastics (military helmets)

The helmet shells were formed using a 408 tonne (900,000 lb) thermoforming press. Figure 3 illustrates the steps of the process as it was performed for the helmet fabrication.

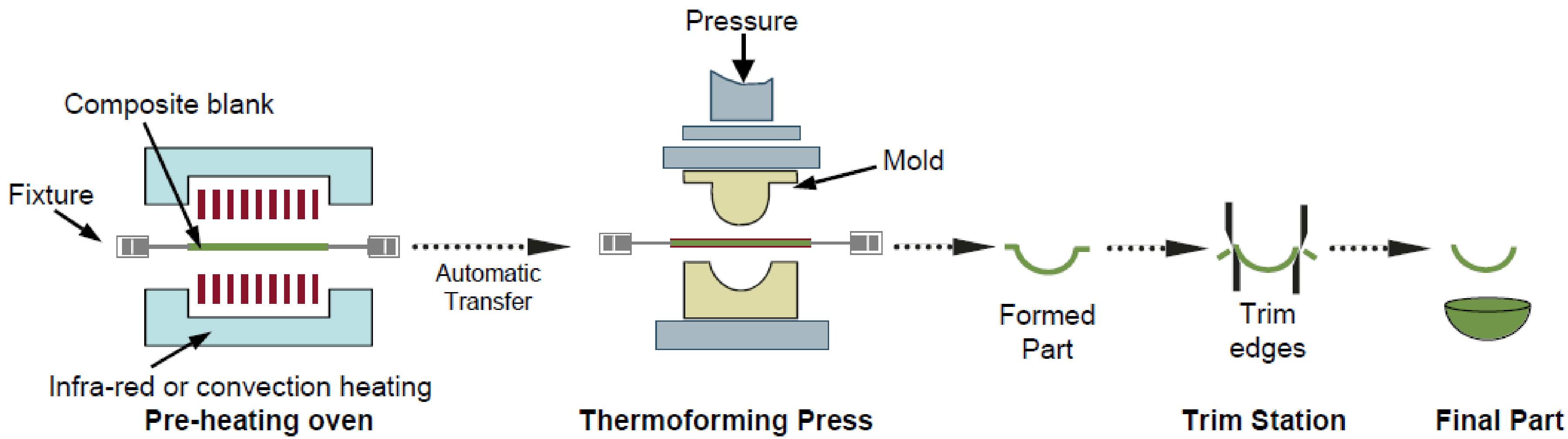


Figure 3. Thermoforming process steps

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- High-strength, lightweight materials for transportation
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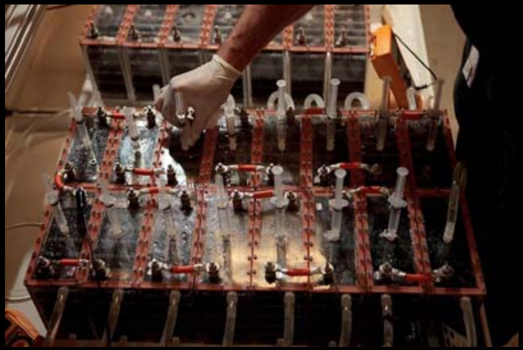
  - Wide band gap semiconductors (SiC, ZnO, diamond, ...)
  - Hard and soft magnetic materials
- Photovoltaic materials and processes
- Energy storage materials
- High temperature materials

Power Conversion & Energy Storage

Today | Future

And
Smart!

10,000 lbs | 100 lbs

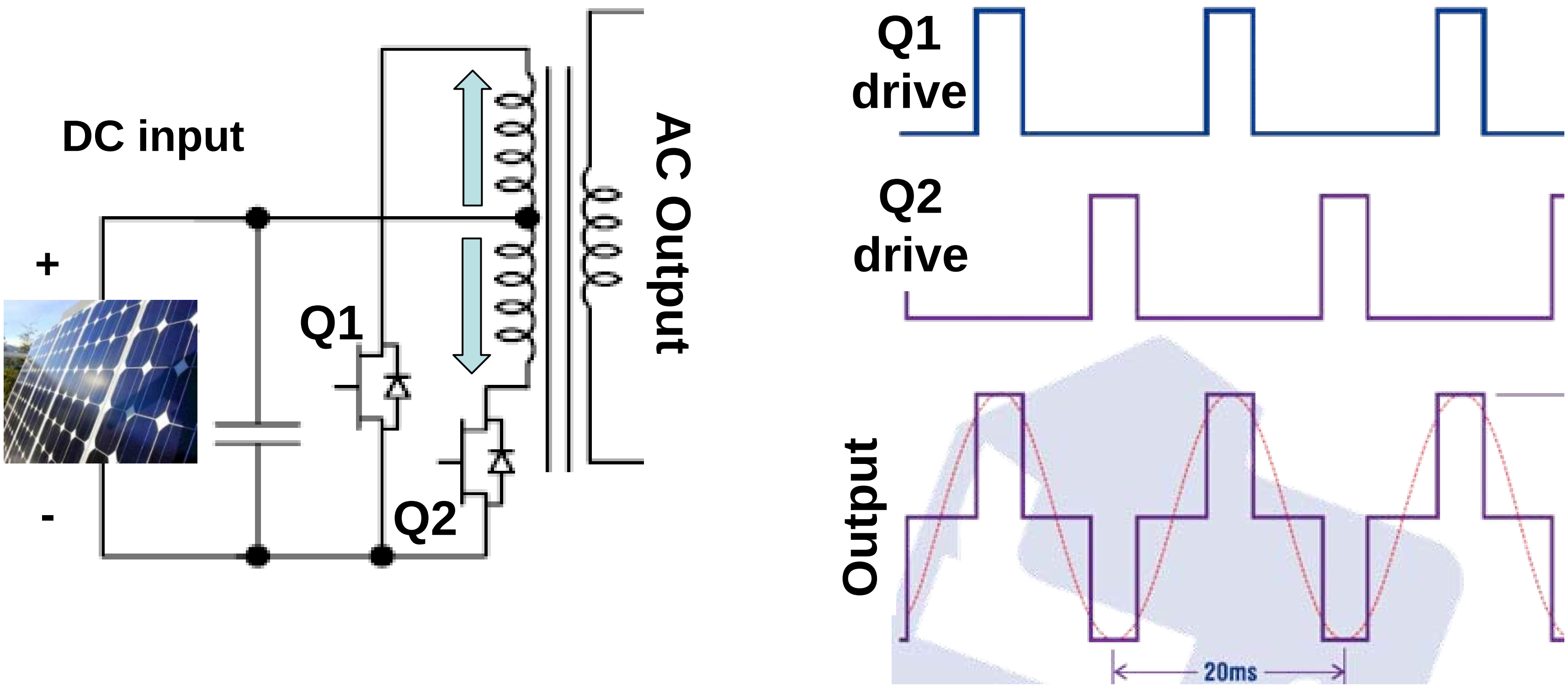


Anywhere
In the
world

$100/kWh | $100/kWh

2010: 30% of all electric power flows through power electronics
2030: 80% of all electric power will flow through power electronics

A Tutorial on DC to AC converters



• Current pulse when Q1 is conducting (on) and Q2 is off

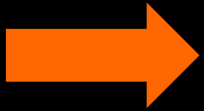
• Current pulse when Q2 is on and Q2 is off. The induced current and voltage on the output side of the transformer is reversed

• Inductors (L) and Capacitors (C) smooth the AC

The size of transformers for inverters (DC ⇔ AC), converters (DC ⇔ DC), and for step up and down voltage scales roughly as the inverse of switching frequency.

Today

10,000 lbs



Future

100 lbs

And Smart!

2010: 30% of all electric power flows through power electronics
2030: 80% of all electric power will flow through power electronics

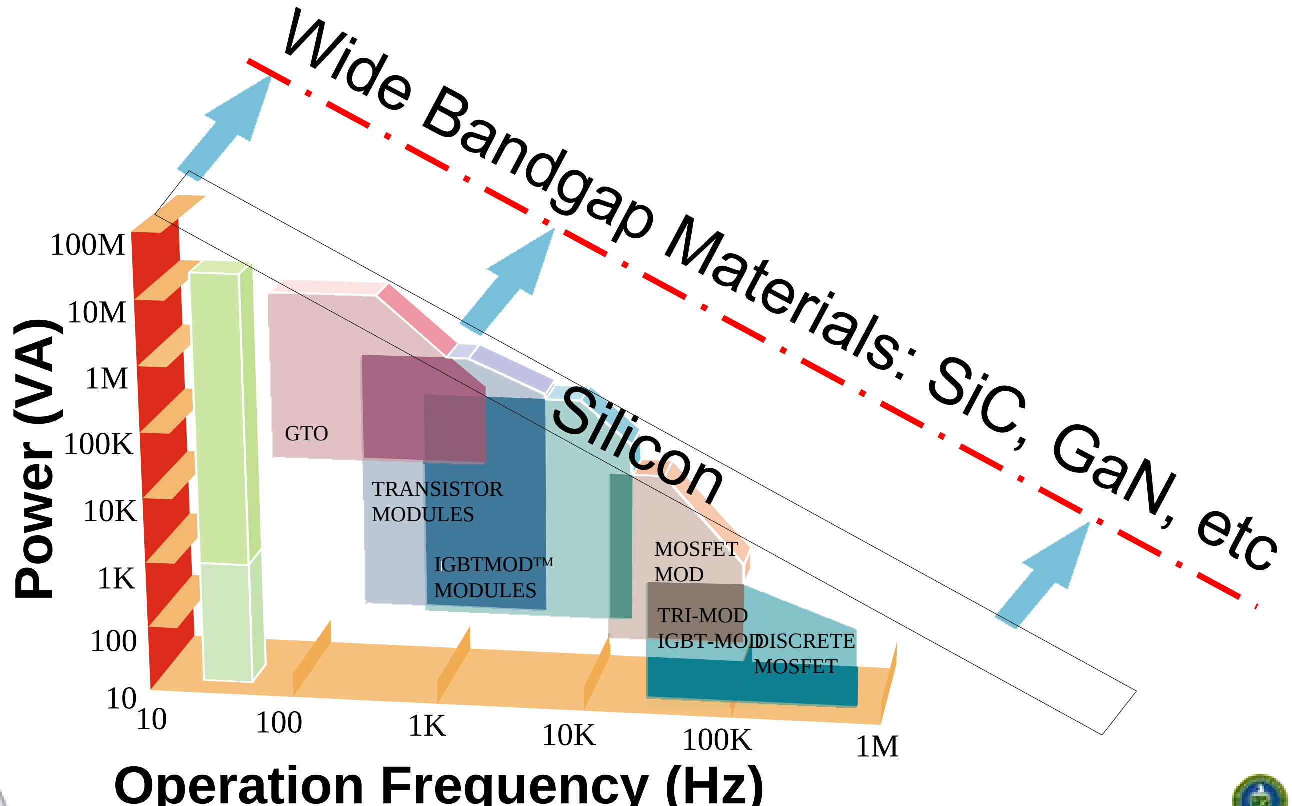
Miniature (Fast) Magnetics Needs Fast Switches

Bandgap (energy to 'free electron') increases
⇩
Breakdown voltage increases
⇩
Drift region can be decreased

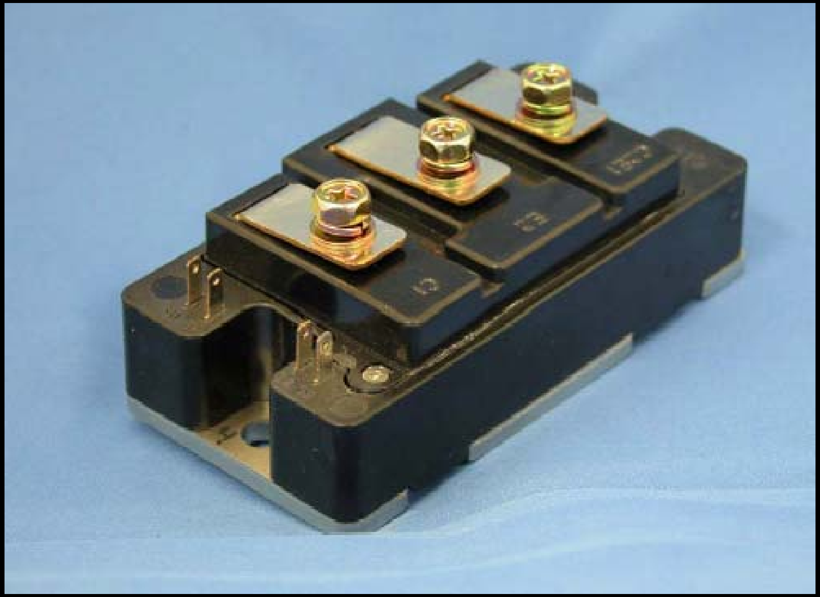
Reduces transit time

Increases frequency

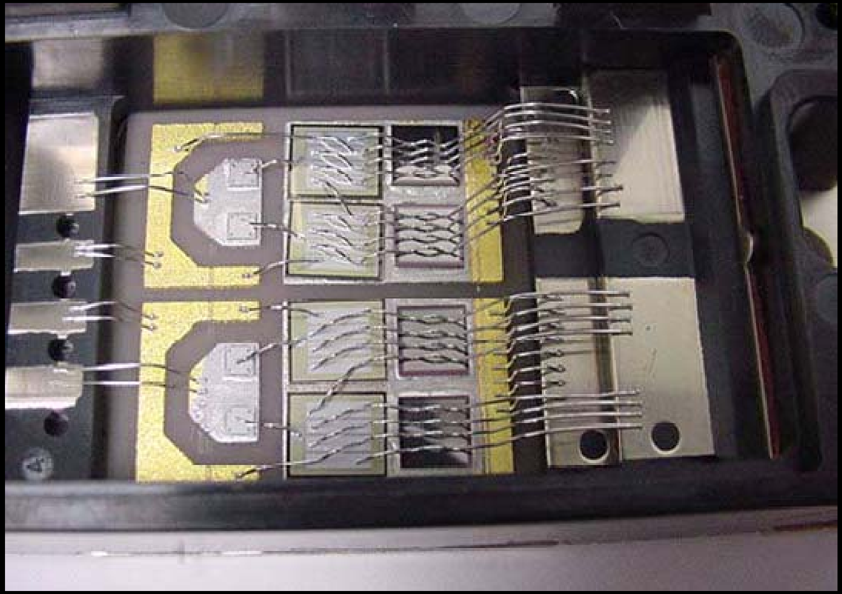
Reduces on-resistance



SiC power modules operate at 1200V and 880 amps. (1MW)



1.2 kV/100A SiC module

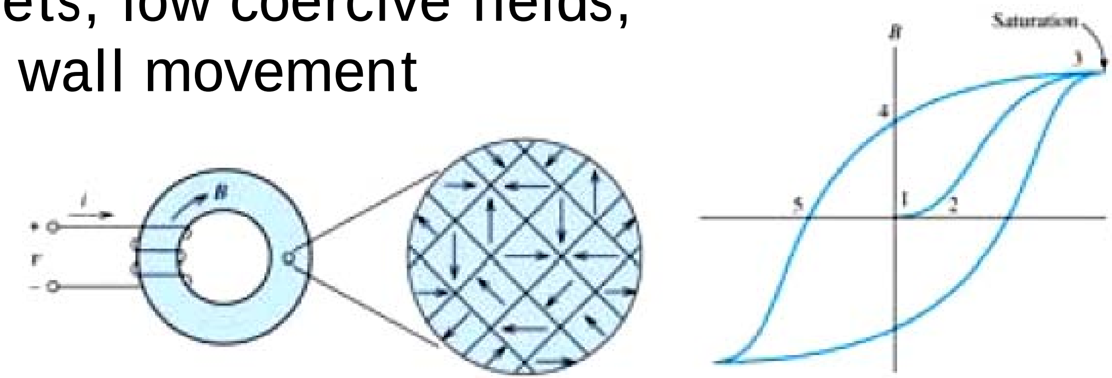


Internal view: 2 80 A SiC MOSFETs and 2 50 A SiC JBS diodes

Latest news is that a > 1 kV, 1 MW ***single*** SiC transistor has been demonstrated.

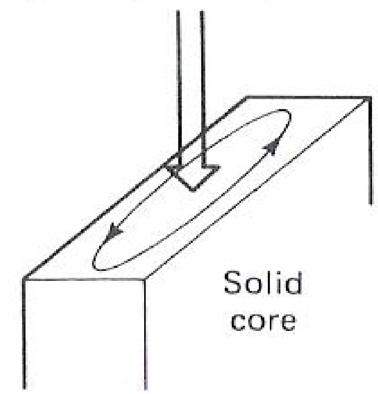
LIMITS TO SCALING WITH FREQUENCY & POWER

Energy lost in rotating recalcitrant domains…
- requires soft magnets, low coercive fields, little or no domain wall movement



(a) Sample and coil for applying H (b) Magnetic domains (c) Hysteresis loop in the B – H plane

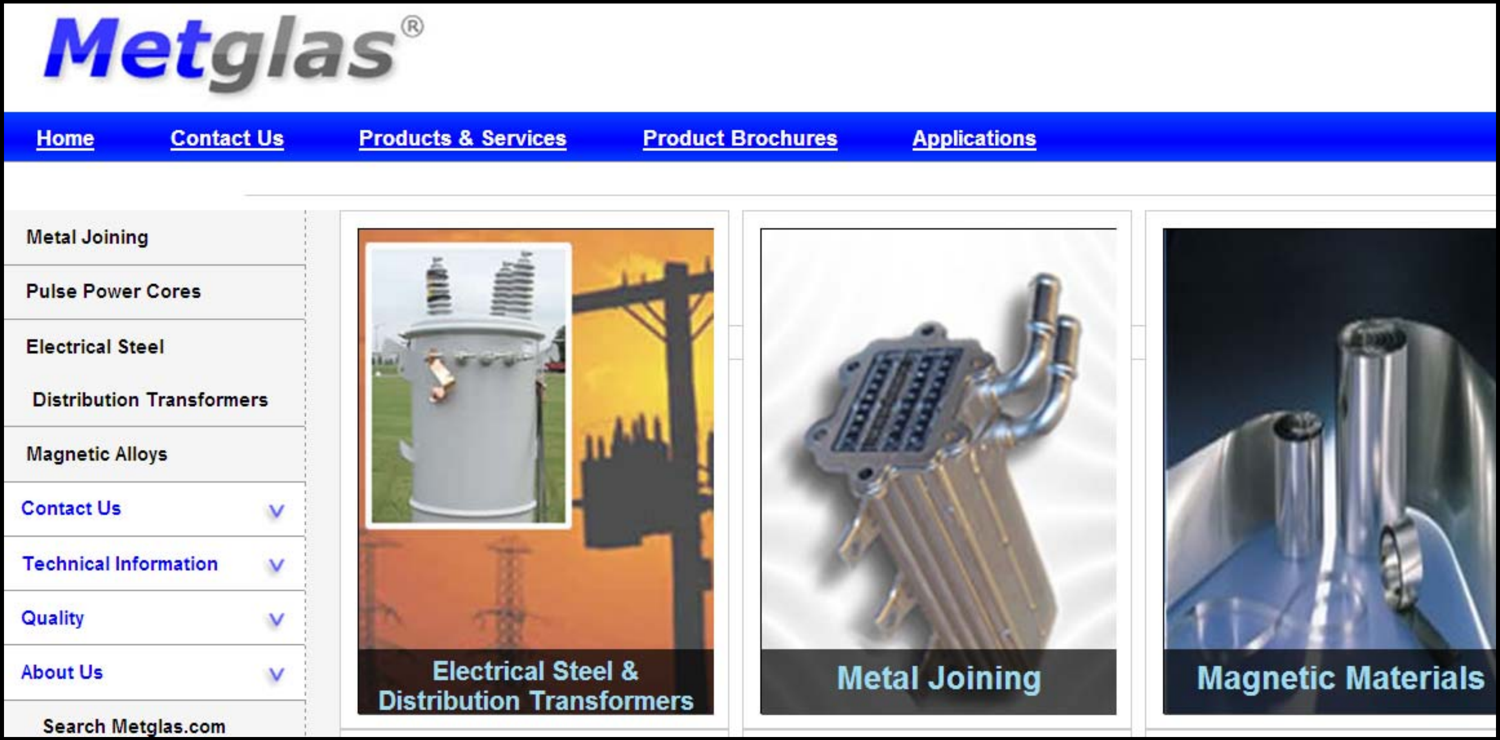
Energy lost induced electrical current
- requires poor electrically conductivity or insulating material (no eddy- currents)



Efficient transformer and high field magnets

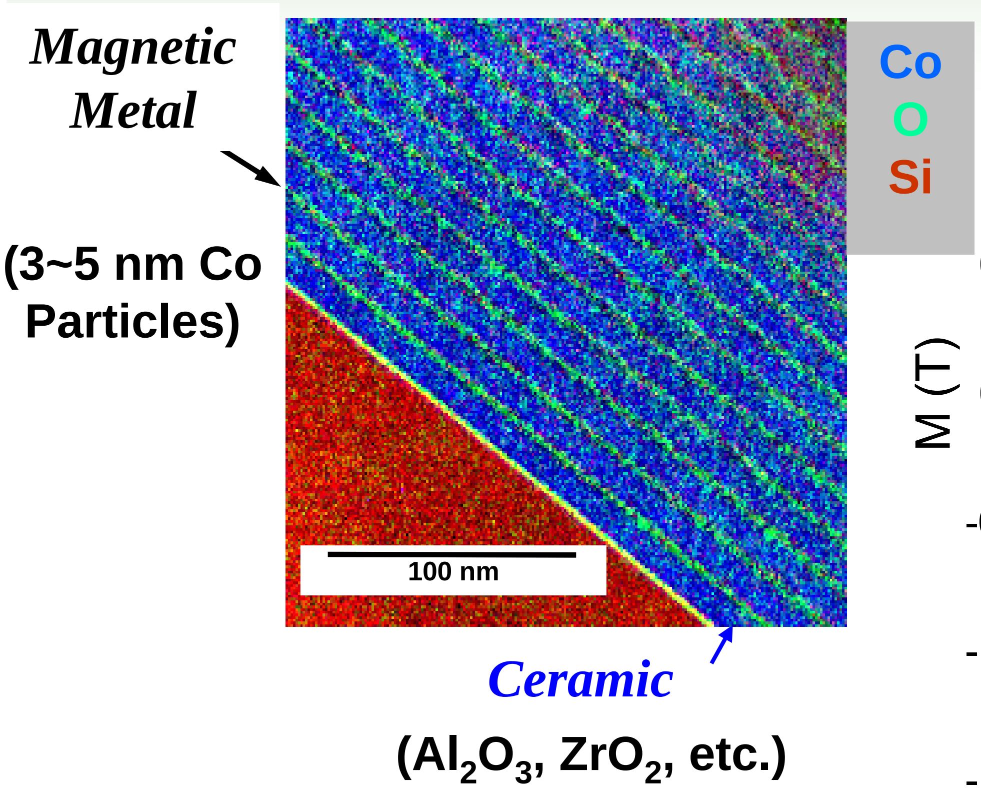
Metglas is a thin amorphous metal alloy ribbon produced by using rapid (10^6 °C/s) solidification. AlliedSignal began research in the 1970s. The *Advanced Technology Program of NIST* provided 50% cost share in a research program in the 1990s.

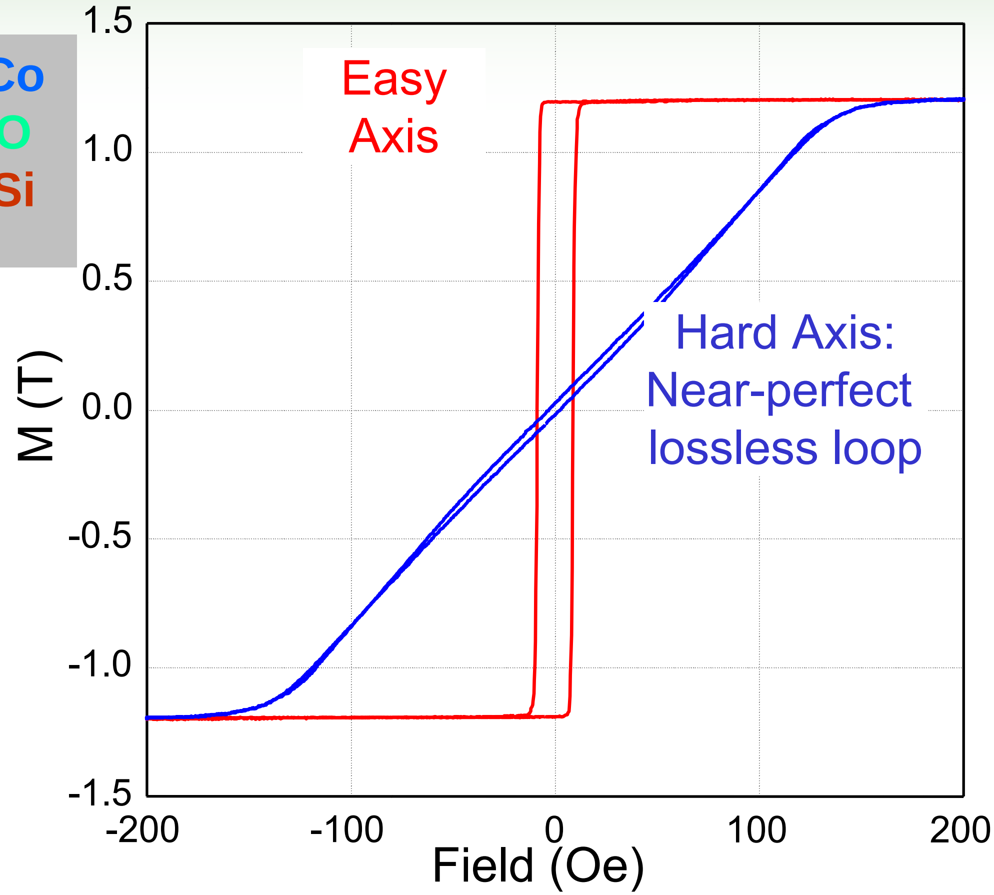
The best commercial metallic glass material has power losses of ~15% of the best silicon-iron grades.



http://www.atp.nist.gov/eao/sp950-3/honeywell.pdf

New Materials: Metal Nano-composites





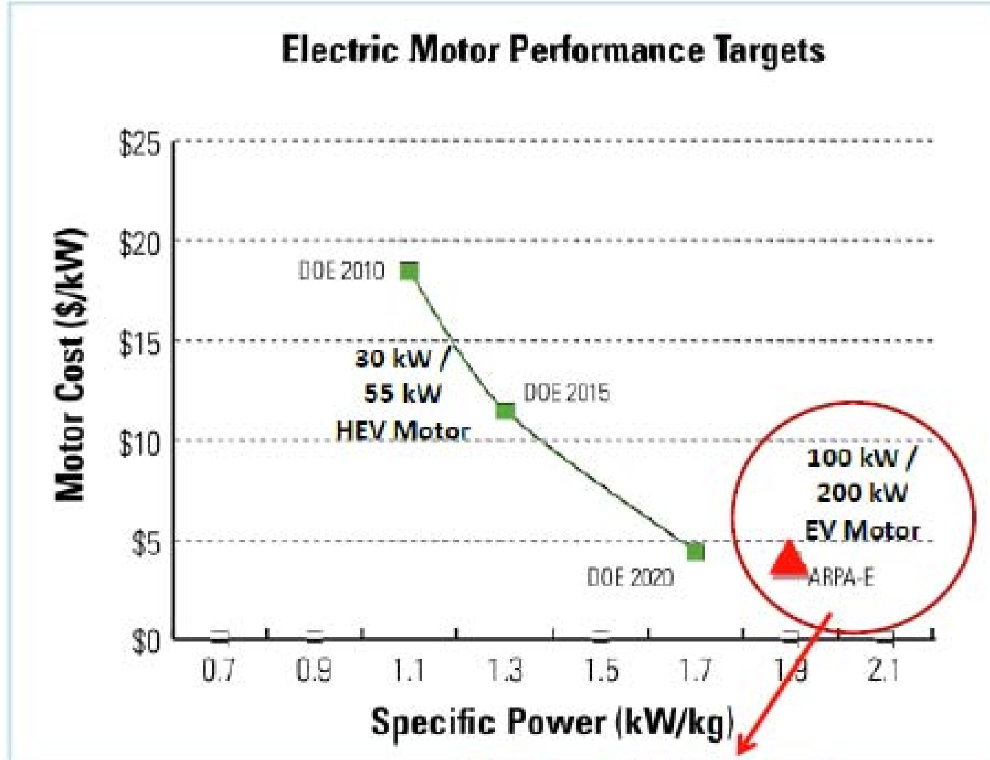
- Ferromagnetic (coupled particles)
- High resistivity (300 ~ 600 μΩ·cm) decreases eddy-current loss independent of flux direction.
- Some have strong anisotropy for low permeability and low hysteresis loss

Source: C Sullivan, et al.

ADVANCED ELECTRIC MACHINES FOR ELECTRIC VEHICLES

Enabling Larger, More Powerful Electric Vehicles

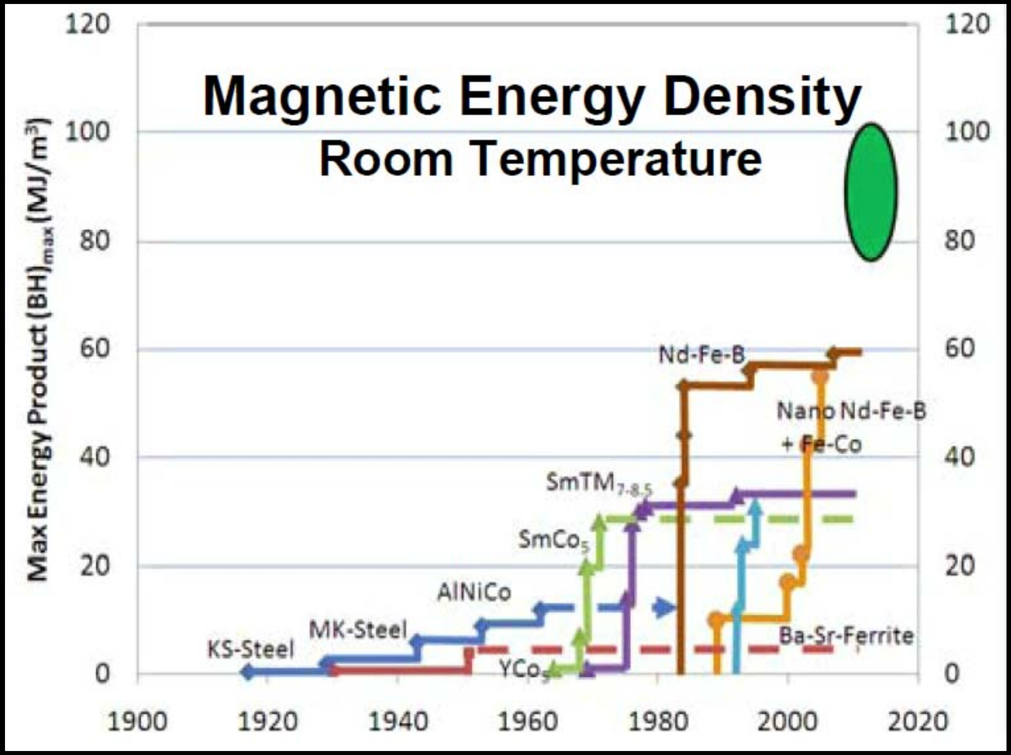
80 kW motor ~$1,500 ⇒ $320



and Order of Magnitude Reduction in Rare Earth Content: less than 0.33kg/kW

China produces ~ 95% of the rare earth metals

Rare Earths are used in motors/generators,
advanced batteries, displays, fluorescent and LED lighting

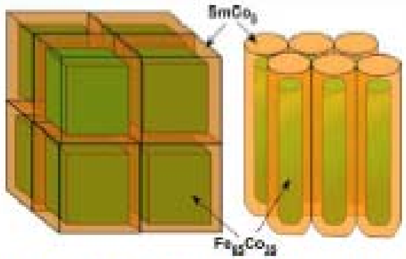


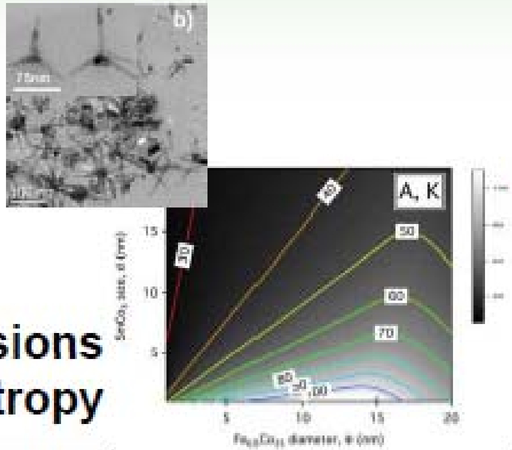
Critical Rare Earth Free Magnetic Materials – New Structures

Hard on Soft Nanoparticle

"Scalable Exchange Coupling"

BH_{max} = 50–100 MGOe



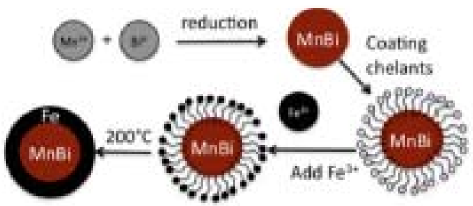


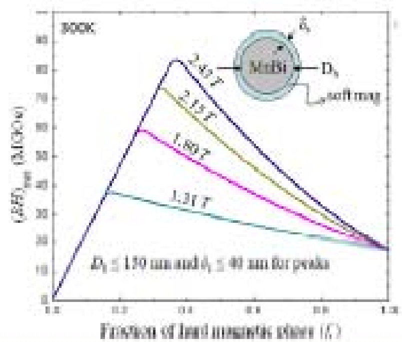
Maintain Critical Dimensions and Anisotropy

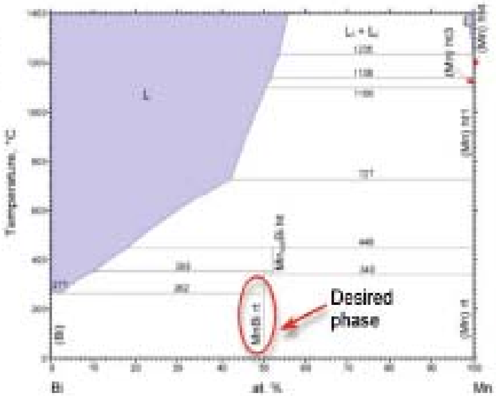
BiMn on Fe

"Elevated Temperature Stability"

BH_{max} = 40 MGOe (200C)







MnBi core / Fe shell

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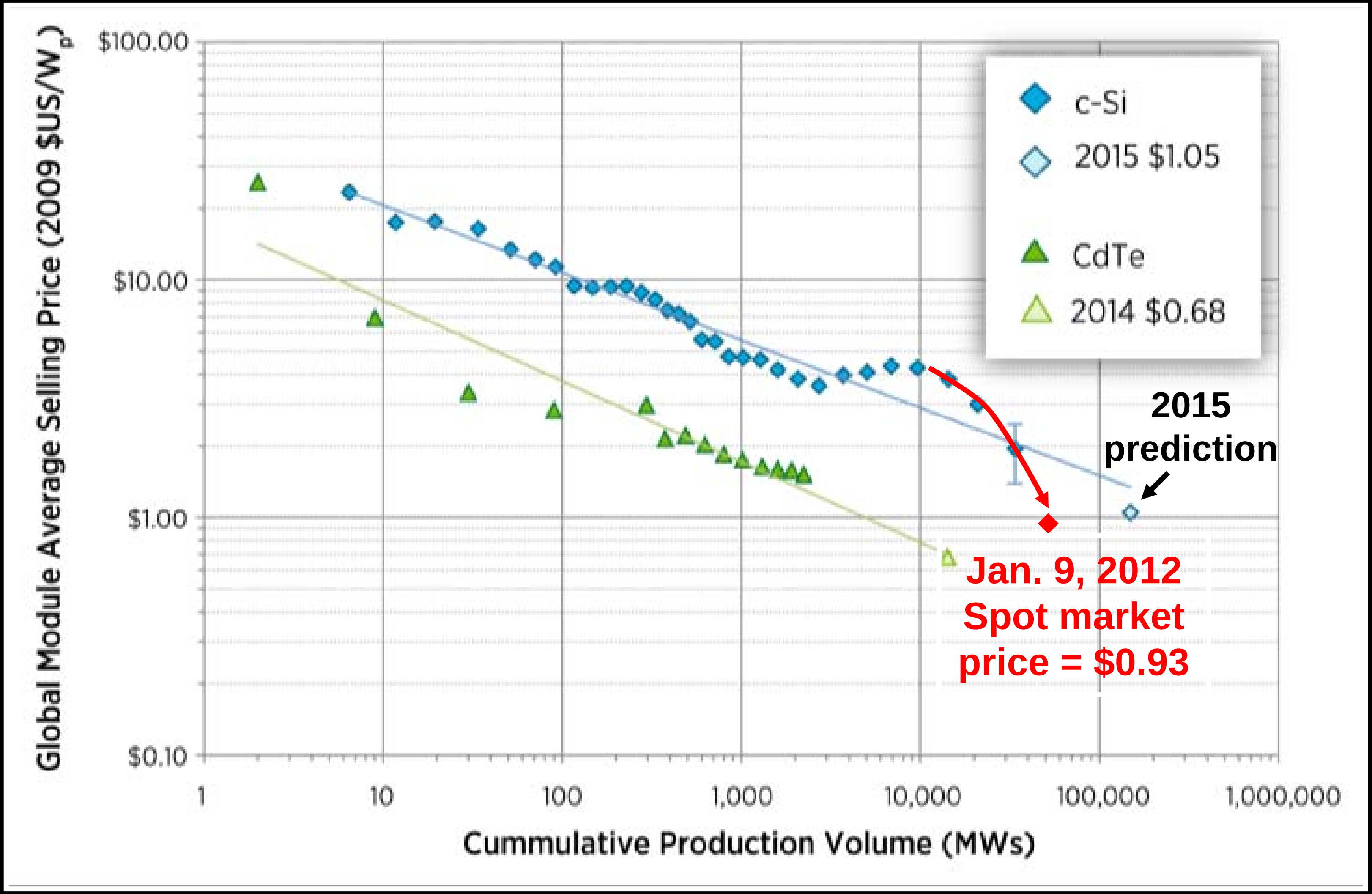
- Photovoltaic materials and processes

- Energy storage materials

- High temperature materials

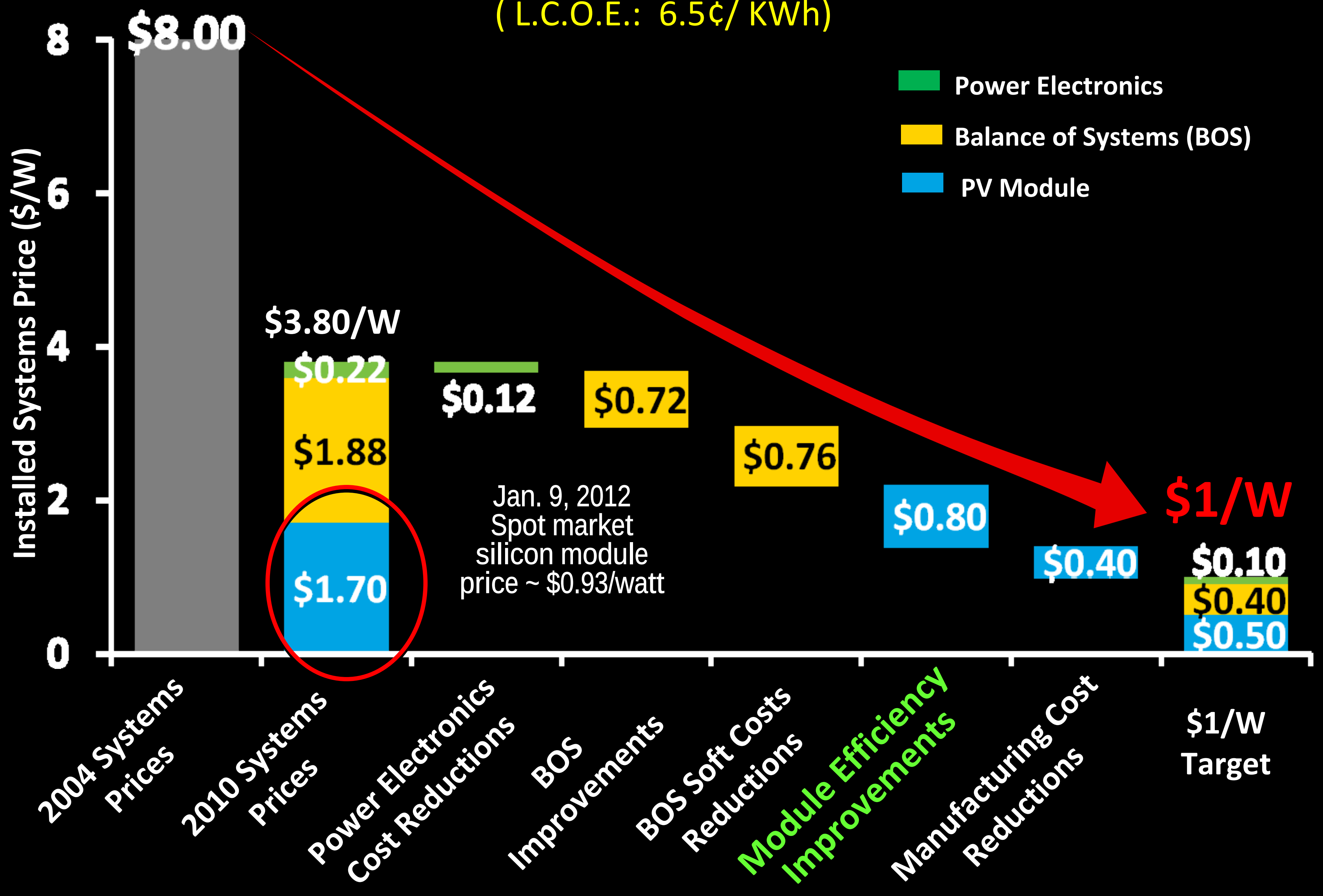
Cost of PV modules are dropping below the power law experience curves

Source: (CdTe) First Solar Earnings Presentation, SEC Filings; (c-Si) Navigant, Bloomberg NEF, NREL internal cost models

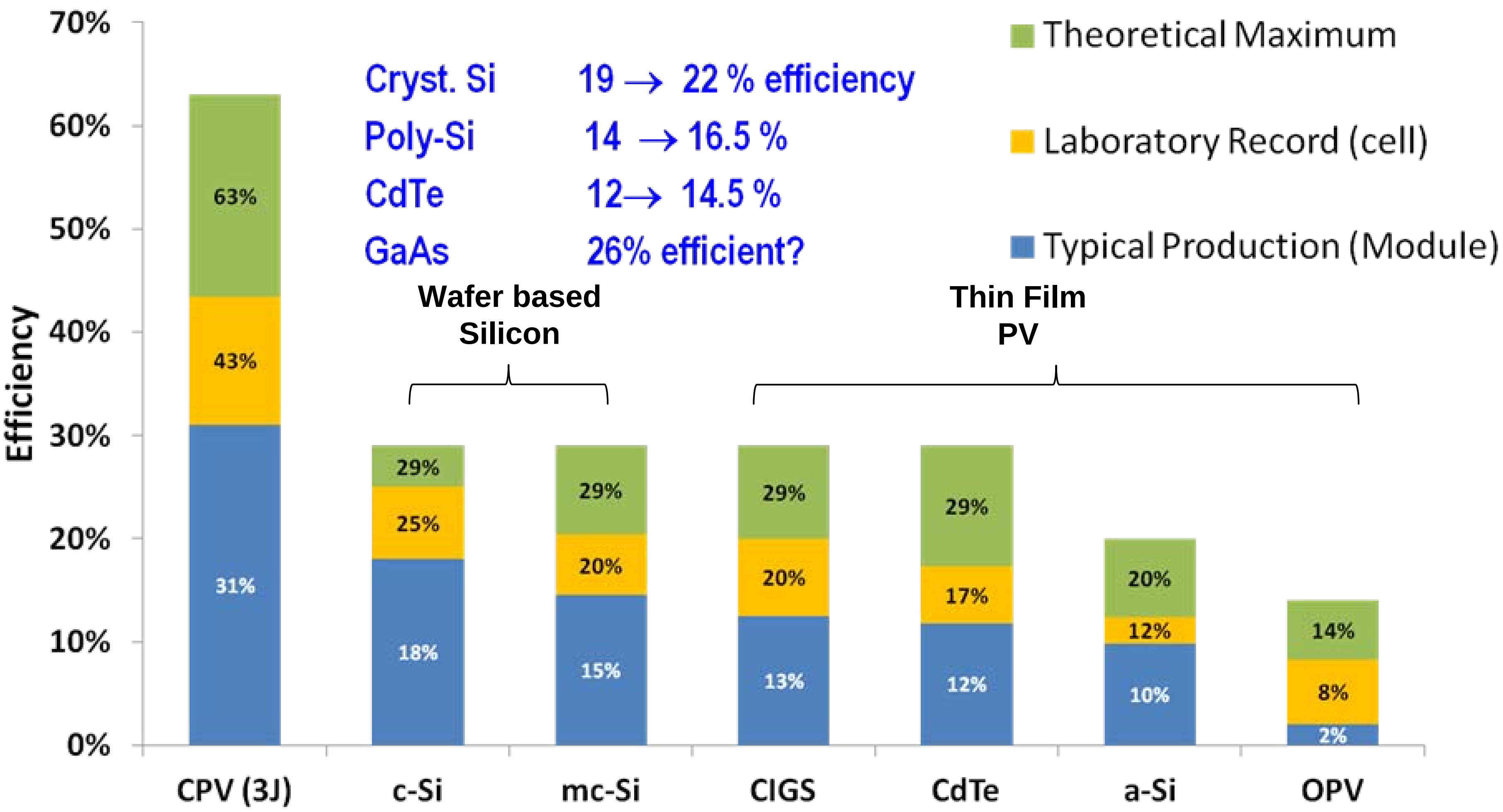


SunShot goal: Cost Competitive Solar by 2020

(L.C.O.E.: 6.5¢/ KWh)



A Materials Science Approach to Enhancing Cell and Module Efficiency



PROGRESS IN PHOTOVOLTAICS: RESEARCH AND APPLICATIONS
Prog. Photovolt: Res. Appl. 2011; 19:565–572

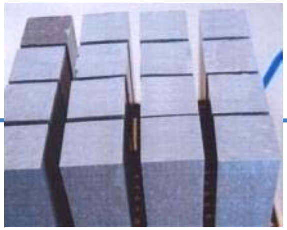
Opportunities in Silicon

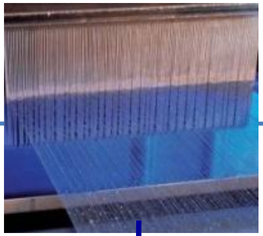
Conventional approach

Standard

1. Cast Ingot
2. Cut Brick
3. Grind & Polish Brick
4. Saw Wafers

Pure Silicon

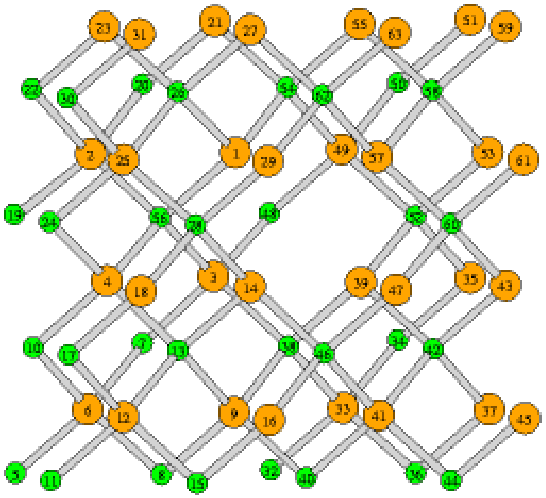




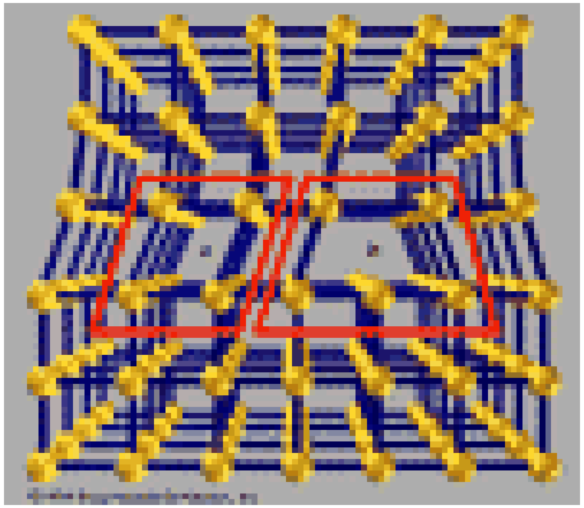
Wastes 50% of Silicon

1366 Direct Wafe

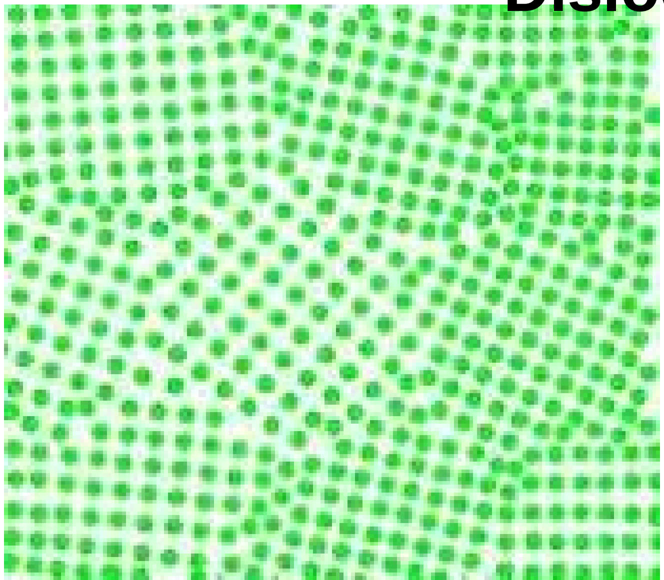
CdTe – Getting to 23% Efficiency through Fundamental Materials Science



Point Defects- Cd Vacancies



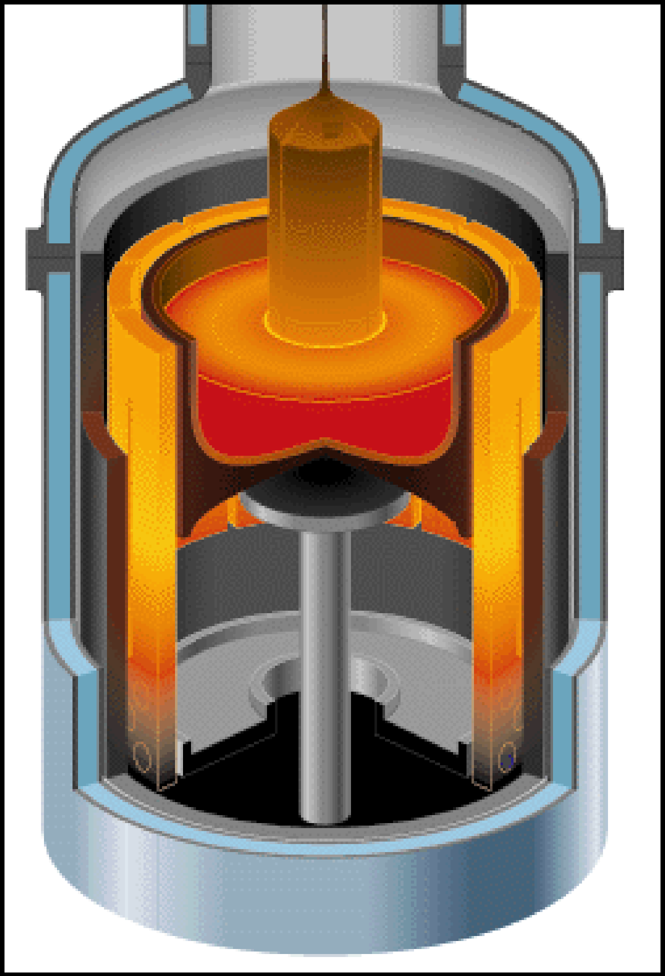
Line Defects : Dislocations



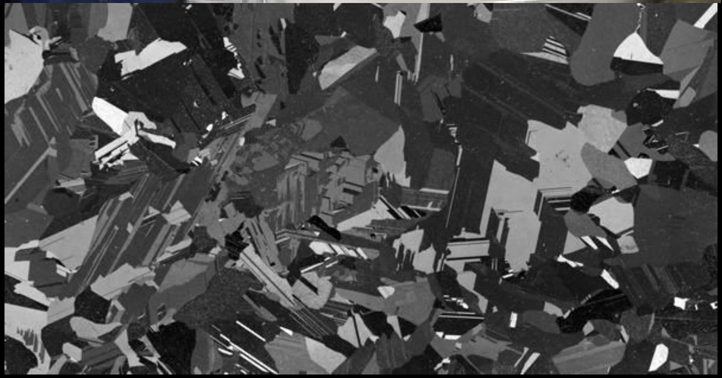
Grain Boundary Control

Silicon Crystal Growth

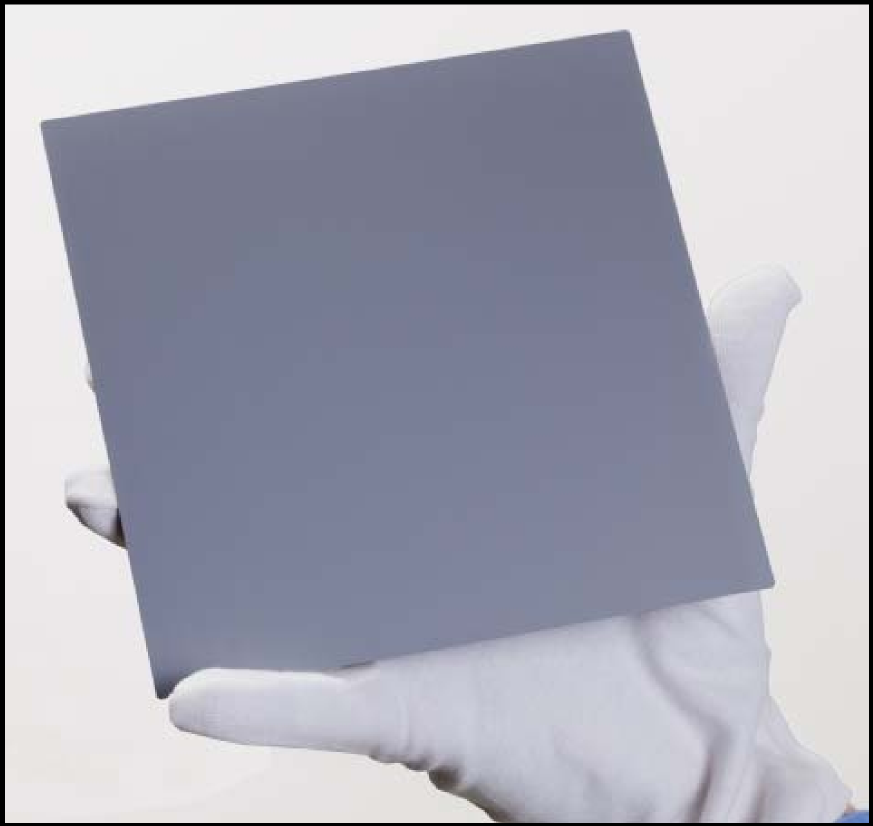
Czochralski growth



Directional solidification



Casting Single Crystal Wafers



In 2007, the DOE supported research of BP Solar in the U.S. to make large single crystals of silicon in directional solidification method. A proto-type version of this technology achieved 20% efficiency, better than many CZ mono wafers in production.

Before the technology was taken to the manufacturing scale, intense competition with Chinese manufacturers caused BP Solar shut down operations in the US.

This technology has been improved in China. JA Solar and may soon go into production of single crystal silicon using directional solidification.

Innovation in Energy

New materials and transportation efficiency

Power electronics

Solar photo-voltaics

Batteries

Research Roadmap for 2015 and Beyond

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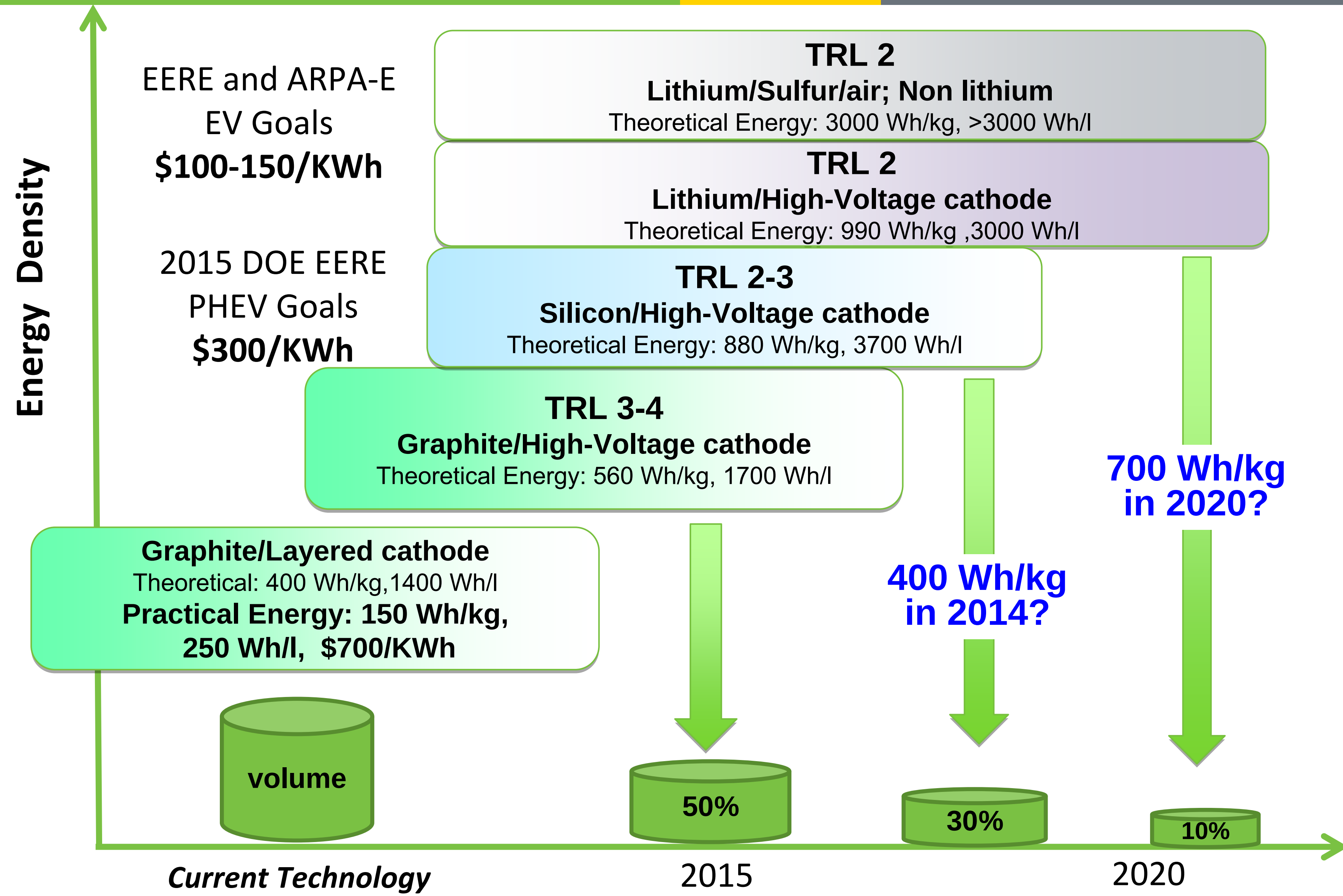


Reclaiming Leadership in Advanced Batteries

Research discoveries made by scientists at Argonne National Lab allowed them to, develop a new lithium-manganese ion battery.

- 50-100% cathode energy density increase
- Less costly to manufacture
- Safer

Recent discoveries by an Argonne - U. Illinois – Northwestern collaboration:

Doubling of energy density has been demonstrated in the lab.

Argonne NATIONAL LABORATORY

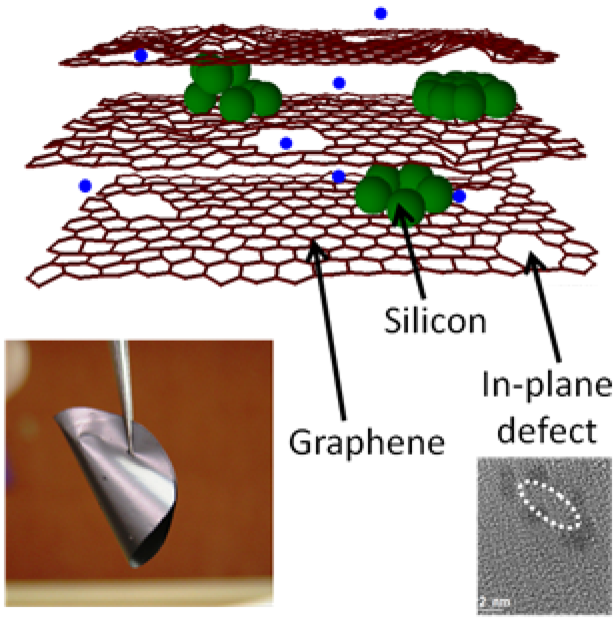
TAILORED INTERFACES CEES
Center for Electrical Energy Storage
Energy Frontier Research Center

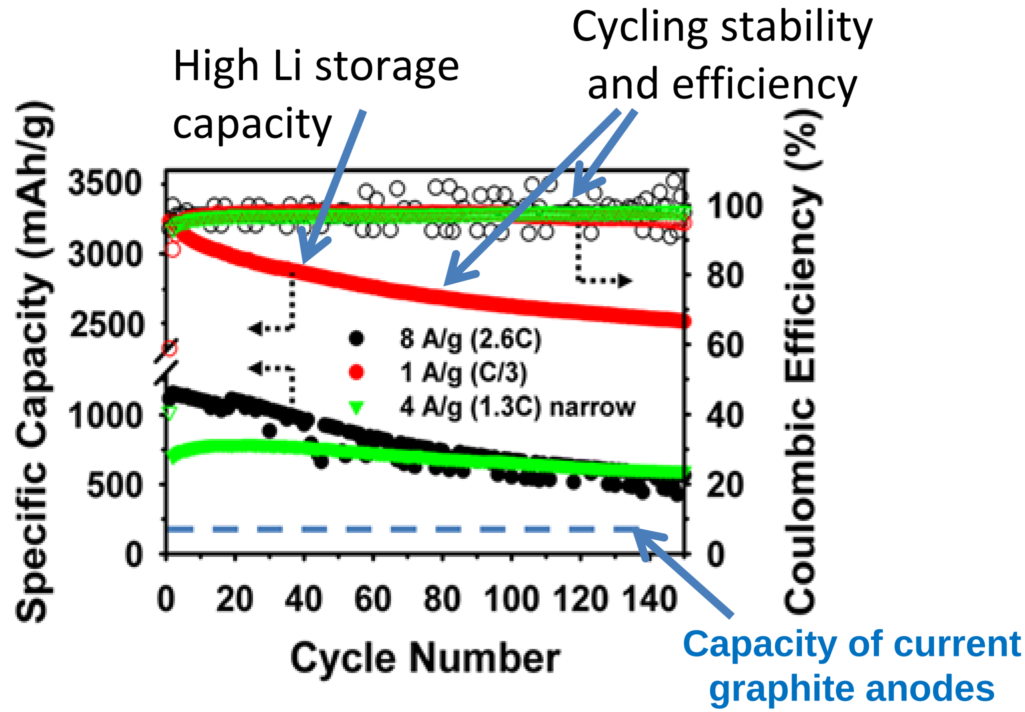
Center for Electrical Energy Storage (CEES)

Architectural Design of a Novel Si-Graphene Anode

In-Plane Vacancy-Enabled High-Power Si–Graphene Composite Electrode for Lithium-Ion Batteries, Kung et al., Adv. Energy Materials, **1**, 1079 (2011).

Nano-particulate silicon embedded within defected graphene sheets provides up to 10x more Li-storage capacity as a conventional graphite anode and can be charged within 15 minutes.



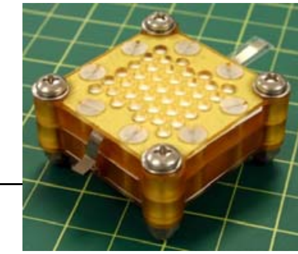


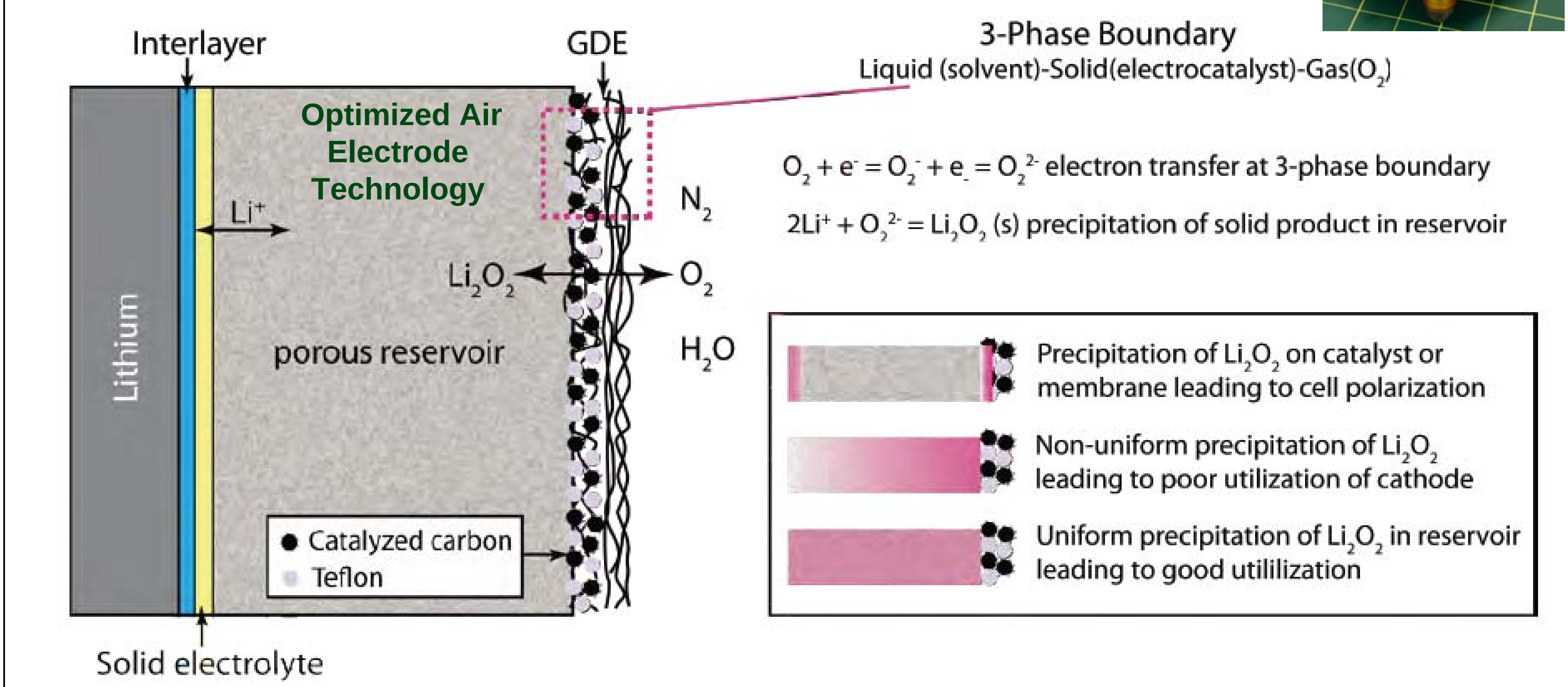
Argonne NATIONAL LABORATORY ILLINOIS UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN NORTHWESTERN UNIVERSITY U.S. DEPARTMENT OF ENERGY

Ultra-High Energy Rechargeable Lithium/Air Battery

Polyplus/Corning: $5M, 2 years

$2\,Li + O_2 \rightarrow Li_2O_2$; V = 3.1V





>3x Li-Ion: 600 Wh/kg & 1000 Wh/L

How to promote domestic manufacturing

- Regulations (mileage, appliance efficiency, pollution standards, etc.) drives innovation.

- Fiscal Polices (R&D tax credits, Master Limited Partnerships, other tax laws) that help companies that take the long term-view and to help guide on-shore investments.

- Corporate and labor leadership.

- Government role as an "early adopter" and other methods to create market draw.

Oh, power electronics and manufacturing engineers ...

Where art thou?

END

How to promote domestic manufacturing

- Regulations (mileage, appliance efficiency, pollution standards, etc.) drives innovation.

- Fiscal Polices that help companies that take the long term-view and to help guide on-shore investments.

- Corporate and labor leadership are essential.

- Government role as an "early adopter" and other methods (e.g. a clean energy standard) to create market draw.

America has the opportunity to lead the world in clean energy technologies and provide a foundation for future prosperity.

We remain the most innovative country in the world … but "Invented in America" is not good enough.

"Invented in America, Made in America, Sold Worldwide"

“The Evolving Structure of the American Economy and the Employment Challenge”

Michael Spence and Sandile Hlatshwayo
Working paper, Council on Foreign Relations (2011)

Tradable jobs: Goods and services that can be produced in one country and consumed in another. Airplanes, cars, electronics …

Non-Tradable jobs: Goods and services that ***have*** to be produced domestically. Government, healthcare, construction, much of legal services because of legal differences across countries.

From 1990 – 2008 employment grew by 27 million jobs. Almost all of it was in the non-tradable side. **There was negligible employment growth on the tradable side of the economy where we compete with other people.**

The forming operation imparts some degree of strain hardening which increases yield strength in bake hardening Type B steels. The paint baking cycle, typically 175°C (350°F) for 20 to 30 minutes, provides another increase in yield strength due to moderate "carbon strain aging". Material properties are generally stable, depending on the process. Figure 1 illustrates the hardening process with bake hardening steels.

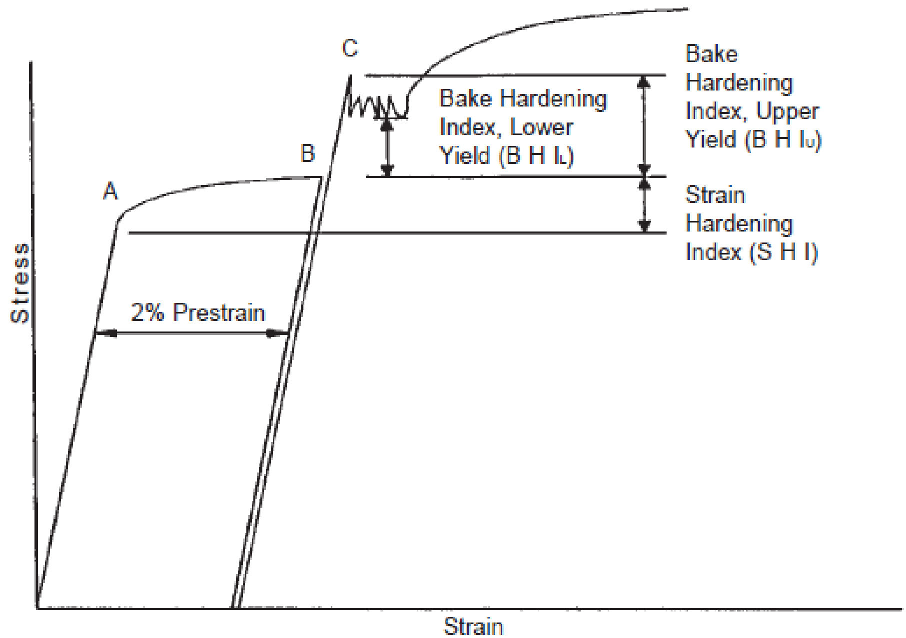


Figure 1 Schematic Illustration Showing Strain Hardening and Bake Hardening Index and the Increase in Yield Strength that Occurs During The Bake Cycle.

General Guidelines for Die Design and Construction

Draw Dies

Higher than normal binder pressure and press tonnage is necessary with H.S.S. in order to maintain process control and to minimize buckles on the binder. Dies must be designed for proper press type and size. In some cases, a double action press or hydraulic press cushion may be required to achieve the necessary binder forces and control. Air cushions or nitrogen cylinders may not provide the required force for setting of draw beads or maintaining binder closure if H.S.S. is of higher strength or thickness.

Draw beads for H.S.S. should not extend around corners of the draw die. This will result in locking out the metal flow and cause splitting in corners of stamping. Draw beads should “run out” at the tangent of the corner radius to minimize metal compression in corners, as shown in figure 16 on page 47.

Better grades of die material may be necessary depending on the characteristics of the HSS, the severity of the part geometry, and the production volume. A draw die surface treatment, such as chrome plating, may be recommended for outer panel applications.

To effectively utilize the automotive structural grades of HSS in the 275 to 420 Mpa (yield strength) range (40 to 60 KSI), most parts should be designed for fabrication in form and flange dies, “draw-action” form dies or open end draw dies. These die processes require the metal to bend and stretch but minimize the metal compression common to closed corners of conventional draw die processes. Structural parts, such as longitudinal rails, motor compartment rails and roof rails can be designed to allow an open-end draw die operation.

It is important that the product designers work closely with the die process planners and the steel suppliers when parts are being designed to avoid improper material/part design/die process combinations. For structural parts such as rails and crossbars, springback on flanges will increase as compared to mild steel. The manufacturing process will therefore require overbend of flanges to allow for springback compensation. The part design should be such that overbend of flanges is possible, particularly for “hat section” parts with opposing sidewalls. Smaller bend radii will minimize springback, but the part design should also allow for a die overbend of at least 6 degrees for HSS parts.