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Accelerating Materials Deployment and Manufacturing via Multi-Scale Modeling and Genomics

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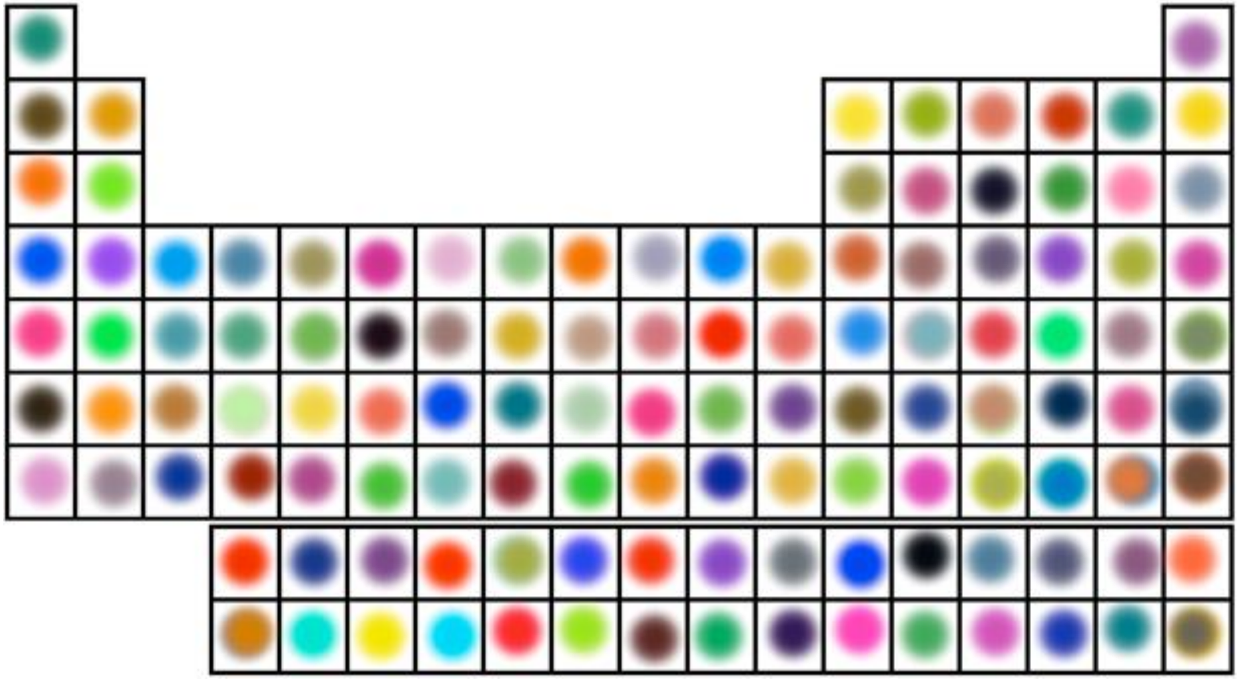
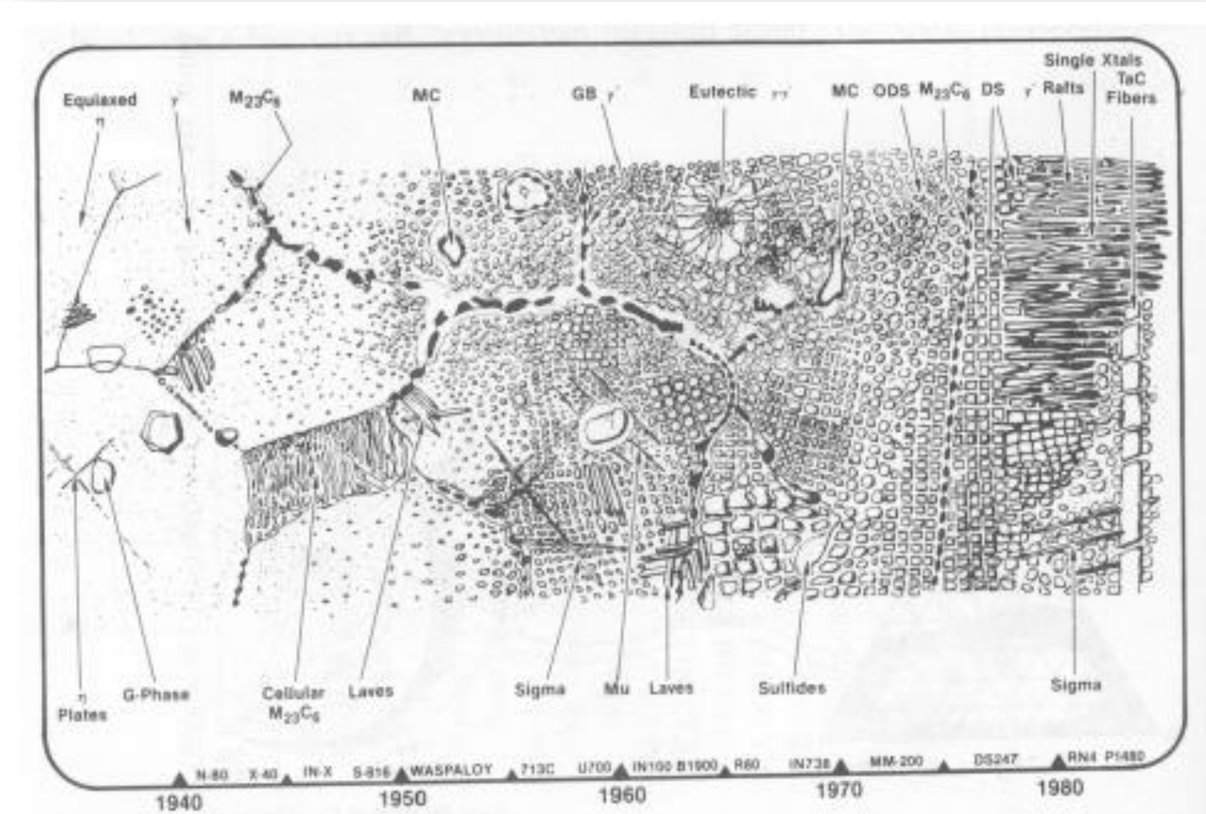
2016 International Forum Korea on Advances in Mechanical Eng. (IFAME)
August 18, 2016 – Daejeon, Korea

Accelerating Materials Deployment – the Iron Man Approach

Possibilities…



Superalloys – Inconel 718

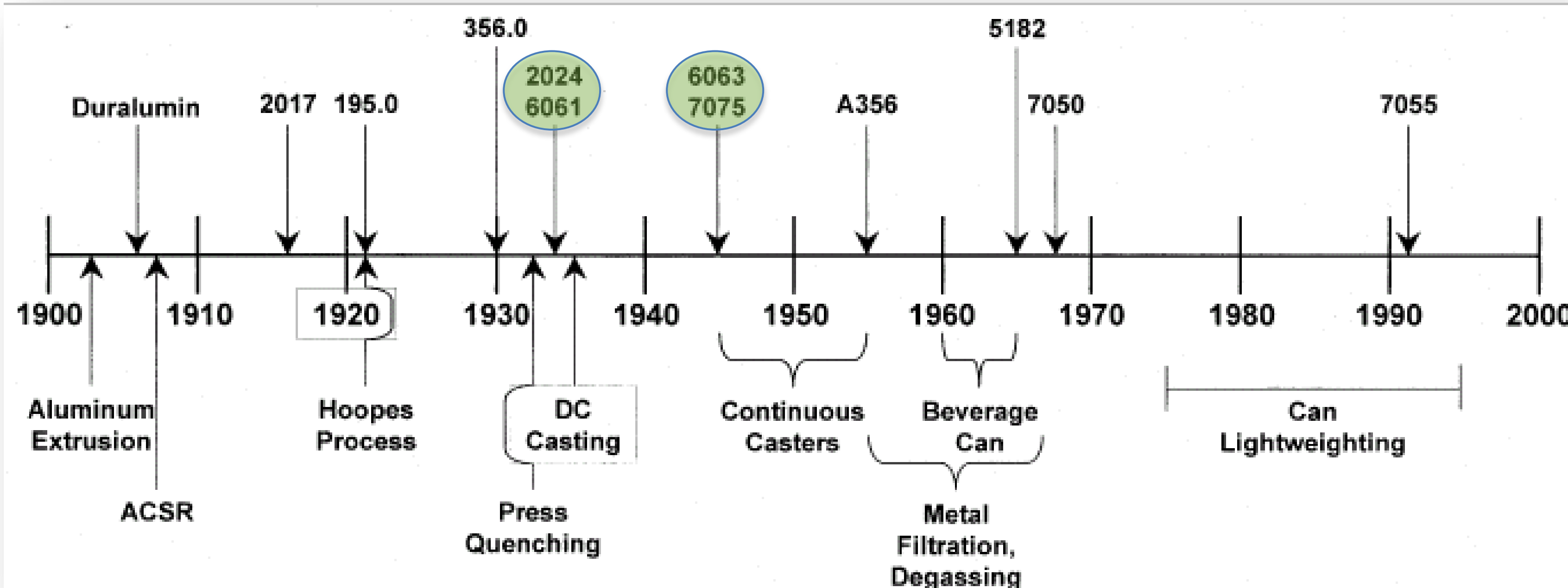


Wagner, H., & Hall, A. (1965). Physical Metallurgy of Alloy 718. DMIC Report 217.

Complicated chemistry, complicated microstructure … developed by: intuition, experimentation

… invented in 1940's by Wiggins Company (England) for steam power plants and then adopted for turbine engine applications by GE and others in the 1960's.

Aluminum Alloys



From: “Technology Innovation in Aluminum Products”, JOM, vol. 53(2), pp. 21-25, 2001

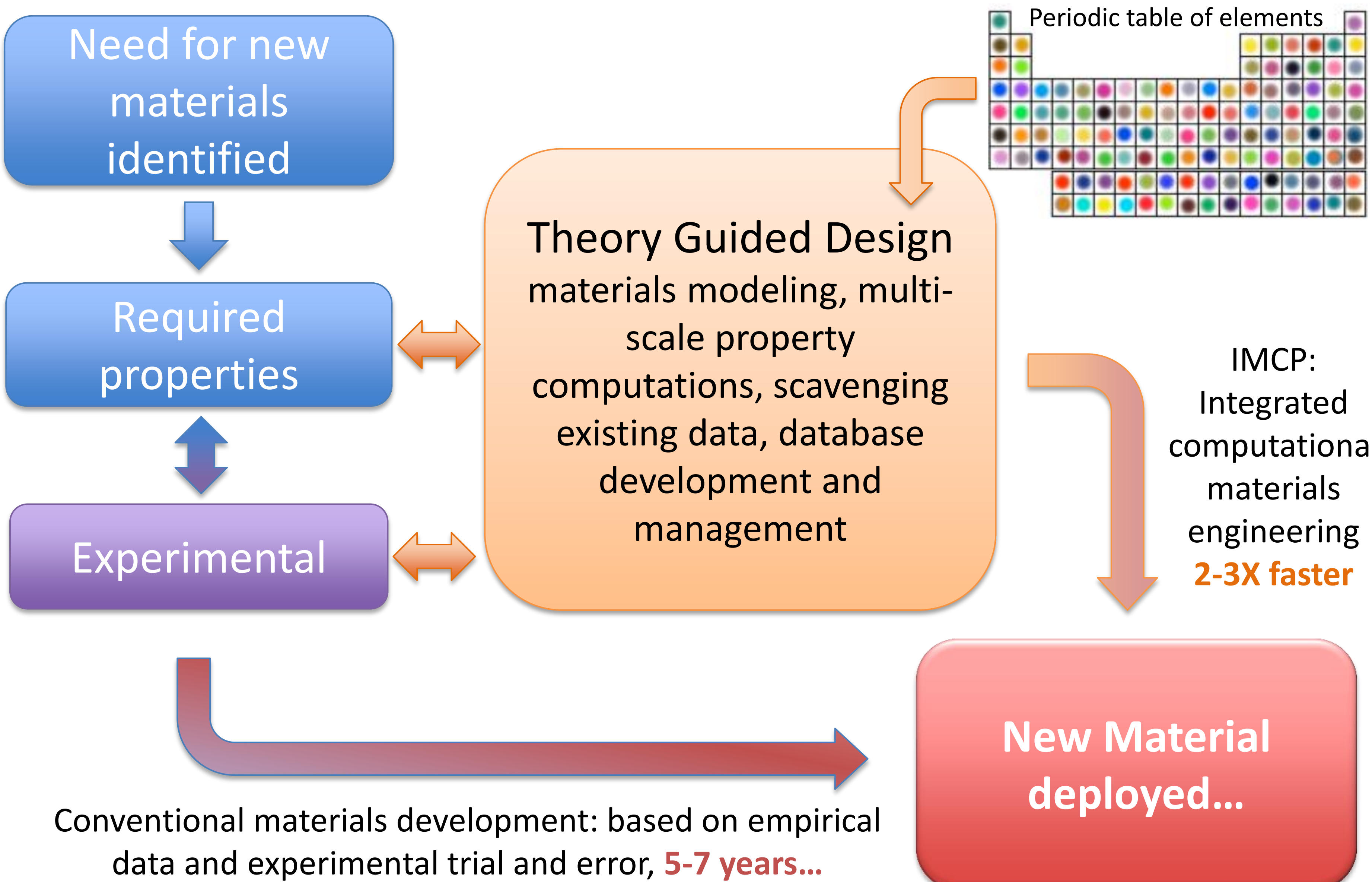
…existing alloys are decades old and are the materials of choice for low weight, high strength applications.

"To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call the Materials Genome Initiative.

The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place. We can do it faster."

-President Obama (6/11)

Accelerating Materials Deployment…



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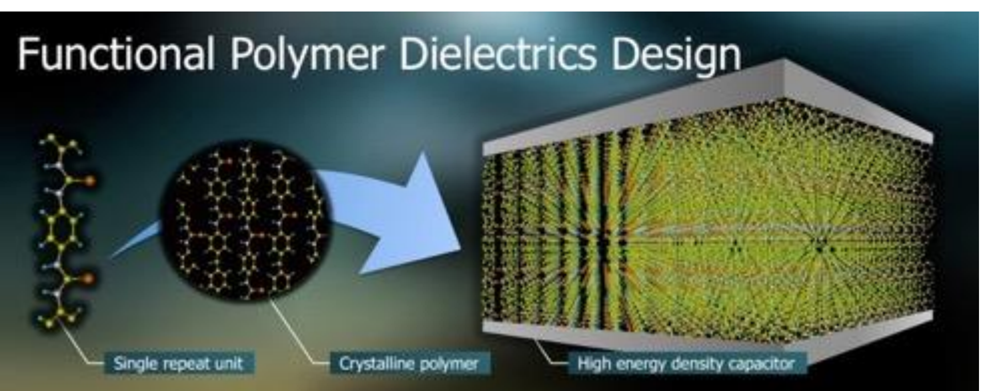
Theory & Modeling – Computational Materials Science
First Steps in Materials Genomics…

Multi-scale modeling through:

- Electronic/atomic – *ab initio* computations
- Atomic – molecular dynamics Monte Carlo

Images courtesy: Rampi Ramprasad; http://rampi.ims.uconn.edu



- Thermodynamics and kinetics
- Phase-field modeling
- Continuum-level modeling – finite element analysis

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Self-Healing, High-Reliability Electrical Contacts

U.S.ARMY

United Technologies Research Center

People…

Mark Aindow
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Yu Sun
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M. Tumerkan Kesim
UConn

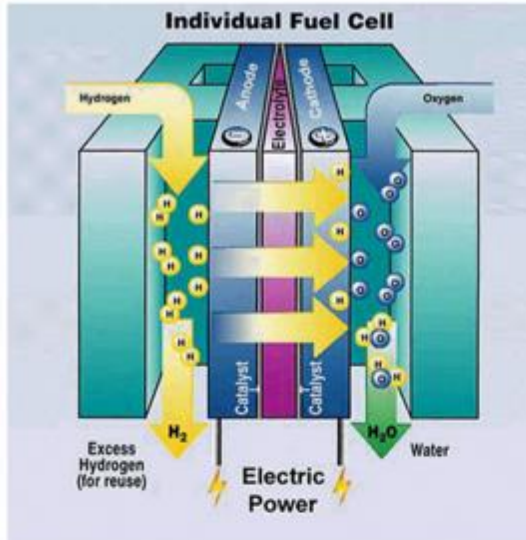
Jonathan Potter
GE Industrial Solutions

Jason Harmon
GE Industrial Solutions

Joe Mantese
UTRC

Electrical Contacts

Non-precious metal catalysts



Inteconnects for Fuel Cells

Interconnects for Solar Cells

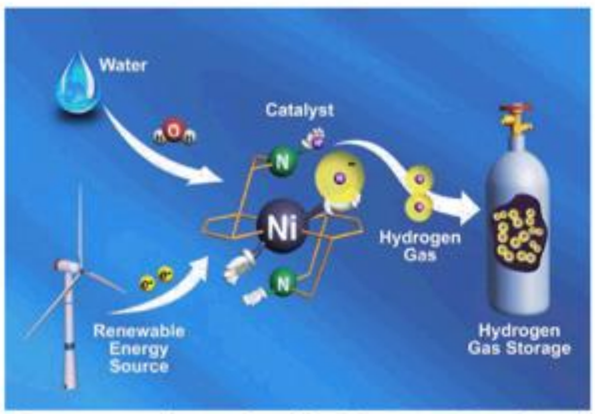
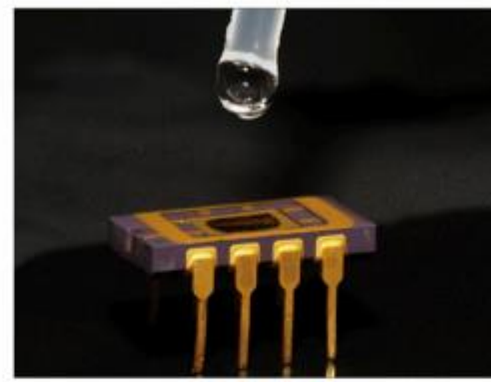


Photo-catalysts for Hydrogen Production

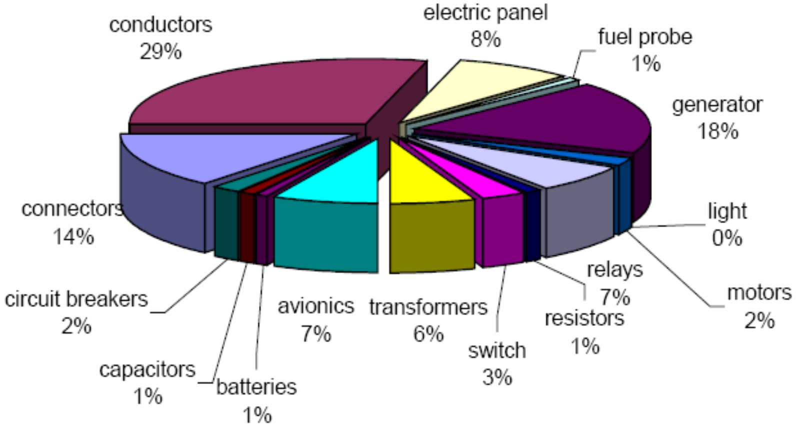
Materials for Electrical Contacts



Selective Surfaces for Chemical Sensing

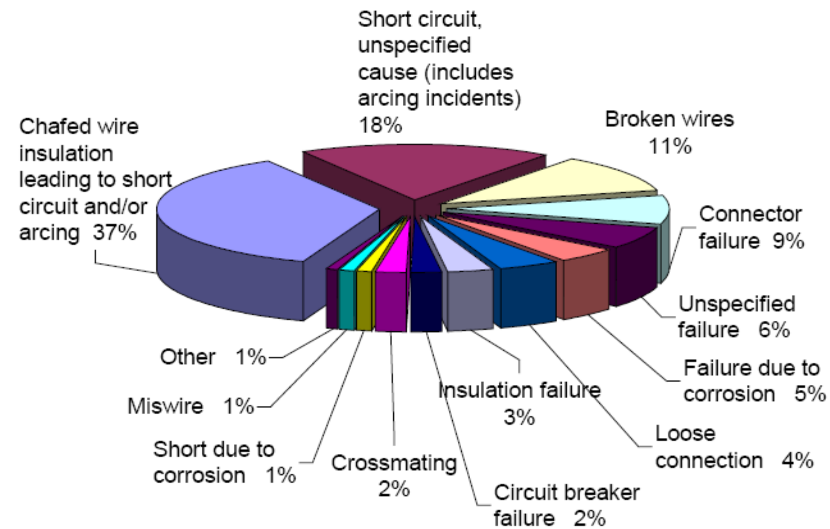
Metallic interfaces are the principal sources of failure in signal and energy sub-systems

Contact Failure



43% of all Electrical Failures Due to Contacts

Based on U.S. Air Force Safety Center Electronics Failure Data for 1989-1999



6% of Contact Failures Due to Corrosion Alone

(Based on U.S. Navy Safety Center Hazardous Incident Data for 1980-1999.)

Failed contacts are the largest source of electrical failures…

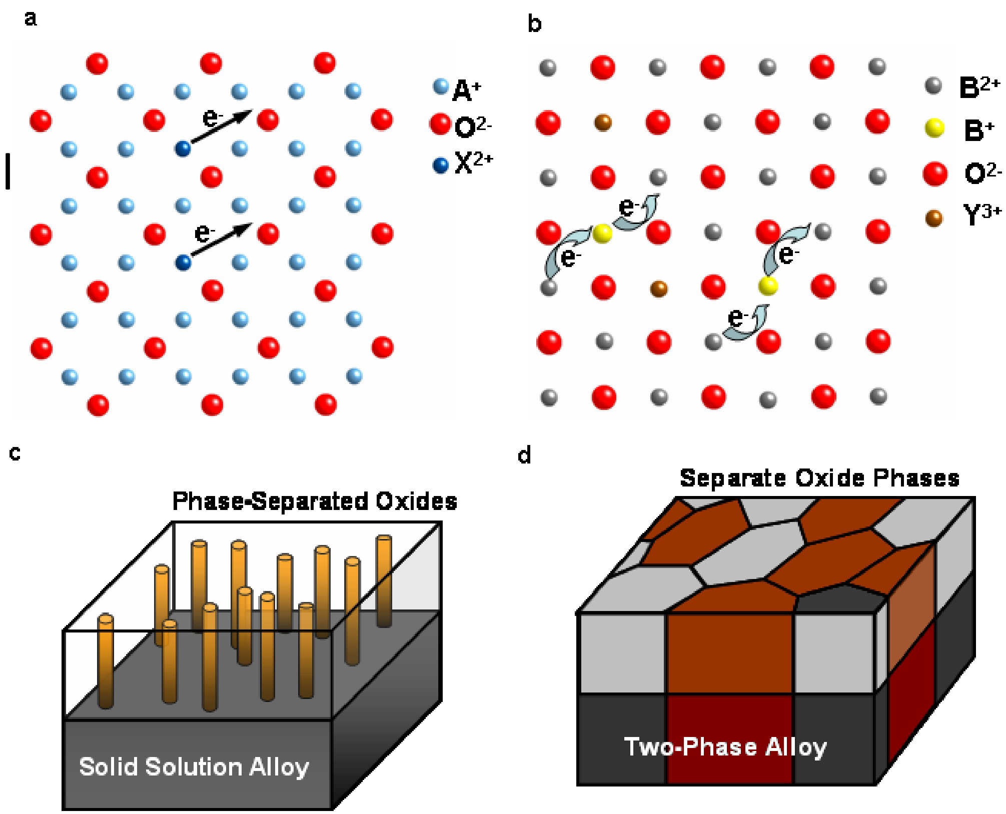
Solutions – Pros and Cons…

Alternatives and augmentations to base metal contacts…

Approach	Advantages	Disadvantages
Solder or Welded Contacts	Metallurgical junction	Field repairs difficult
Tin Coated Base Alloys (e.g. Brass)	Pliable surface that enables metal plowing	Fretting, fritting, whisker, and corrosion failures
Compression Contacts	High contact forces for low resistance contacts	Oxidation and corrosion at interfaces, high engagement forces
Encapsulates and Hermetic Seals	Large diffusion distances for oxidation and corrosion	Large connector footprint, limited field repair
Precious Metals (e.g. Au, Pt, Pd)	Good electrical contact, high corrosion resistance	Prohibitively high costs even for military applications

Materials Development:
Self-Healing Base Metals

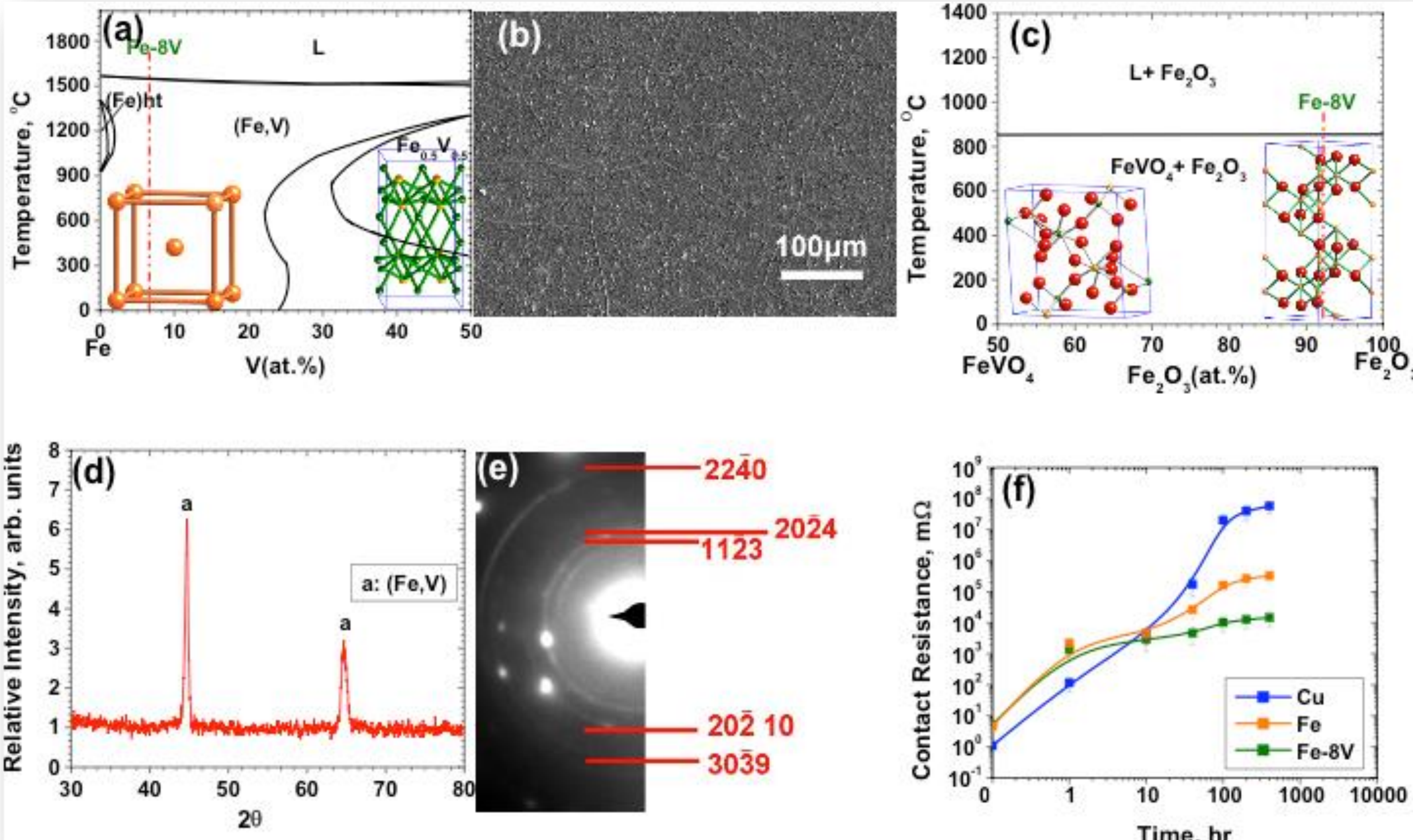
Forming **conducting oxide scales: a) Doping** with cations, **b)** Inducing a **mixed valence state** in the base metal cations (electron/polaron hopping), **c)** Formation of a **mixed oxide scale** wherein oxide phase separation gives percolative conducting pathways through the insulating base metal oxide, **d)** Forming a **two-phase base metal alloy** where the second phase forms a inherently conductive native scale.



The Midas Touch: Turning Base Metals into "Gold"
by Developing Alloys that Form Naturally Conductive Oxides

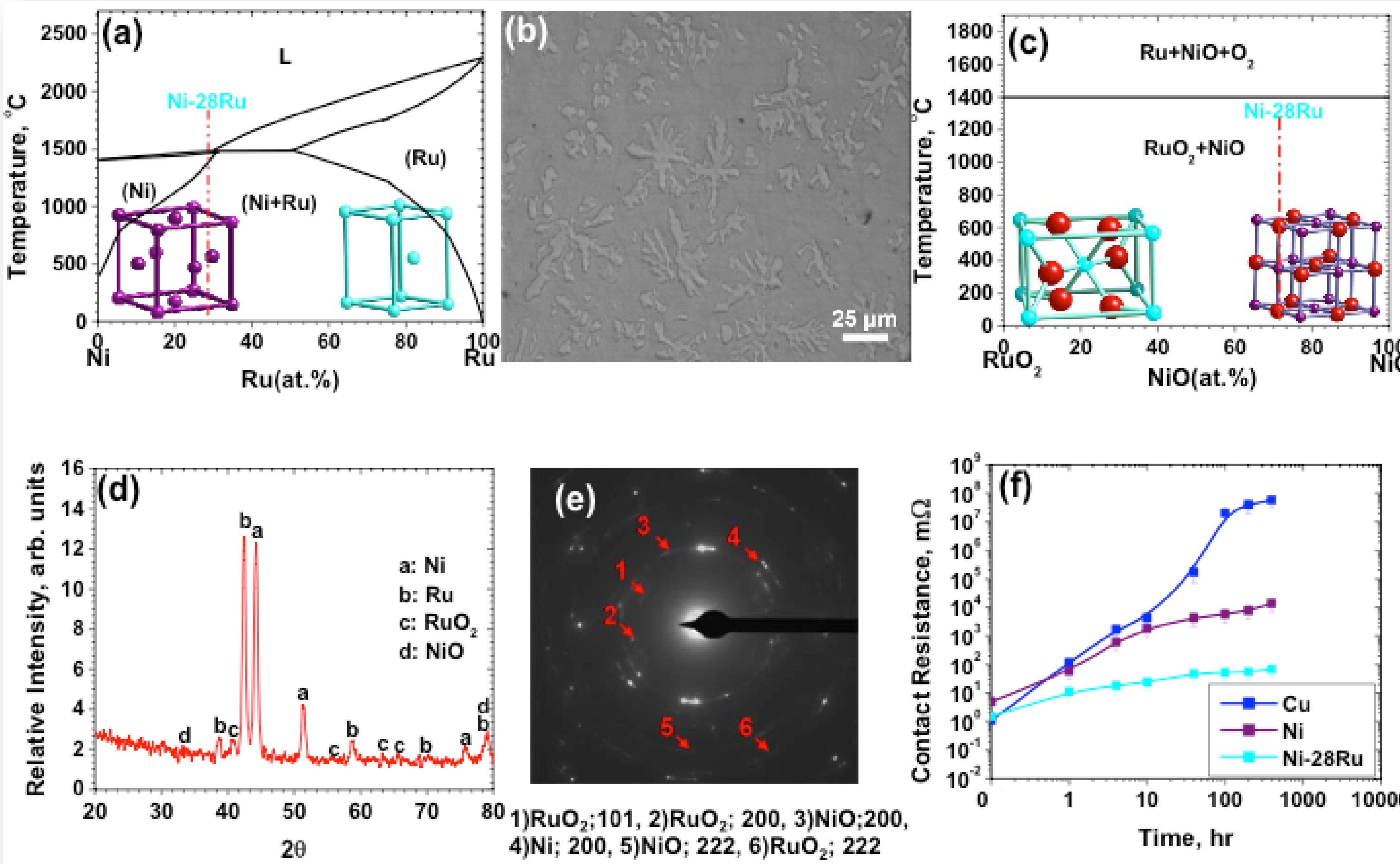
M. Aindow, S. P. Alpay, Y. Liu, J. V. Mantese and B. S. Senturk, "Base Metal Alloys with Self-Healing Native Conductive Oxides for Electrical Contact Materials," Appl. Phys. Lett. **97**, 152103 (2010)

Alloy Development: Fe-V



Fe-8V shows a $>10^3$X improvement in FOM over Cu

Alloy Development: Ni-Ru



Ni-28Ru shows a >10^5X improvement in FOM over Cu

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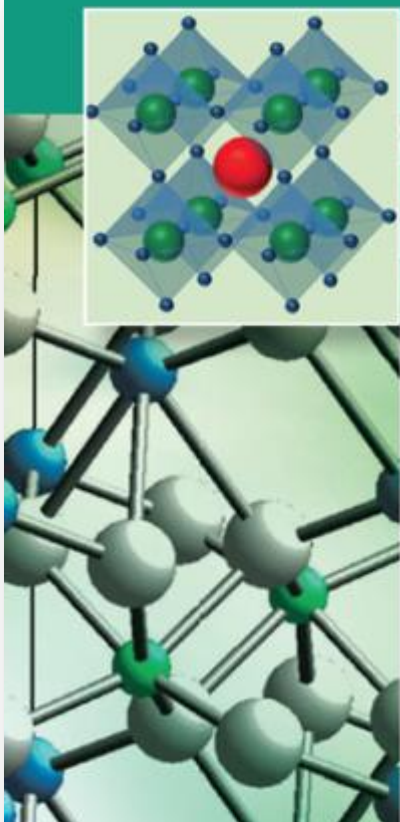
Waste Heat Recovery through Pyroelectric Energy Conversion

U.S.ARMY

United Technologies Research Center

A Good Overview…



MRS Bulletin

Next-generation electrocaloric and pyroelectric materials for solid-state electrothermal energy interconversion

S. Pamir Alpay, Joseph Mantese, Susan Trolier-McKinstry, Qiming Zhang, and Roger W. Whatmore

MRS BULLETIN • VOLUME 39 • DECEMBER 2014 • www.mrs.org/bulletin 1099

People…

George Rossetti, Jr.
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Serge Nakhmanson
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Gursel Akcay
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Sabanci University

Claire Weiss Brennan
ARL, UTC Aerospace

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UIUC, Rutgers

Hamidreza Khassaf
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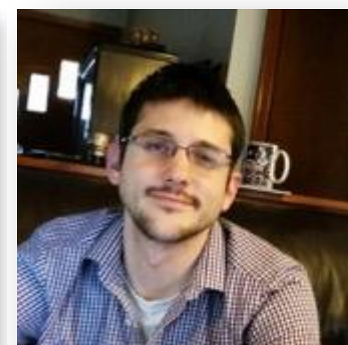
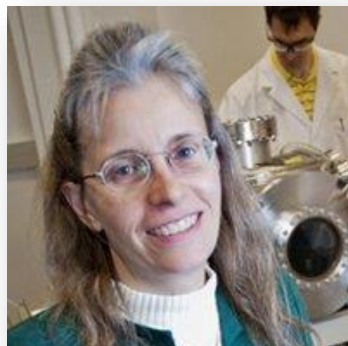


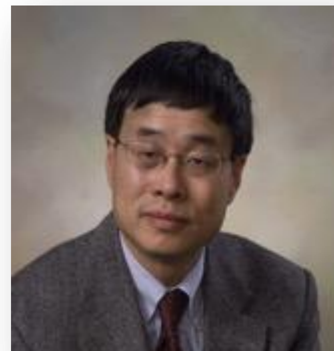
John Mangeri
UConn

People…

Joe Mantese
UTRC



Susan Trolier-McKinstry
Penn State



Qiming Zhang
Penn State

Roger W. Whatmore
Tyndall NRI, Imperial College, UK

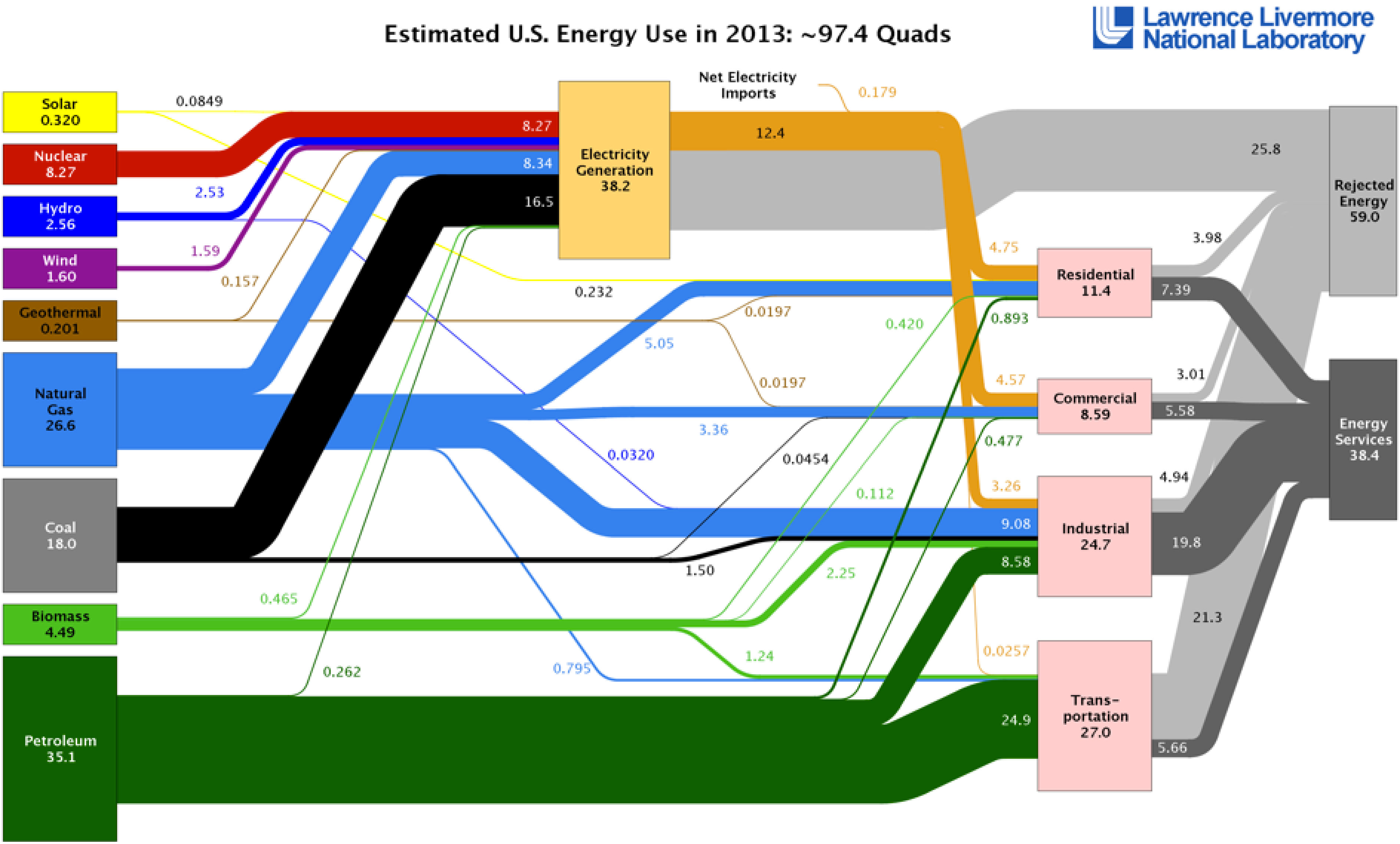
United Technologies Research Center

PENNSTATE 1855

Tyndall National Institute

SCIENTIA

Great Potential for Waste Energy Recovery



Source: LLNL 2014. Data is based on DOE/EIA-0035(2014-03), March, 2014. If this information or a reproduction of it is used, credit must be given to the Lawrence Livermore National Laboratory and the Department of Energy, under whose auspices the work was performed. Distributed electricity represents only retail electricity sales and does not include self-generation. EIA reports consumption of renewable resources (i.e., hydro, wind, geothermal and solar) for electricity in BTU-equivalent values by assuming a typical fossil fuel plant "heat rate." The efficiency of electricity production is calculated as the total retail electricity delivered divided by the primary energy input into electricity generation. End use efficiency is estimated as 65% for the residential and commercial sectors 80% for the industrial sector, and 21% for the transportation sector. Totals may not equal sum of components due to independent rounding. LLNL-MI-410527

Electrothermal Applications

Fire Detection

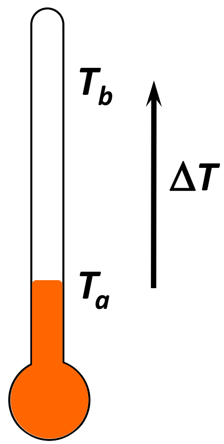
Solid State Cooling Devices

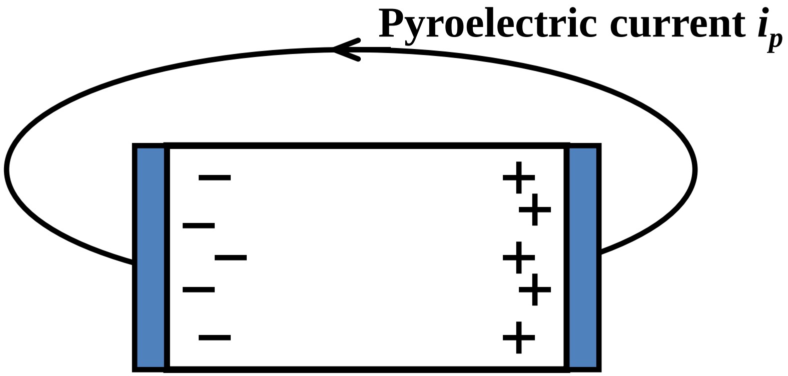
Thermal Imaging

Intruder Alarms

- Large electrocaloric and pyroelectric response
- Low loss
- Low leakage currents
- High breakdown voltage
- Low dielectric constant

Pyroelectric Coefficient

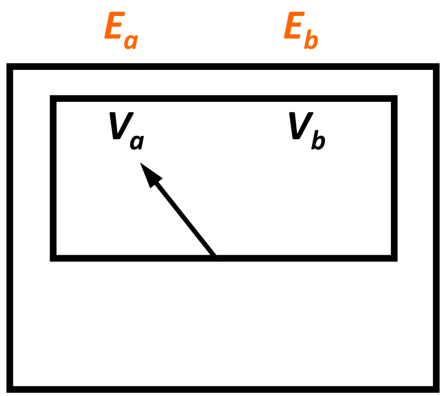


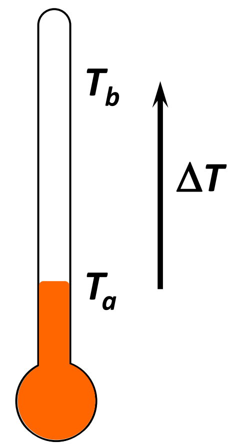


Pyroelectric (PE) Effect: the change in the charge density (polarization) in response to a change in temperature *T*.

$$p(T,E) = \frac{dP}{dT} = \frac{dP_S}{dT} + \int_0^E \left(\frac{\partial \varepsilon}{\partial T}\right)_E dE$$

Electrocaloric (EC) Effect

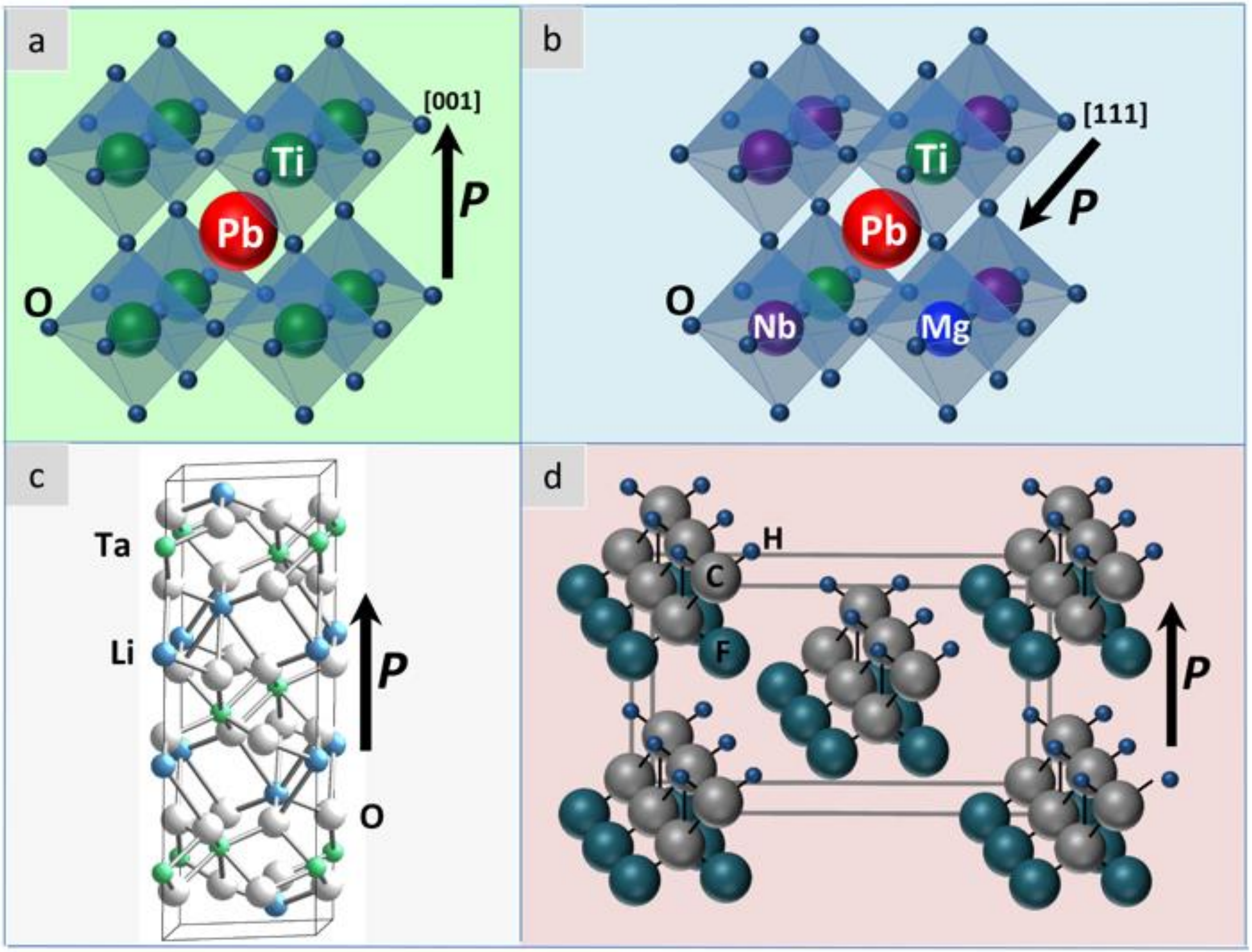




Electrocaloric (EC) Effect: change in temperature *T* under adiabatic conditions in response to an applied electric field *E*.

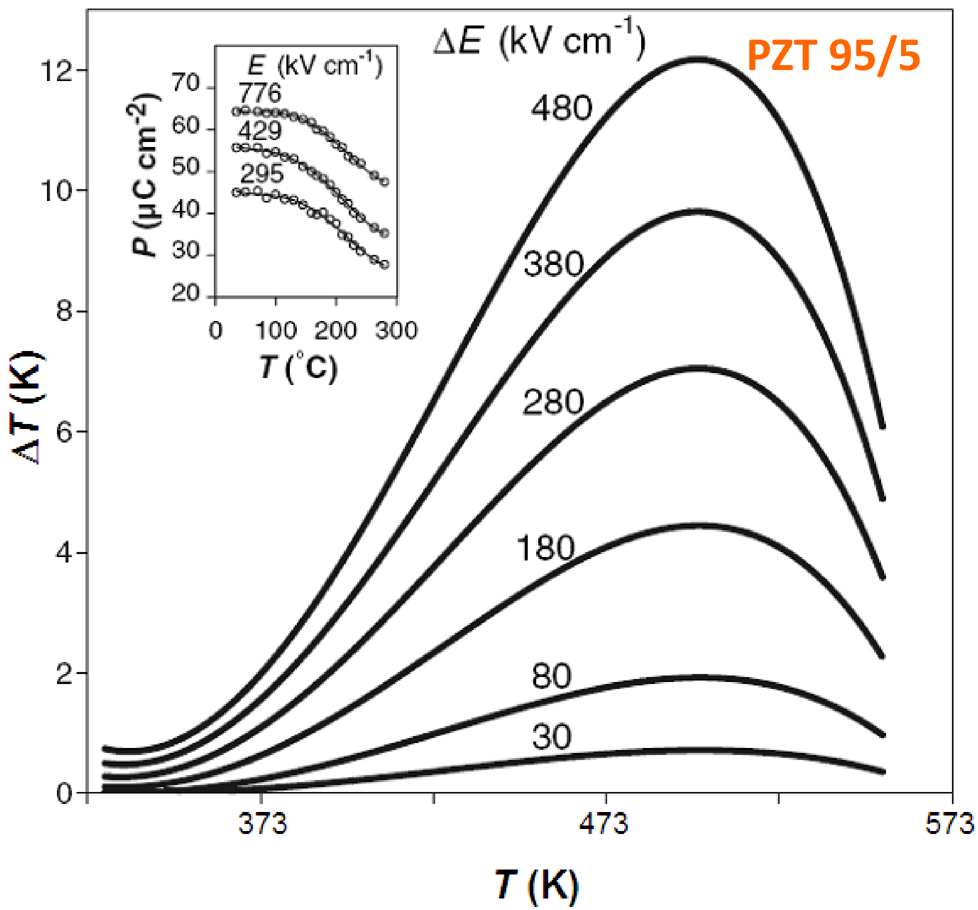
$$\Delta T(T,E,u) = -\int_{E_a}^{E_b} \frac{T}{C_E(T,E,u)} \left(\frac{\partial P(T,E,u)}{\partial T} \right)_E dE$$

Ferroelectric Materials



Crystal structures of four most common pyroelectric materials: **a.** $PbTiO_3$, **b.** $x\cdot Pb(Mg_{1/3}Nb_{2/3})O_3-(1-x)\cdot PbTiO_3$ (PMN-PT) in the rhombohedral phase, **c.** $LiTaO_3$, and **d.** polyvinylidene difluoride (PVDF), $-(C_2H_2F_2)_n-$.

Background: EC Effect in FE Thin Films



Experimental data for PZT 95/5 and $0.9\cdot PbMg_{1/3}Nb_{2/3}O_3$-$0.1\cdot PbTiO_3$ on Pt(111)/Ti/SiO_2/Si show that there is a **large EC response** in FE thin films.

FE films have higher breakdown electric fields. Thus, higher electric fields (~500 kV/cm or more) can be applied and temperature changes (ΔT) ~10 K can be realized.

Mischenko *et al*., Science **311**, 1270 (2006);
Mischenko *et al*., Appl. Phys. Lett. **89**, 242912 (2006).

Q. M. Zhang et al. demonstrated **large EC effects in PVDF-based polymeric systems.**

Neese *et al*., Science, **321**, 821 (2008).

Background: Since then…

Table I. Properties of several pyroelectric materials when used for thermal energy harvesting in either a resistive (linear) or the Ericsson cycle.[a]

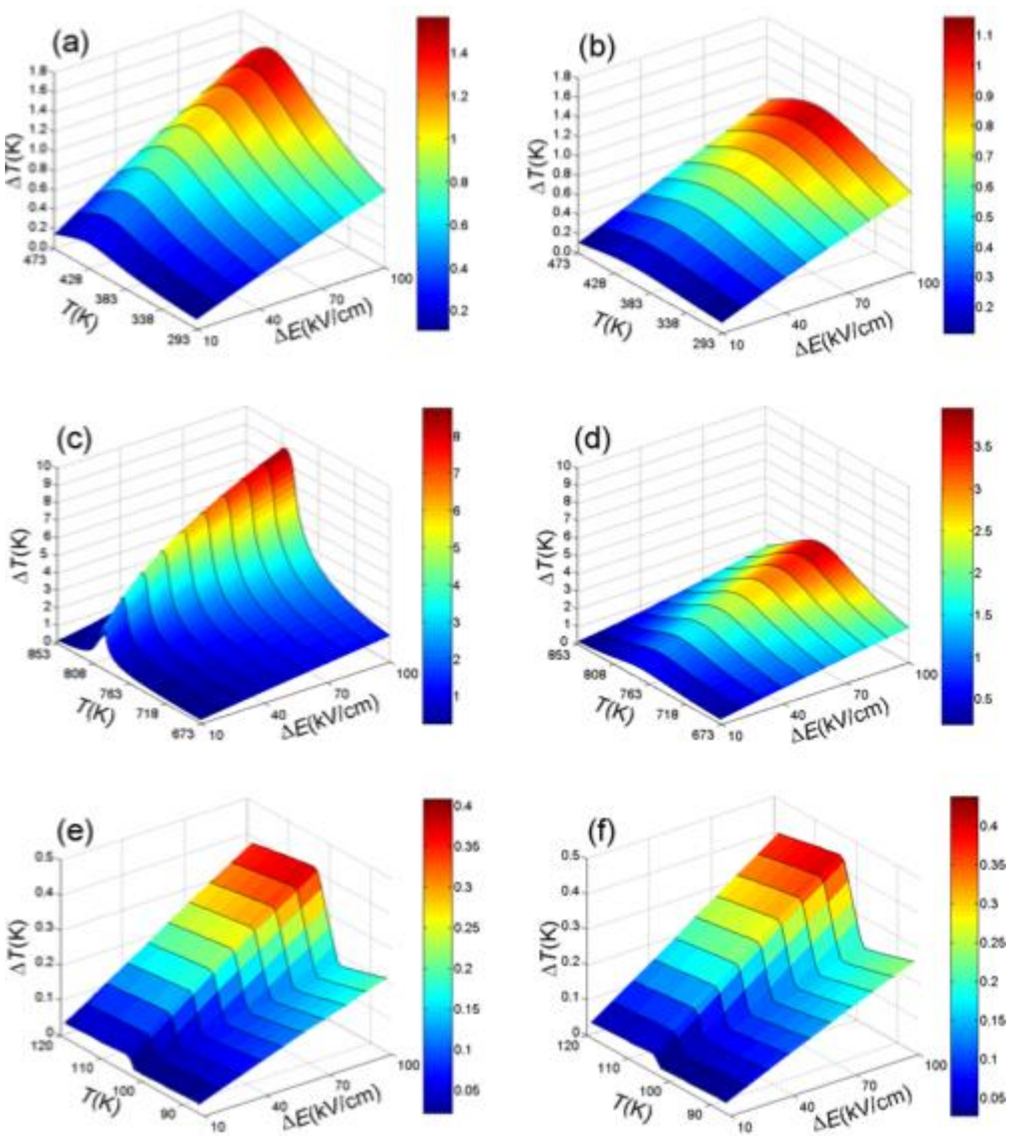
Linear Materials Employed in a Resistive Cycle									
Material[b]	Type[c]	p	ε	c'	T	W_{cycle}[a]	η_{Carnot}	η_{Res}/η_{Carnot}	Ref.
		$\mu Cm^{-2}K^{-1}$		$MJm^{-3}K^{-1}$	°C	kJm^{-3}			
$LiTaO_3$	X	230	54	3.2	100	8.7	2.6%	0.81%	8,24
0.72 PMN-0.28 PT	X (111)	1071	660	2.5	75	15.4	2.8%	1.85%	25
PZFNTU	C	380	290	2.5	100	4.4	2.6%	0.53%	26
PZT30/70-0.01Mn	F	300	380	2.5	100	2.1	2.6%	0.25%	27
PVDF	P	30	11	2.5	37	0.7	3.2%	0.09%	28
PVDF-TrFE 60/40	P	45	29	2.3	77	0.6	2.8%	0.08%	29
Non-Linear Materials Employed in Ericsson Cycle									
Material[b]	Type[c]	Q_{ECE}	E_1	c'	T	W_{cycle}[a]	η_{Carnot}	$\eta_{Eric}/\eta_{Carnot}$	Ref.
		$MJ\ m^{-3}$	$MV\ m^{-1}$	$MJ\ m^{-3}K^{-1}$	°C	$kJ\ m^{-3}$			
0.95PST-0.05PSS	C	4.2	2.5	2.5	–5	154	3.7%	14%	30
0.90PMN-0.1PT	C	1.4	3.5	2.5	30	45	3.2%	5%	23
0.75PMN-0.25PT	X (111)	3.2	2.5	2.5	75	91	2.8%	11%	31
0.75PMN-0.25PT	F	15	90	2.5	100	397	2.6%	38%	32
PZT95/05	F	31	78	2.5	220	631	2.0%	56%	33
PVDF-TrFE 55-45	P	38	200	2.3	37	1206	3.2%	62%	34,35
PVDF-TrFE-CFE	P	61	350	2.3	77	1718	2.8%	73%	35,36

[a]Computed parameters assume a temperature cycle of ±5°C about T.
[b]Material codes defined in text, with the following exceptions: PST = $PbSc_{1/2}Ta_{1/2}O_3$; PSS = $PbSc_{1/2}Sb_{1/2}O_3$; PZFNTU = $Pb(Zr_{0.58}Fe_{0.2}Nb_{0.2}Ti_{0.02})_{0.995}U_{0.005}O_3$; PZT$x$/1 – x = $PbZr_xTi_{1-x}O_3$, where 0.01 Mn means doped with 1% Mn.
[c]Types: C = ceramic; X = single crystal; F = thin oxide film; P = thin polymer film.

$BaTiO_3$, $PbTiO_3$, $SrTiO_3$ Films (Clamped)

Bulk

Clamped



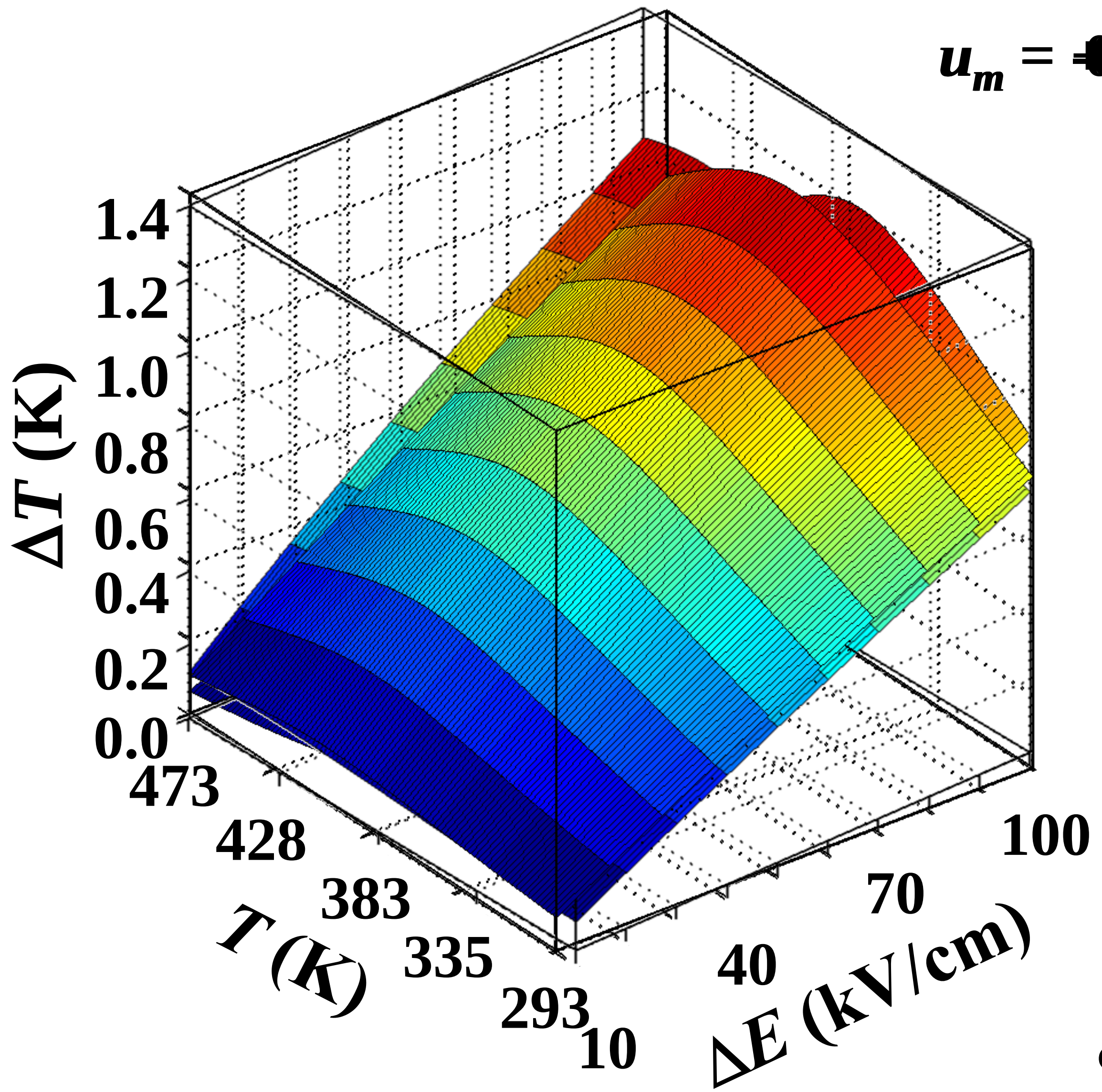
BTO

PTO

STO

J. Zhang, A. A. Heitmann,
S. P. Alpay, and G. A. Rossetti, Jr.,
J. Mater. Sci. **44**, 5263 (2009).

$BaTiO_3$ Thin Films – Misfit Strain

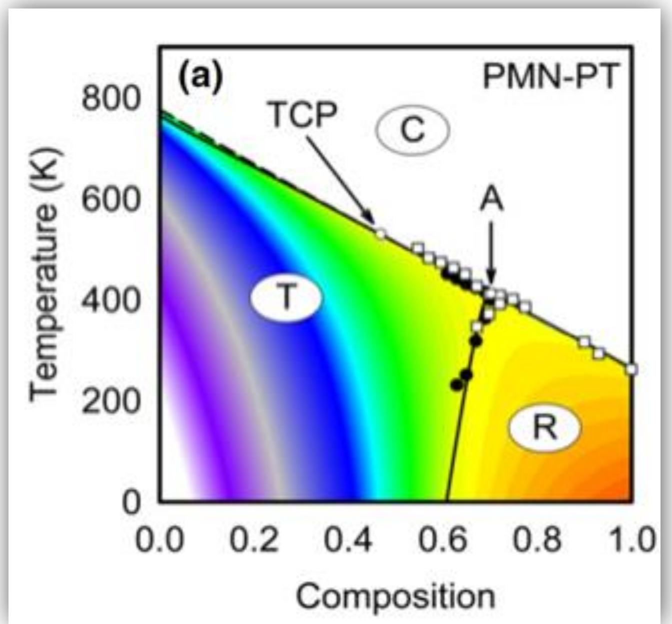


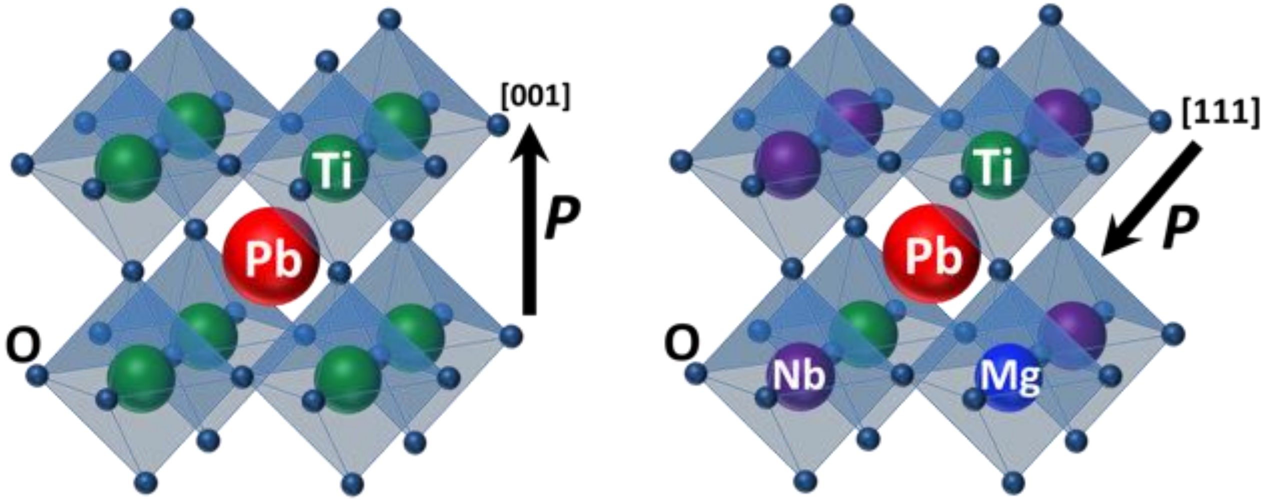
Compressive → Tensile

T_{max} ↓ and ΔT_{max} ↑

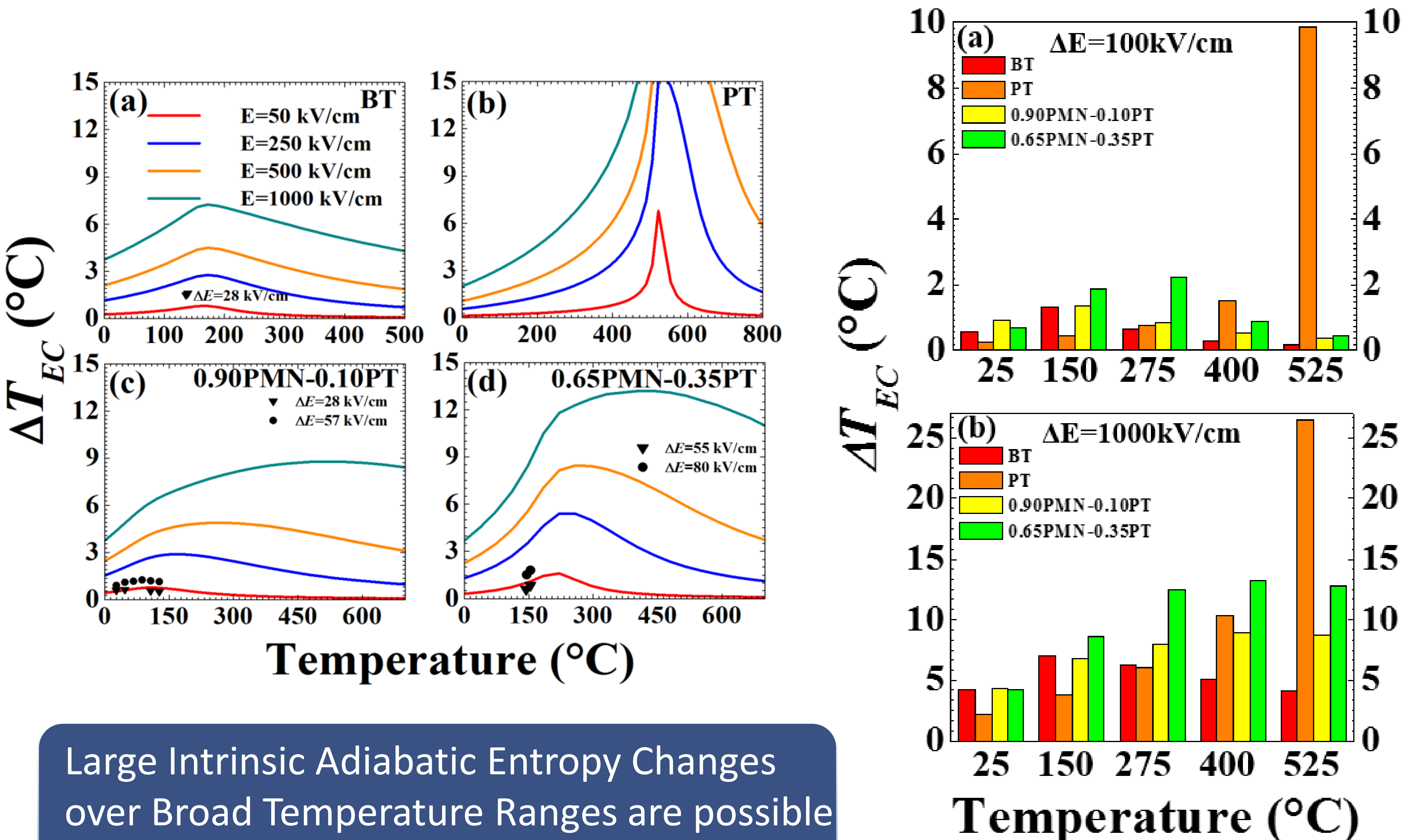
J. Zhang, A. A. Heitmann, S. P. Alpay, and G. A. Rossetti, Jr., J. Mater. Sci. **44**, 5263 (2009).

Relaxor – FE Solid Solutions?





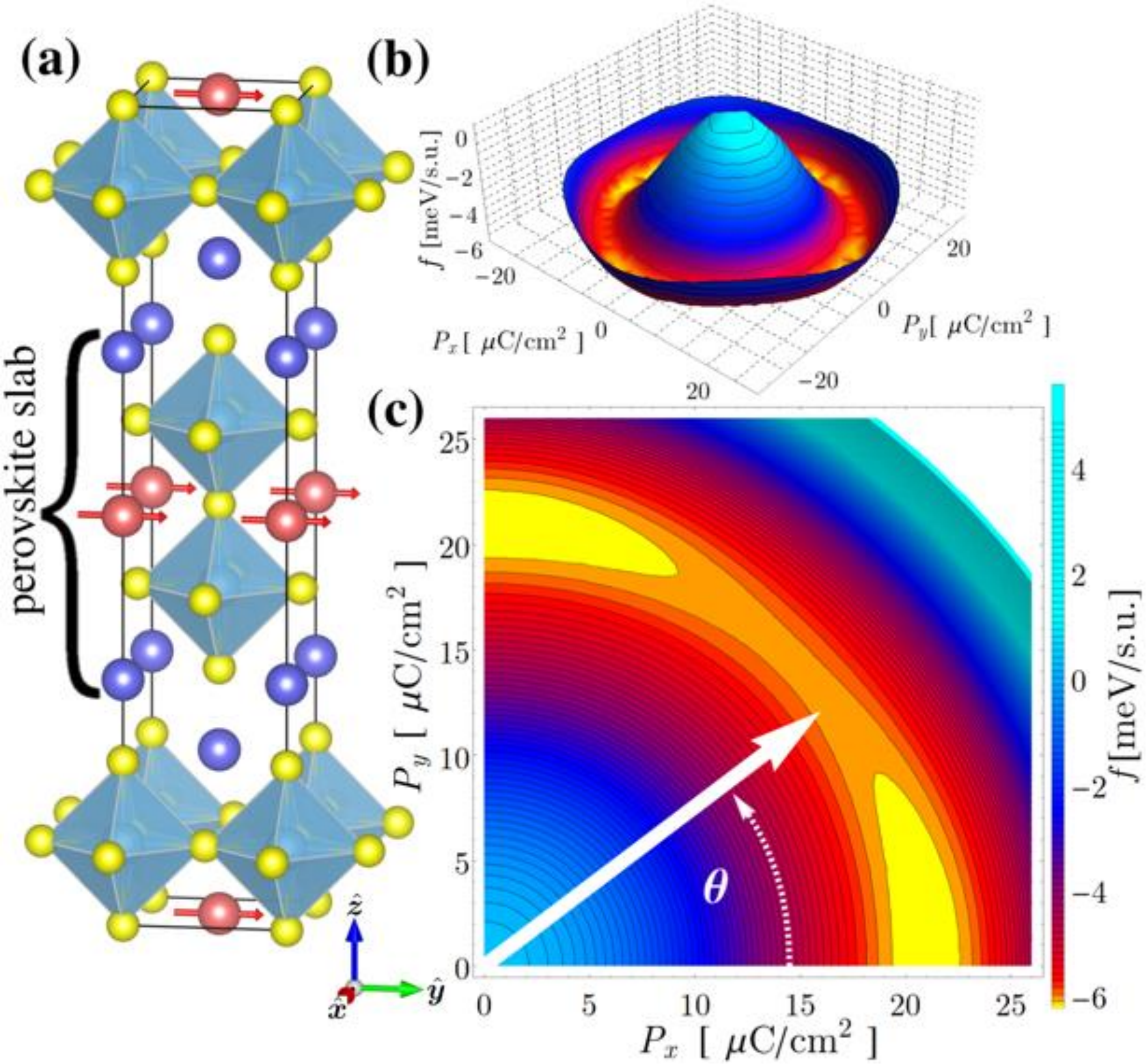
Relaxor – FE Solid Solutions: PMN – PT



Large Intrinsic Adiabatic Entropy Changes over Broad Temperature Ranges are possible

H. Khassaf, J. V. Mantese, N. Bassiri–Gharb, Z. Kutnjak, S. P. Alpay, "Ferroelectrics and Relaxor-Ferroelectric Solid Solutions with Large Intrinsic Electrocaloric Response over Broad Temperature Ranges," J. Mater. Chem. C. 4, 4763 (2016)

Can we do better?

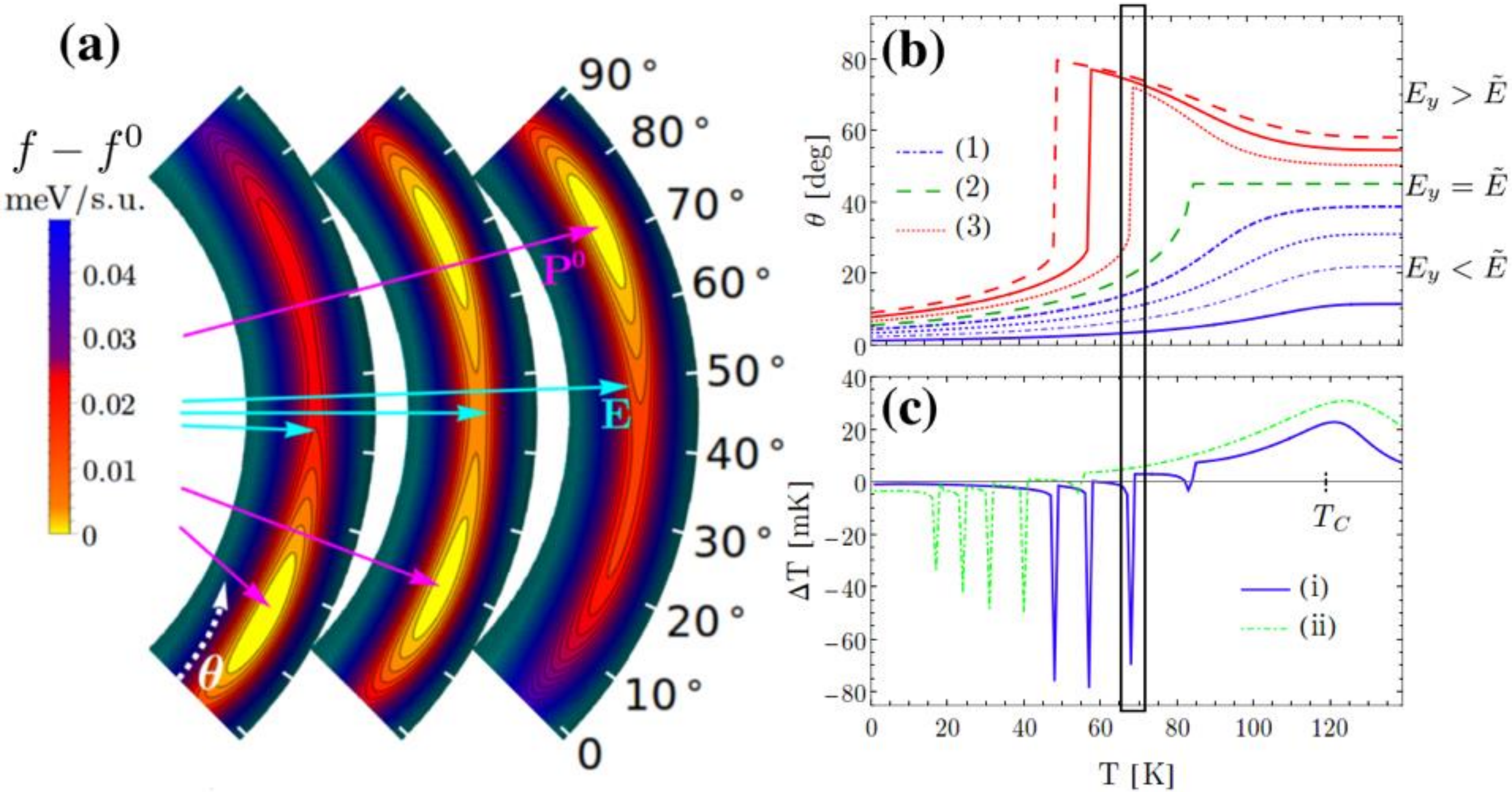


Can electrothermal properties of ferroelectrics be enhanced by designing artificial multilayers?

Crystal structure and free energy landscape of $PbSr_2Ti_2O_7$ and Goldstone-like energy surface

J. Mangeri, K. C. Pitike, S. P. Alpay, and S. M. Nakhmanson, "Amplitudon and Phason Modes of Electrocaloric Energy Interconversion," npj Computational Materials 2, 16020 (2016).

Additional, *Independent* Entropy Channels…



J. Mangeri, K. C. Pitike, S. P. Alpay, and S. M. Nakhmanson, "Amplitudon and Phason Modes of Electrocaloric Energy Interconversion," *npj Computational Materials* 2, 16020 (2016).

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UCONN | ADDITIVE MANUFACTURING INNOVATION CENTER

Design of Custom Aerospace Alloys for Additive Manufacturing

PRATT & WHITNEY
DEPENDABLE ENGINES

UTC Aerospace Systems

UCONN

materials & ENGINEERING science

People…

Rainer Hebert
UConn

Venkat Vedula
UTAS

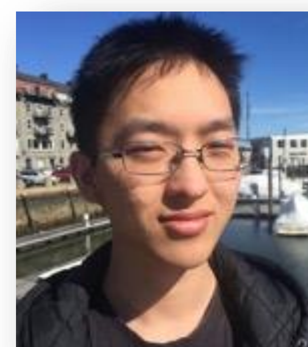
David Furrer
Pratt & Whitney

Jason Hancock
UConn

Sanjeev Nayak
UConn

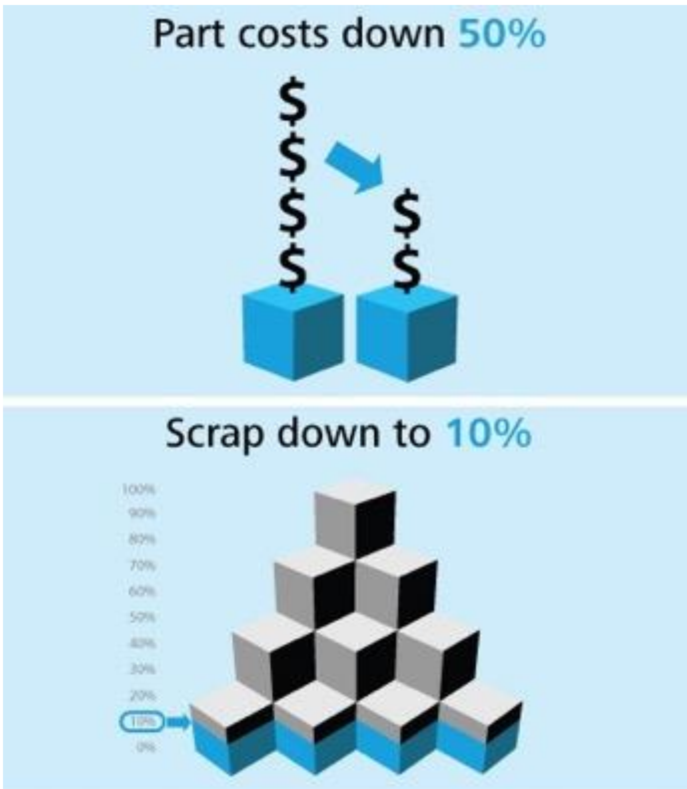
Sanjubala Sahoo
UConn

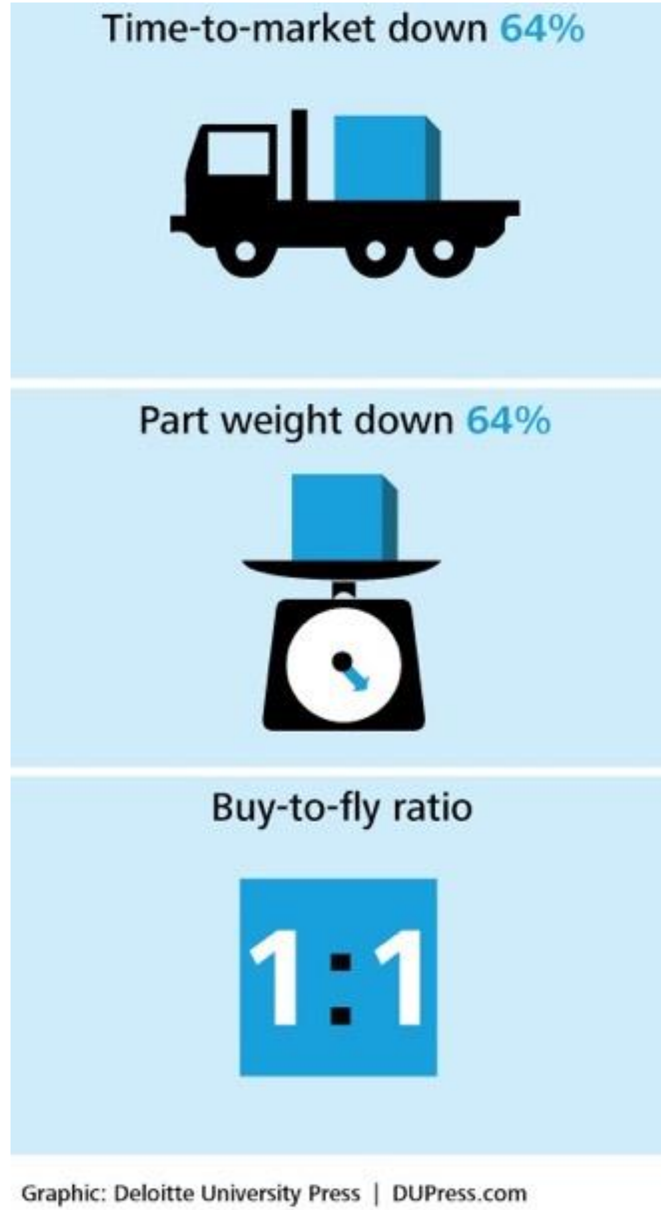
Tulsi Patel
UConn - KIMM



Cain Hung
UConn

Benefits of Additive Manufacturing



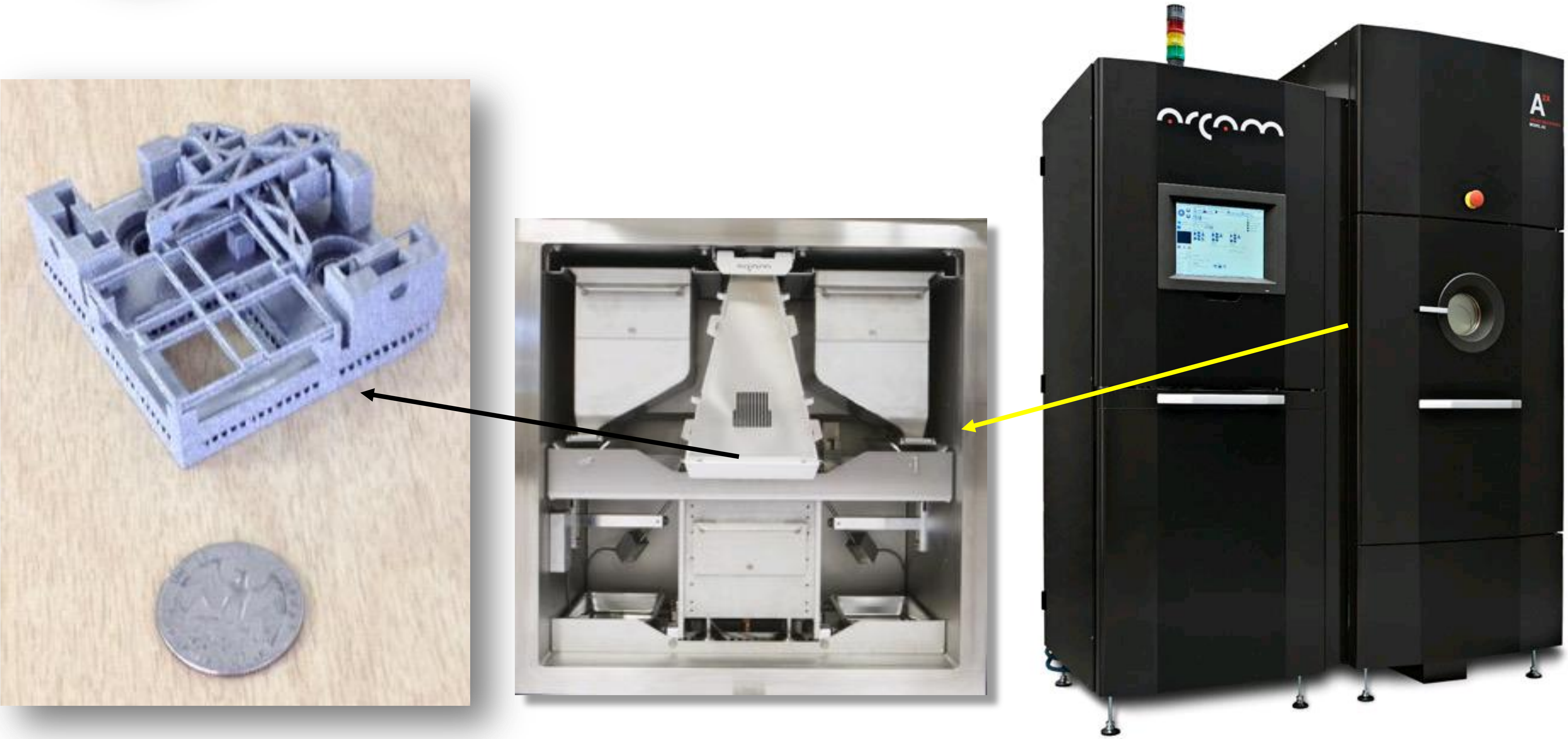


Key Industries Using AM

GE fuel nozzle: 19 individual parts combined into one

- Biomedical (personalized)
  - Dental crowns, implants
  - Joint replacements
- Printed electronics
  - RFID devices
- Aerospace
  - Fuel nozzles
  - Brackets
  - Turbine blades with complex cooling channels
- Tools/Molds
- Automotive

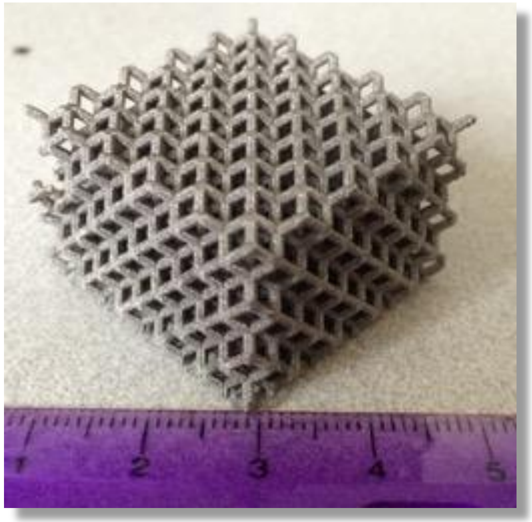
P&W Additive Manufacturing Innovation Center



Arcam A2X Electron beam melting technology

Build volume: 200 mm x 200 mm x 340 mm, Ti-6Al-4V, Inconel-718

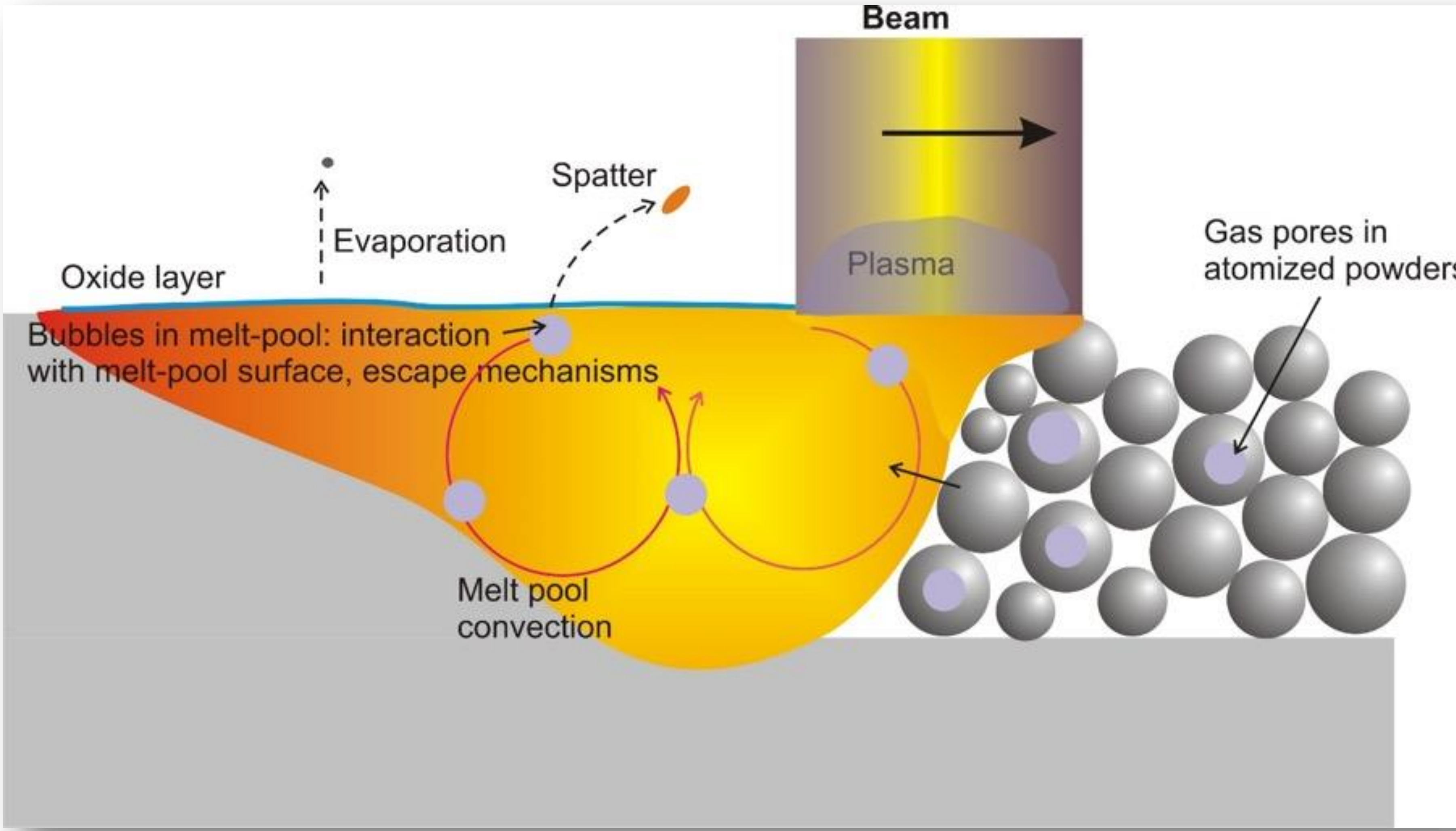
P&W Additive Manufacturing Innovation Center



3DSystems ProX-300, 500 W laser

Build Volume 250 mm x 250 mm x 300 mm, stainless steel, Al-alloys

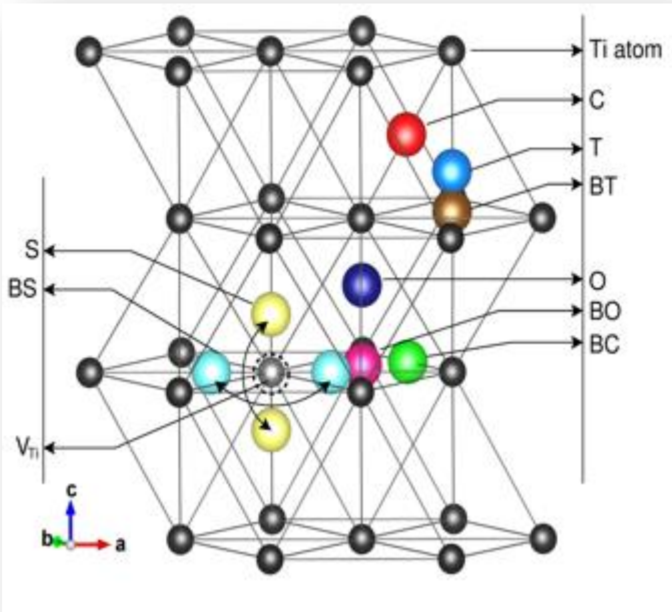
Additive Manufacturing of Metallic Alloys



… is an extremely complicated

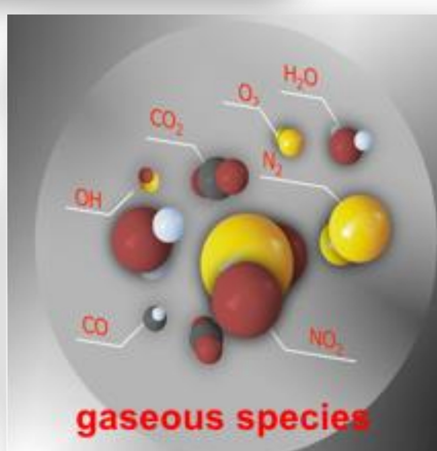
Modeling Impurity Effects in Additive Manufacturing

Defect chemistry of Ti



Surface chemistry of Ti

base metal



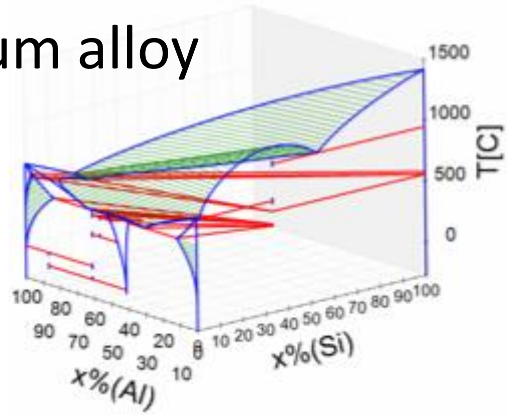
Impurities impact the surface tension/gradient and melting behavior, formation of voids

First-principles computations are used to probe chemical effects on interactions in Ti and select alloys

Surface tension of Ti-6Al-4V particles as a function of temperature, impurity content in atmosphere and the particle

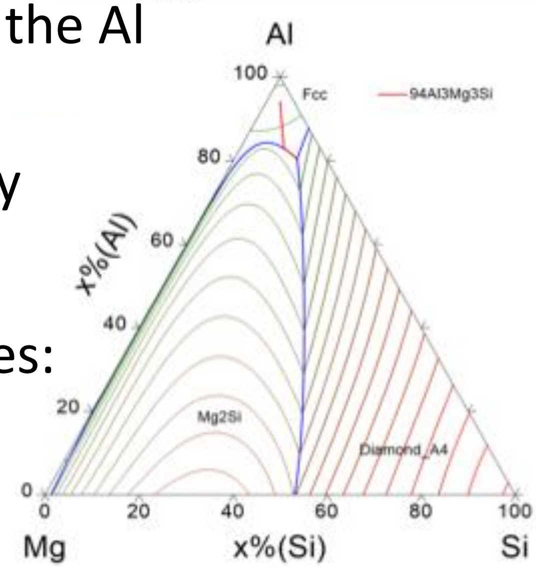
Searching for descriptors for strengthening Al alloys

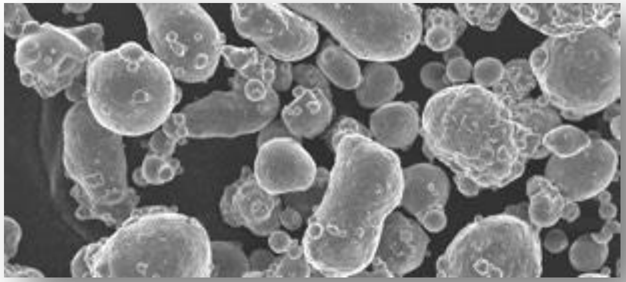
- Theory assisted design of high strength aluminum alloy
- Density functional electronic structure theory



Potential descriptors

- High strength: Large bulk modulus
- Must form coherent/semicoherent interface with the Al matrix: Lattice mismatch
- Immiscible in Al matrix: Solubility, interface energy
- Temperature stability: Ab initio thermodynamics
- Constructing large database of materials properties: Materials genomics



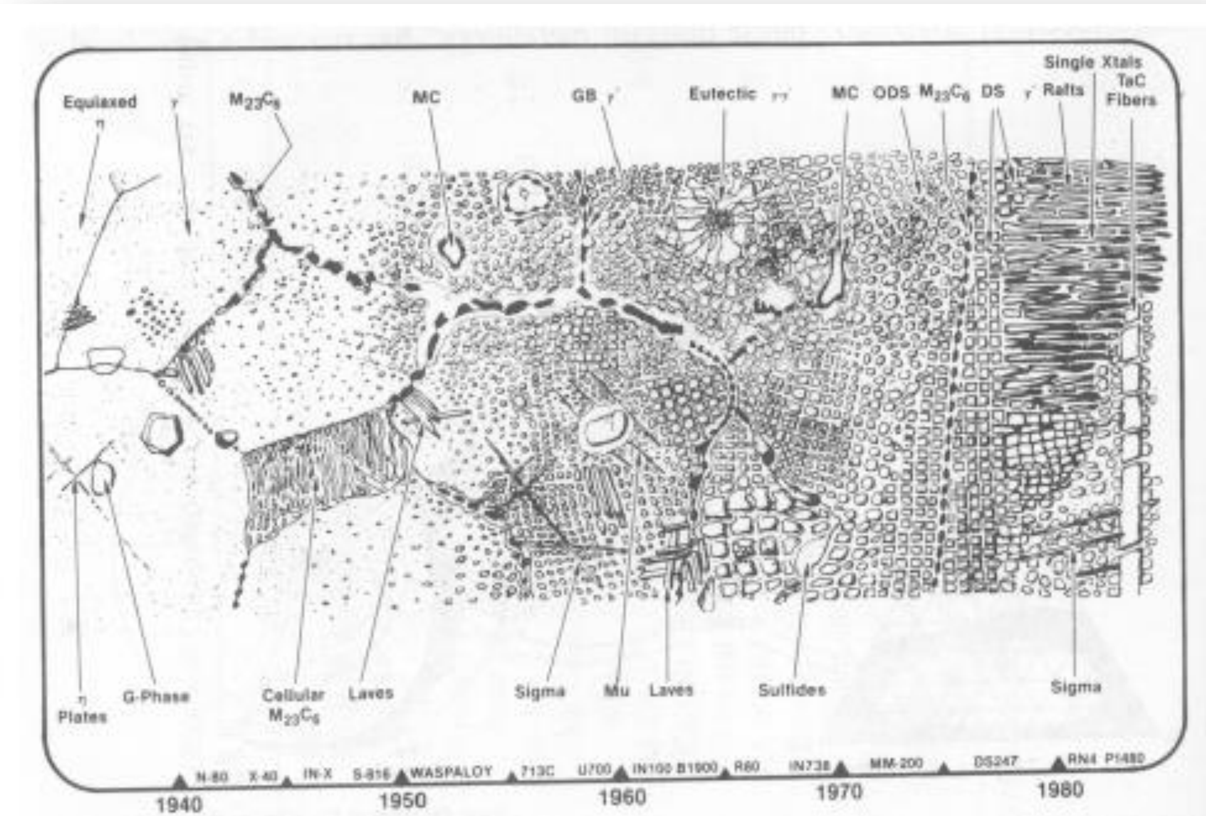


Al 6061 powder, average powder size 10 microns

Summary

Accelerating Materials Deployment and Manufacturing via Multi-Scale Modeling and Genomics

Superalloys – Inconel 718

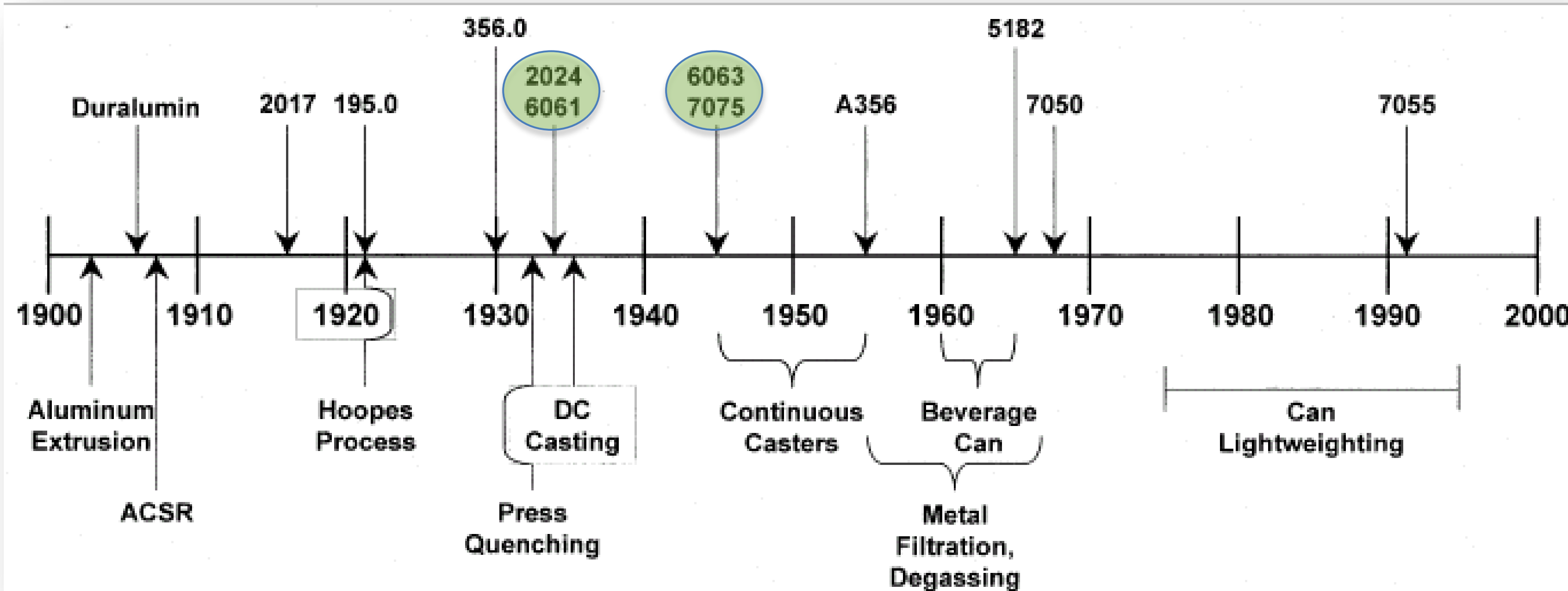


Wagner, H., & Hall, A. (1965). Physical Metallurgy of Alloy 718. DMIC Report 217.

Complicated chemistry, complicated microstructure … developed by: intuition, experimentation

… invented in 1940's by Wiggins Company (England) for steam power plants and then adopted for turbine engine applications by GE and others in the 1960's.

Aluminum Alloys

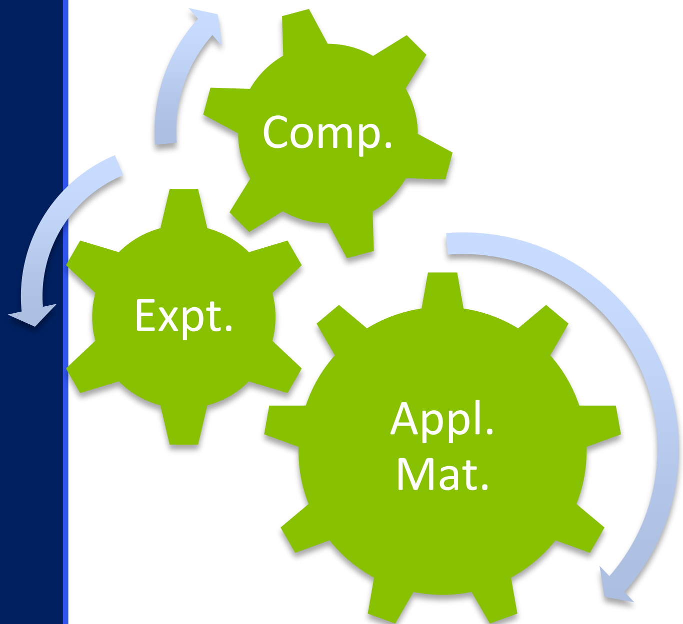


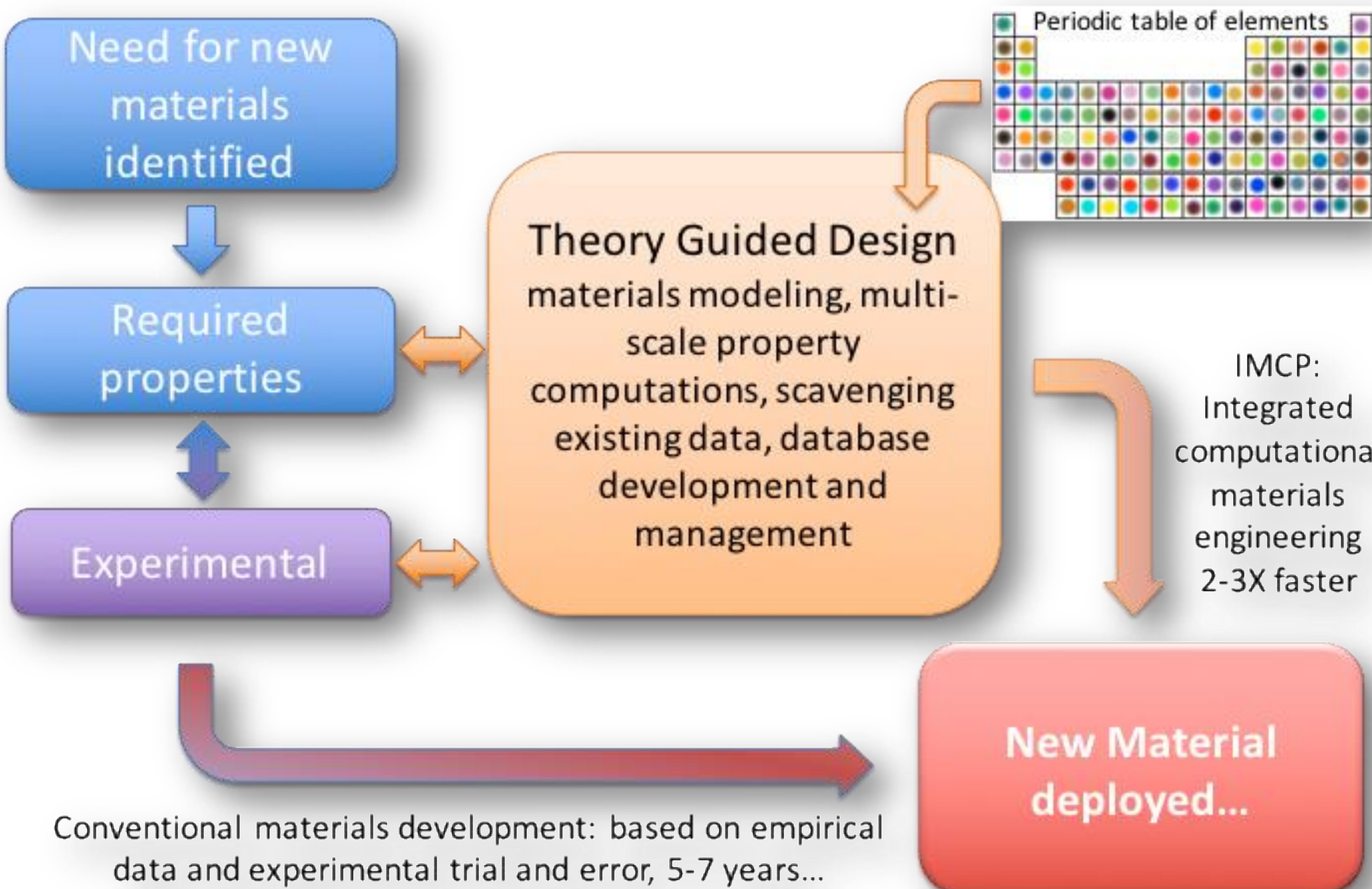
From: “Technology Innovation in Aluminum Products”, JOM, vol. 53(2), pp. 21-25, 2001

…existing alloys are decades old and are the materials of choice for low weight, high strength applications.

What is needed? Computational Guidance…

- Systematic materials discovery and design studies are needed to optimize properties
- Identification of descriptors…
- Materials Genomics – multi-scale screening of materials, *ab initio*, molecular dynamics, thermodynamics, phase field, continuum, data base development
- Provide materials properties to systems level analysis for CoP/FoM computations




Need for new materials identified
Required properties
Experimental
Periodic table of elements
Theory Guided Design
materials modeling, multi-scale property computations, scavenging existing data, database development and management
IMCP:
Integrated computational materials engineering
2-3X faster
New Material deployed...
Conventional materials development: based on empirical data and experimental trial and error, 5-7 years...