MODULE 1: INTRODUCTION

Materials Data Science

I. What is Materials Data Science

What is CMSE and ICME?

- Computational Materials Science and Engineering

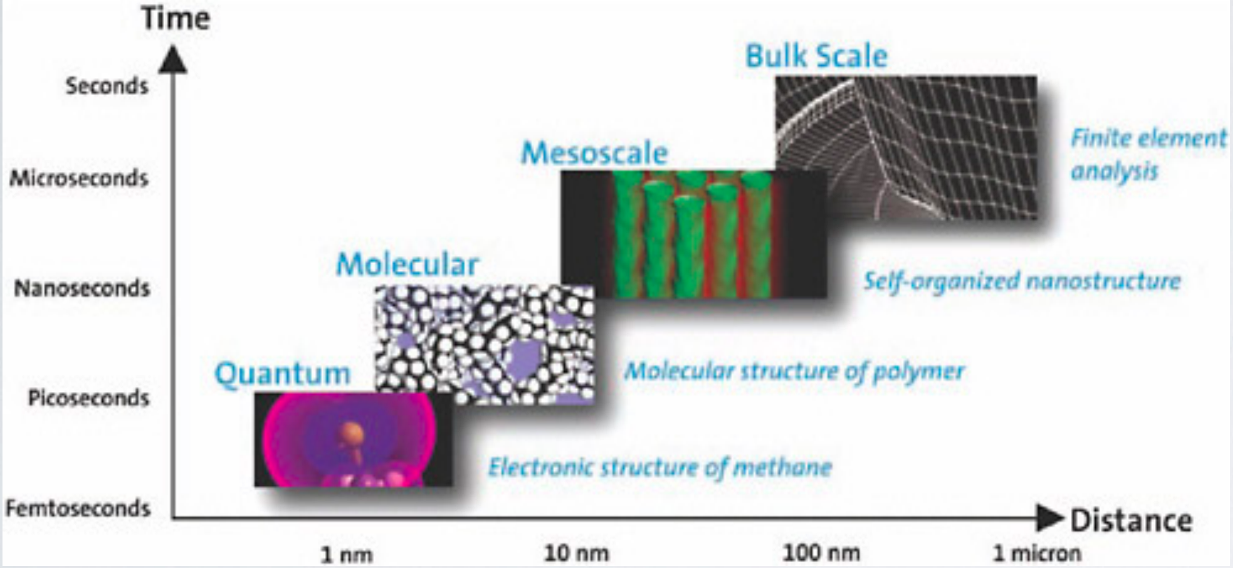
The application of computational tools to materials discovery, characterization, design, testing, and optimization.

- Integrated Computational Materials Engineering

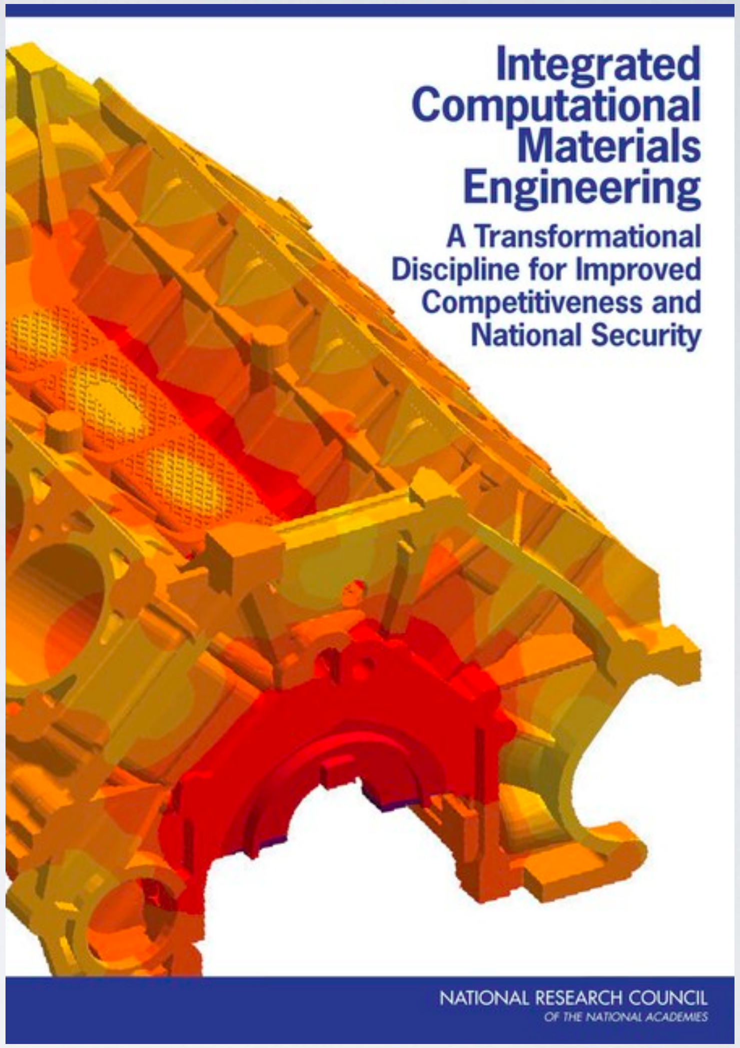
Integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing process simulation.

- NAE ICME Report (2008)

What is CMSE and ICME?



The Theory



Integrated Computational Materials Engineering

A Transformational Discipline for Improved Competitiveness and National Security

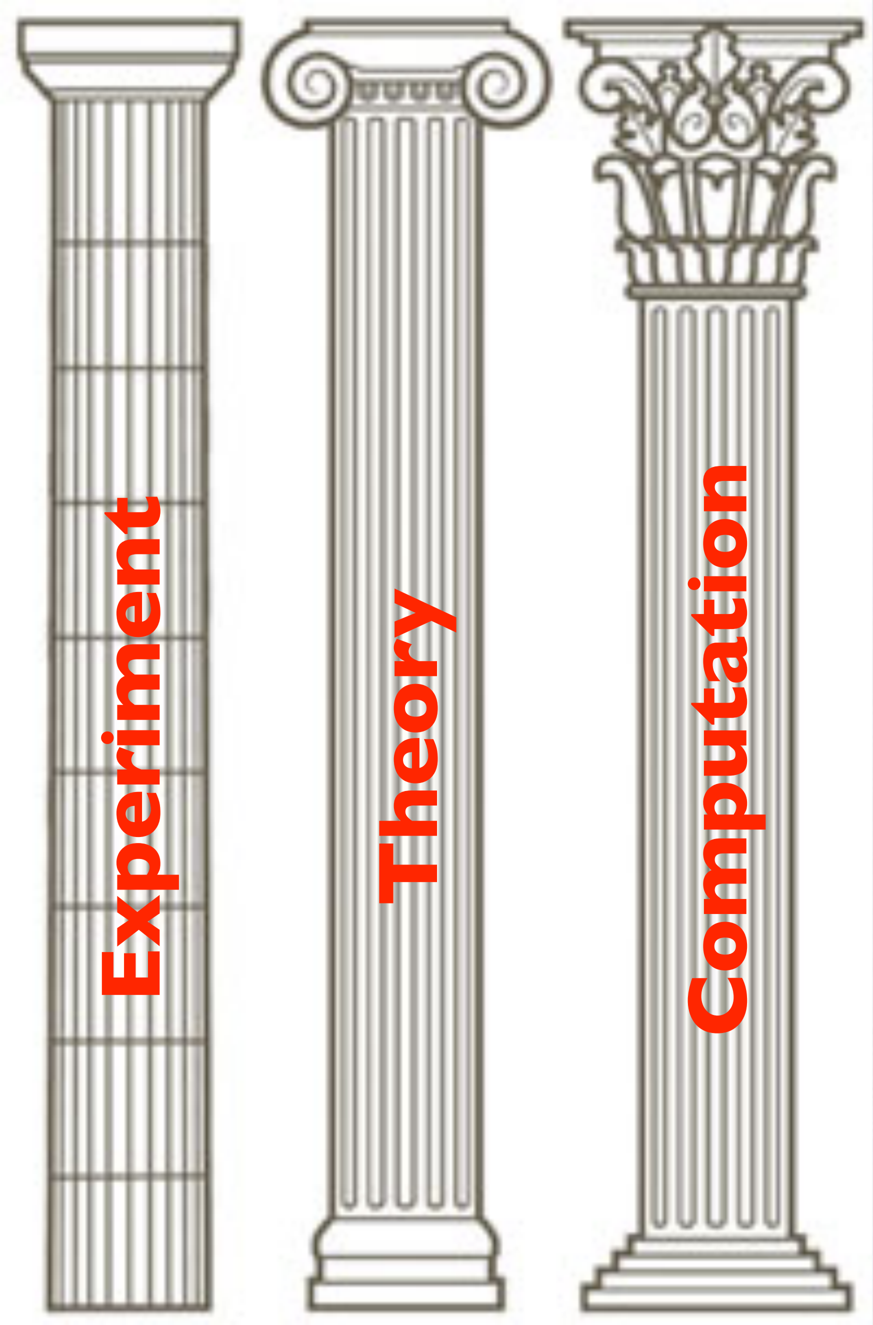
NATIONAL RESEARCH COUNCIL
OF THE NATIONAL ACADEMIES

The Will

The Way

Does it work?

- Materials are governed by (mostly known) physical laws
- We can probe materials behavior in three ways:



The third pillar

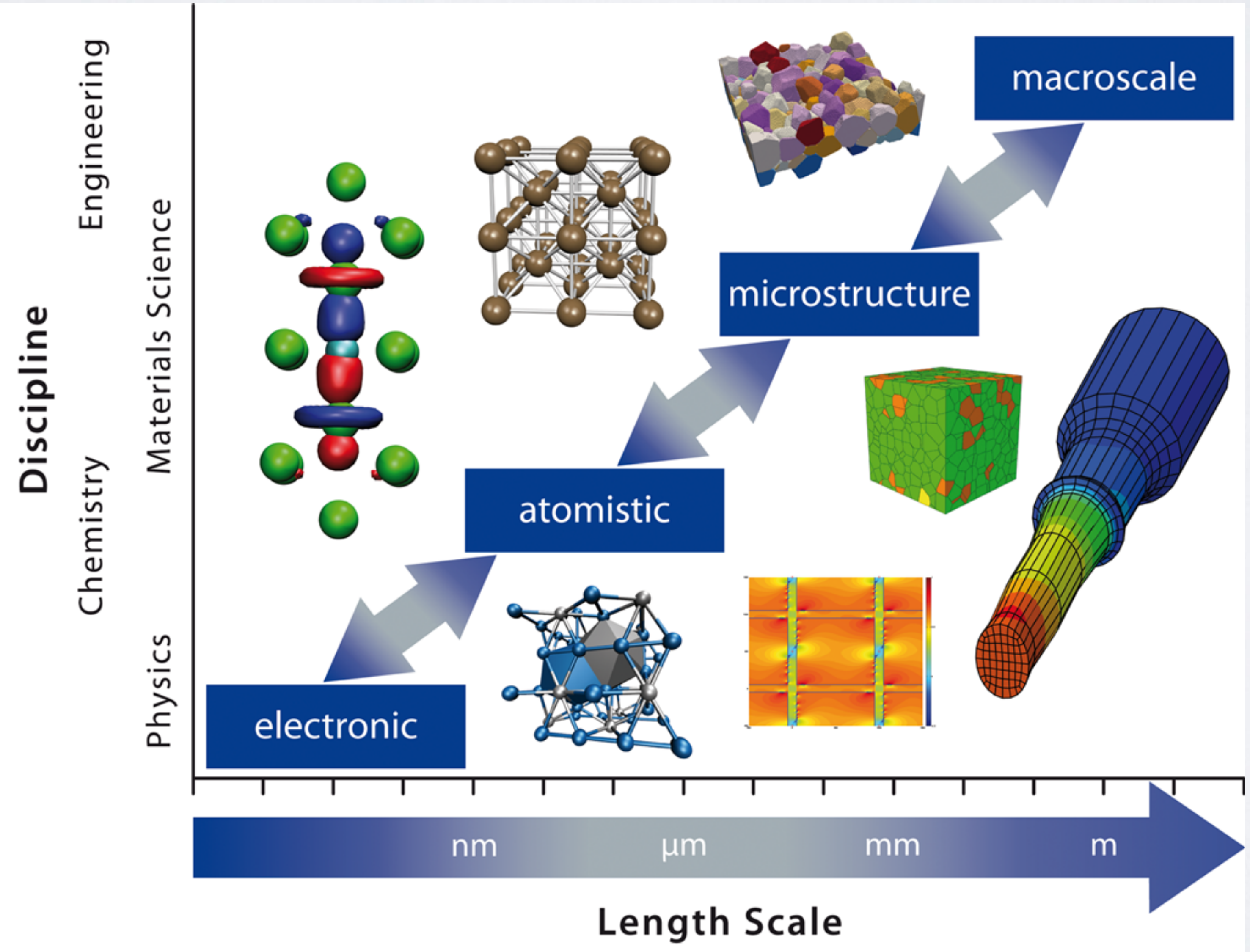
- Computation presents a third way to do science by performing ***in silico* experiments**

- Computer models of materials governed by physical laws allow us to answer similar questions as "real" experiments

properties behavior hypothesis testing "what if..."

MatSE is multiscale

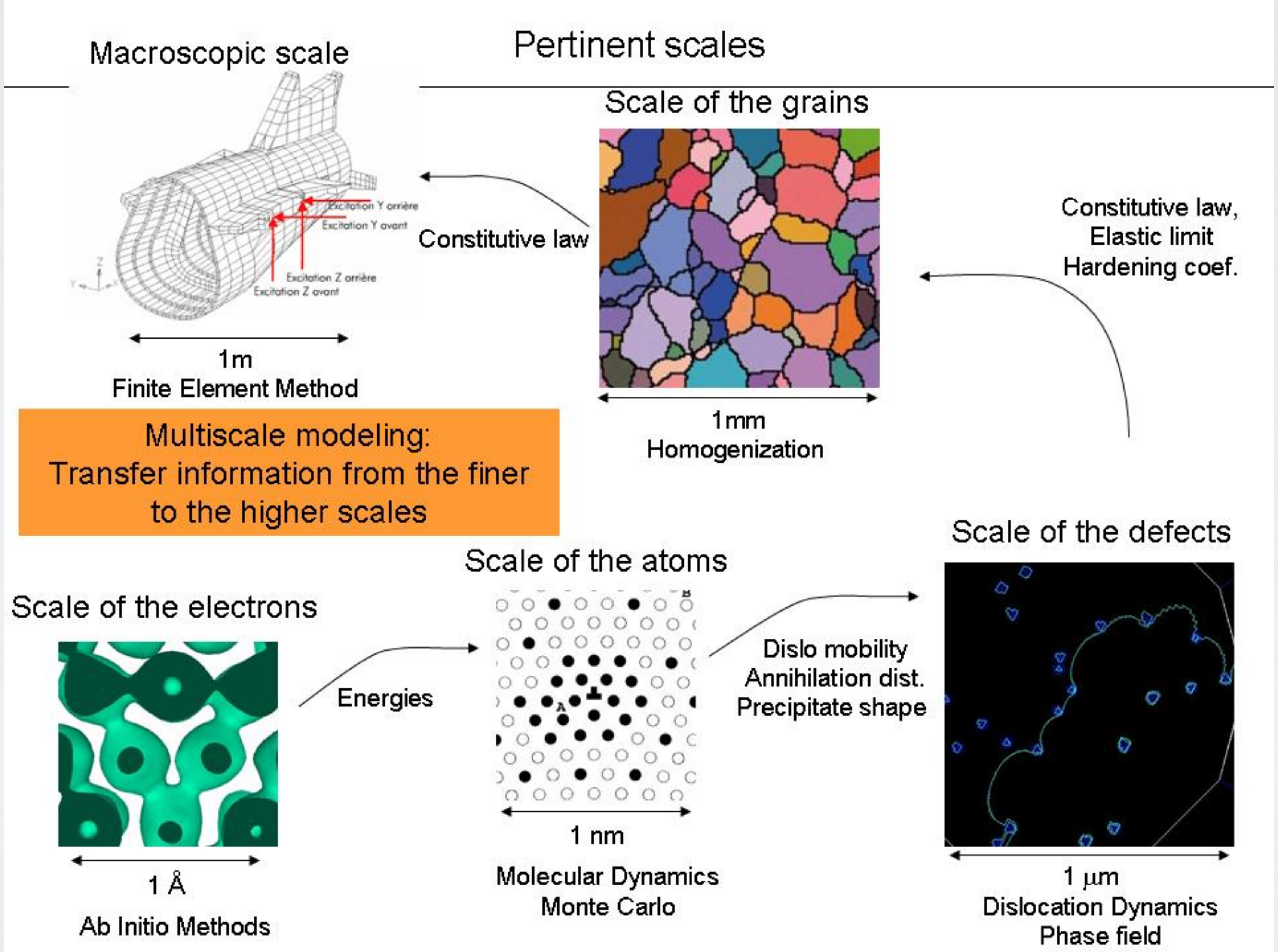
- Physics, chemistry, chemical engineering, mechanical engineering all have long-standing computational traditions
- The "action" in these disciplines tends to be confined to a single scale (smallest - quantum - or largest - continuum)



http://www.icams.de/content/research-at-icams/index.html

MatSE is multiscale

- MatSE is inherently **multiscale** and **multiphysics**
- Relative latecomer to mature computational approaches



Pertinent scales

Macroscopic scale

1m
Finite Element Method

Constitutive law

Scale of the grains

1mm
Homogenization

Constitutive law,
Elastic limit
Hardening coef.

Multiscale modeling:
Transfer information from the finer
to the higher scales

Scale of the electrons

1 Å

Ab Initio Methods

Energies

Scale of the atoms

1 nm

Molecular Dynamics
Monte Carlo

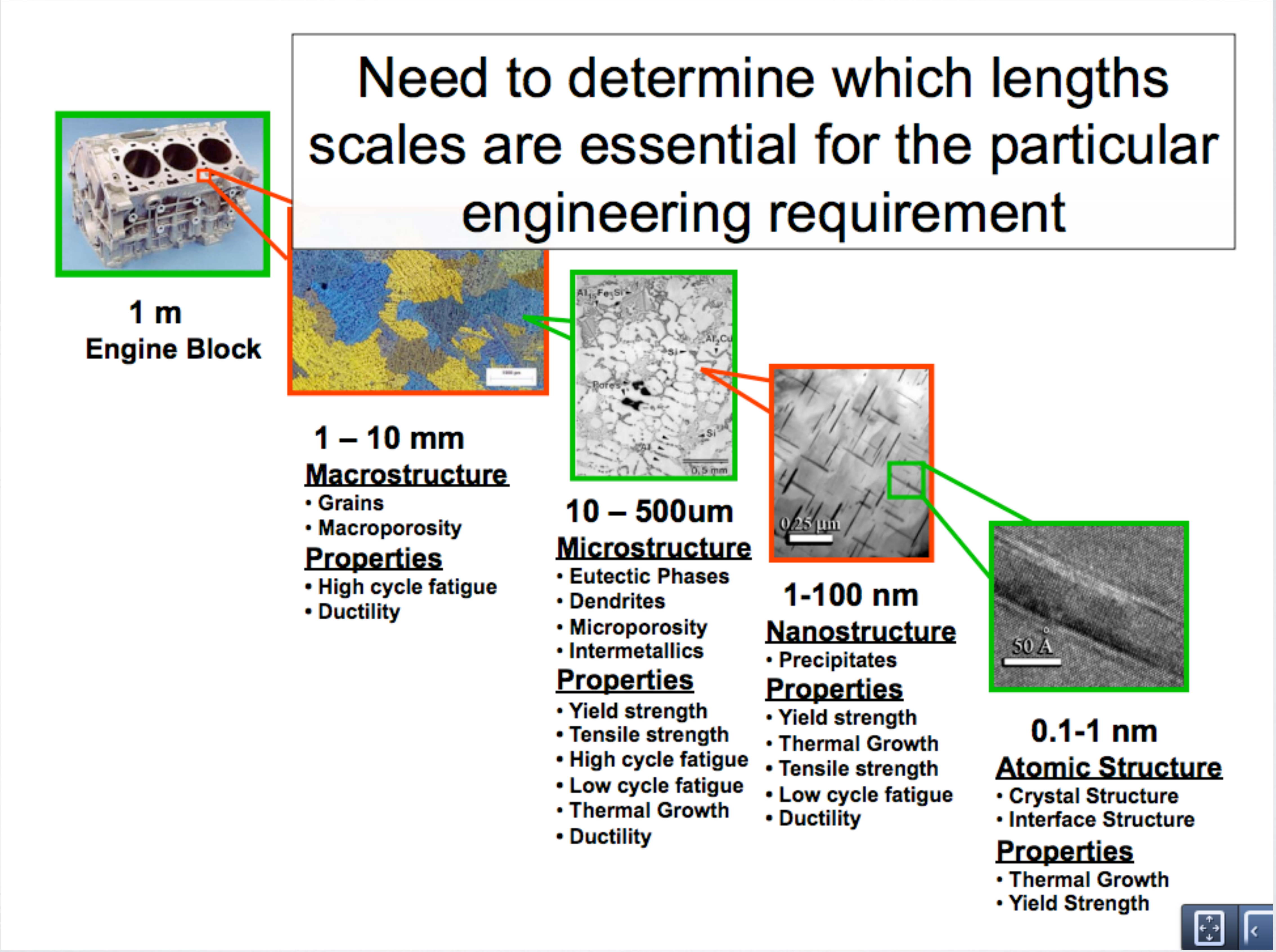
Dislo mobility
Annihilation dist.
Precipitate shape

Scale of the defects

1 μm
Dislocation Dynamics
Phase field

http://drodneygroup.webs.com/

MatSE is multiscale



Need to determine which lengths scales are essential for the particular engineering requirement

1 m
Engine Block

1 – 10 mm

Macrostructure
- Grains
- Macroporosity

Properties
- High cycle fatigue
- Ductility

10 – 500um

Microstructure
- Eutectic Phases
- Dendrites
- Microporosity
- Intermetallics

Properties
- Yield strength
- Tensile strength
- High cycle fatigue
- Low cycle fatigue
- Thermal Growth
- Ductility

1-100 nm

Nanostructure
- Precipitates

Properties
- Yield strength
- Thermal Growth
- Tensile strength
- Low cycle fatigue
- Ductility

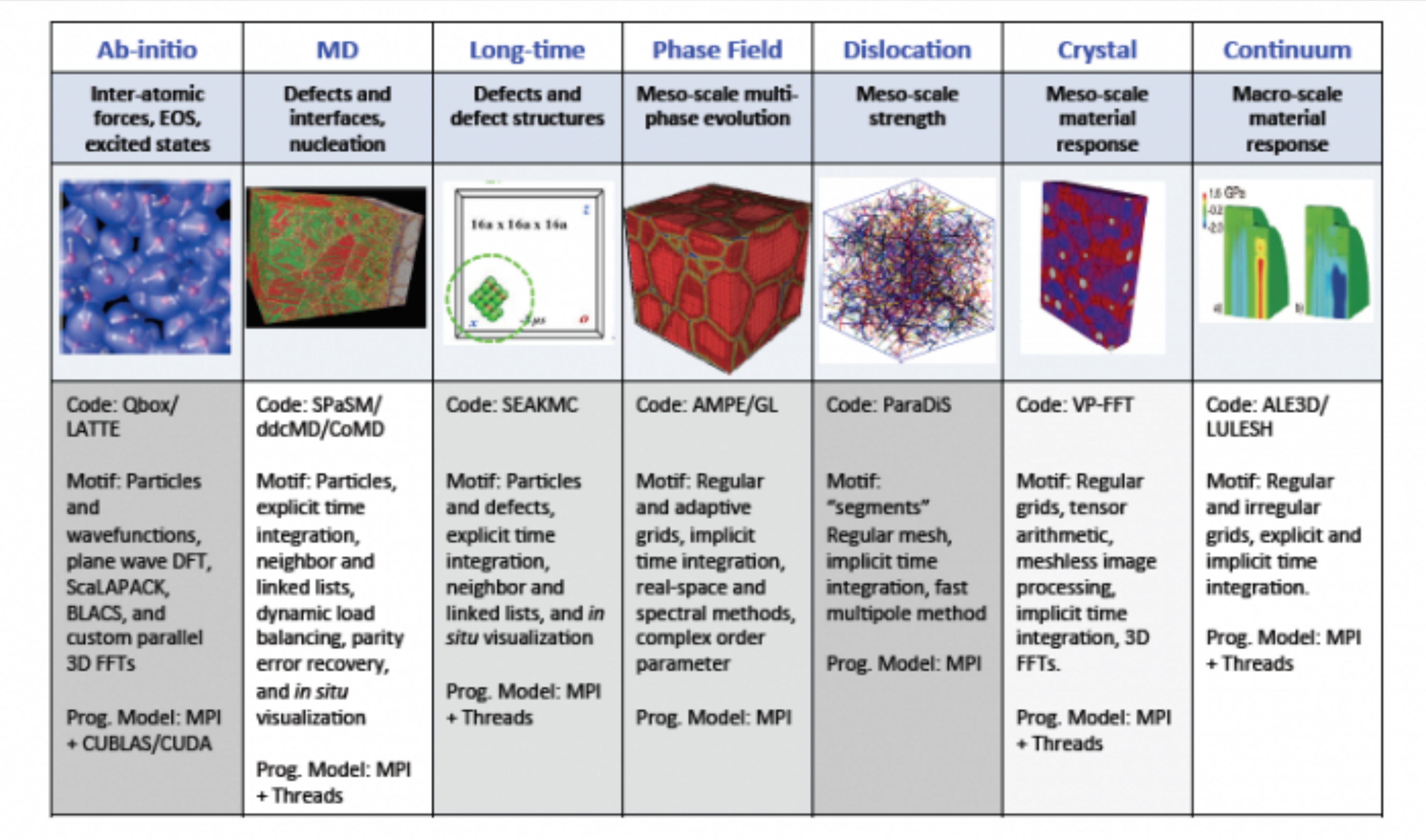
0.1-1 nm

Atomic Structure
- Crystal Structure
- Interface Structure

Properties
- Thermal Growth
- Yield Strength

http://web.ornl.gov/sci/cmsinn/talks/10_allison.pdf

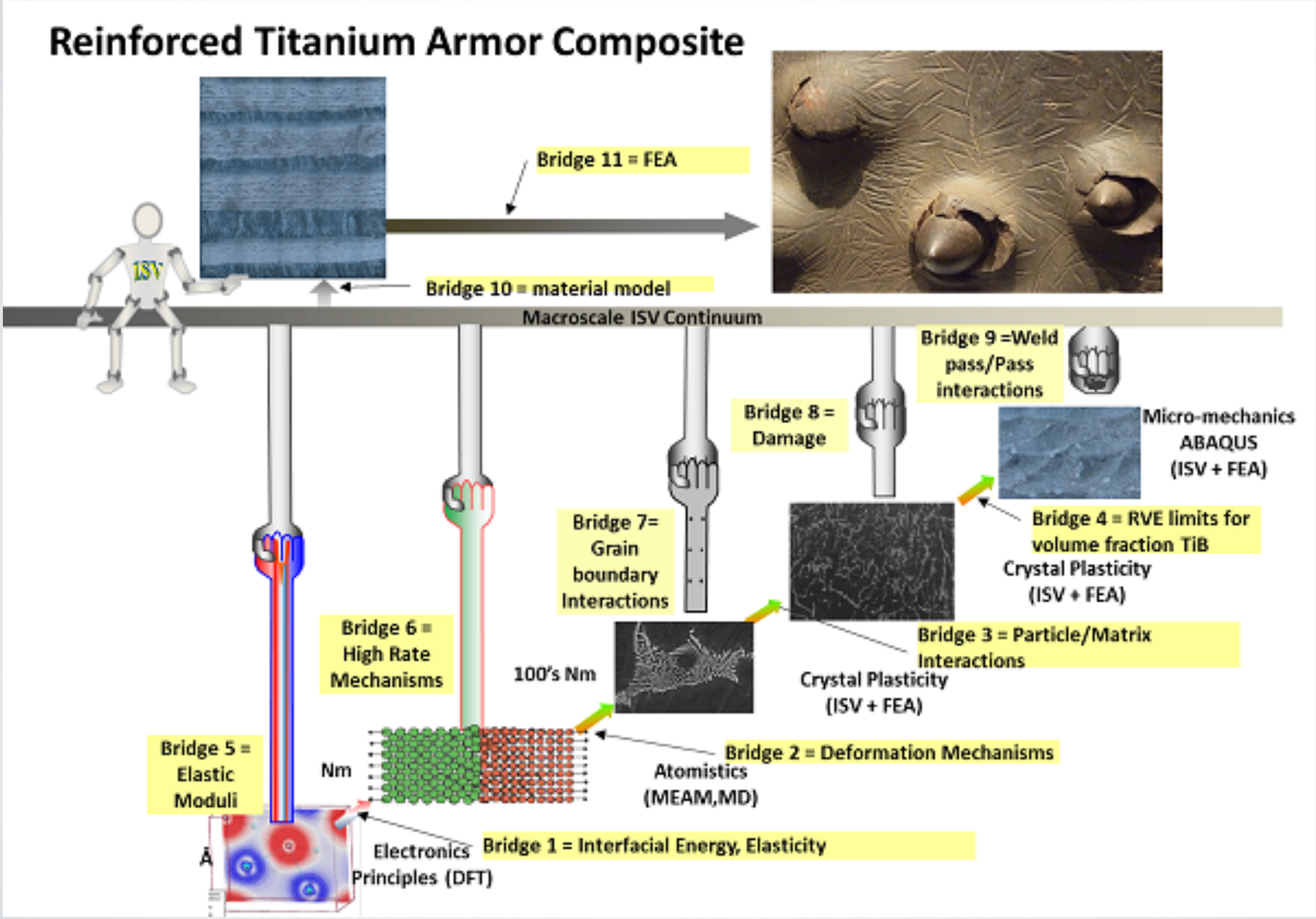
But CMSE is catching up!



Ab-initio	MD	Long-time	Phase Field	Dislocation	Crystal	Continuum
Inter-atomic forces, EOS, excited states	**Defects and interfaces, nucleation**	**Defects and defect structures**	**Meso-scale multi-phase evolution**	**Meso-scale strength**	**Meso-scale material response**	**Macro-scale material response**
Code: Qbox/ LATTE Motif: Particles and wavefunctions, plane wave DFT, ScaLAPACK, BLACS, and custom parallel 3D FFTs Prog. Model: MPI + CUBLAS/CUDA	Code: SPaSM/ ddcMD/CoMD Motif: Particles, explicit time integration, neighbor and linked lists, dynamic load balancing, parity error recovery, and *in situ* visualization Prog. Model: MPI + Threads	Code: SEAKMC Motif: Particles and defects, explicit time integration, neighbor and linked lists, and *in situ* visualization Prog. Model: MPI + Threads	Code: AMPE/GL Motif: Regular and adaptive grids, implicit time integration, real-space and spectral methods, complex order parameter Prog. Model: MPI	Code: ParaDiS Motif: "segments" Regular mesh, implicit time integration, fast multipole method Prog. Model: MPI	Code: VP-FFT Motif: Regular grids, tensor arithmetic, meshless image processing, implicit time integration, 3D FFTs. Prog. Model: MPI + Threads	Code: ALE3D/ LULESH Motif: Regular and irregular grids, explicit and implicit time integration. Prog. Model: MPI + Threads

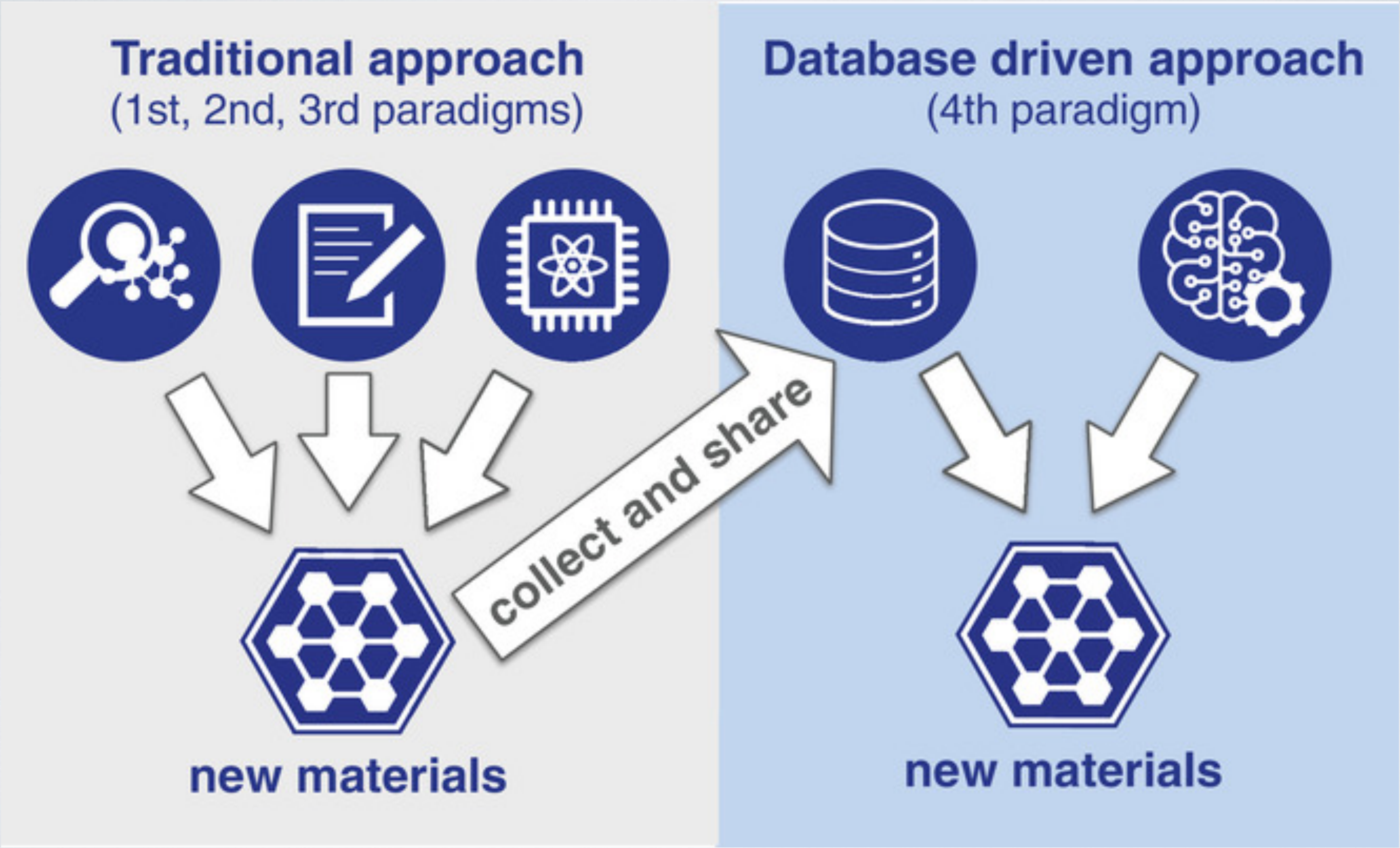
https://www.xstackwiki.com/index.php/ExMatEX

And enabling ICME



https://icme.hpc.msstate.edu/mediawiki/index.php?title=File:Titanium_armor_length_scale_Bridging_plot.png&limit=20

Data-driven design as 4th paradigm



Traditional approach
(1st, 2nd, 3rd paradigms)

new materials

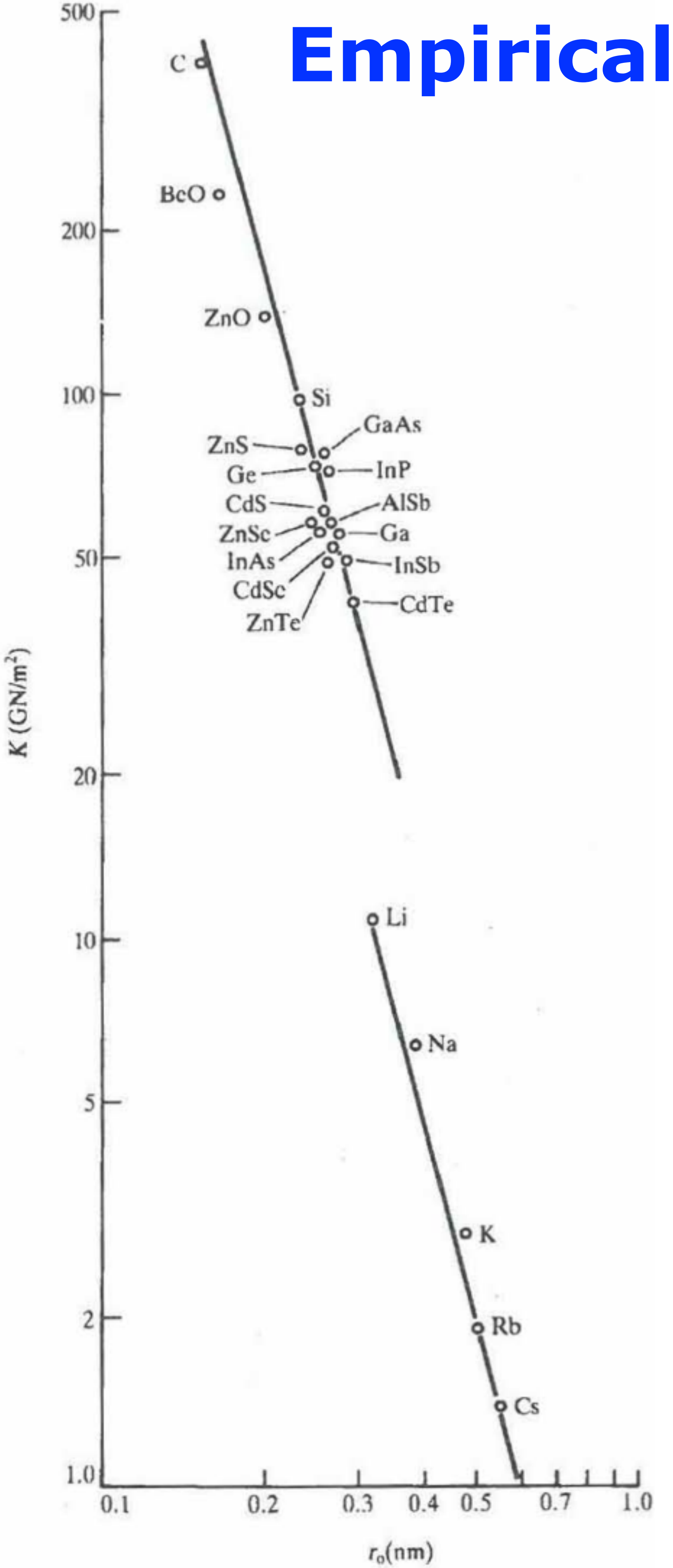
collect and share

Database driven approach
(4th paradigm)

new materials

Advanced Science, Volume: 6, Issue: 21, First published: 01 September 2019, DOI: (10.1002/advs.201900808)

Empirical relations for bulk modulus



$$A \approx U \sim \frac{1}{r} \sim \frac{1}{V^{1/3}}$$

$$\frac{\partial A}{\partial V} \sim \frac{1}{V^{4/3}}$$

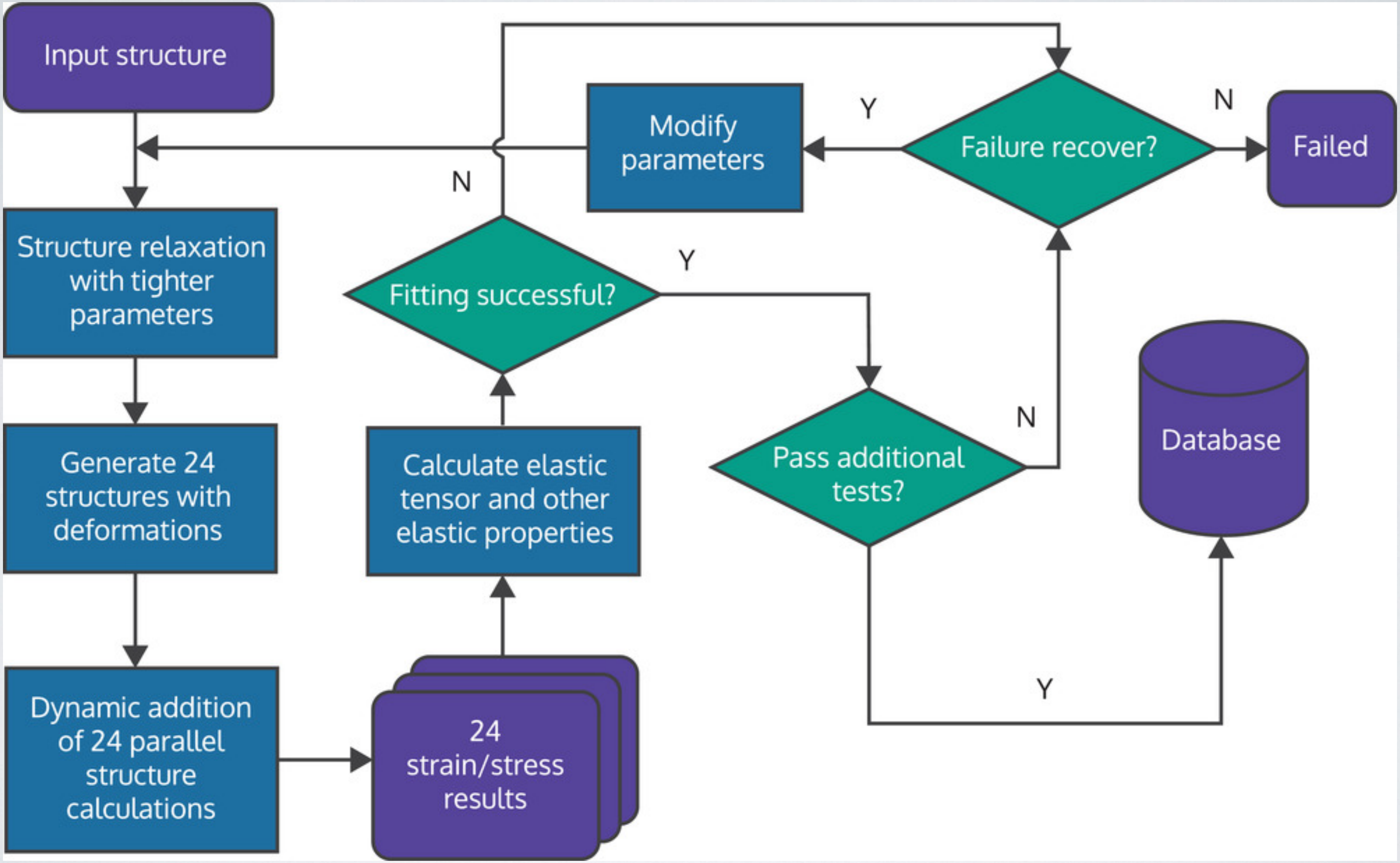
$$\frac{\partial^2 A}{\partial V^2} \sim \frac{1}{V^{7/3}}$$

$$V_0 \left.\frac{\partial^2 A}{\partial V^2}\right|_{V_0} \approx K \sim \frac{1}{V^{4/3}} \sim r_0^{-4}$$

Cohesive energy = depth of free energy well
Proportional to melting temperature (T_{melt})
Proportional to curvature of well (KV_0)

$$K \approx 100\frac{k_B T_{\mathrm{melt}}}{V_0}$$

Example of high-throughput



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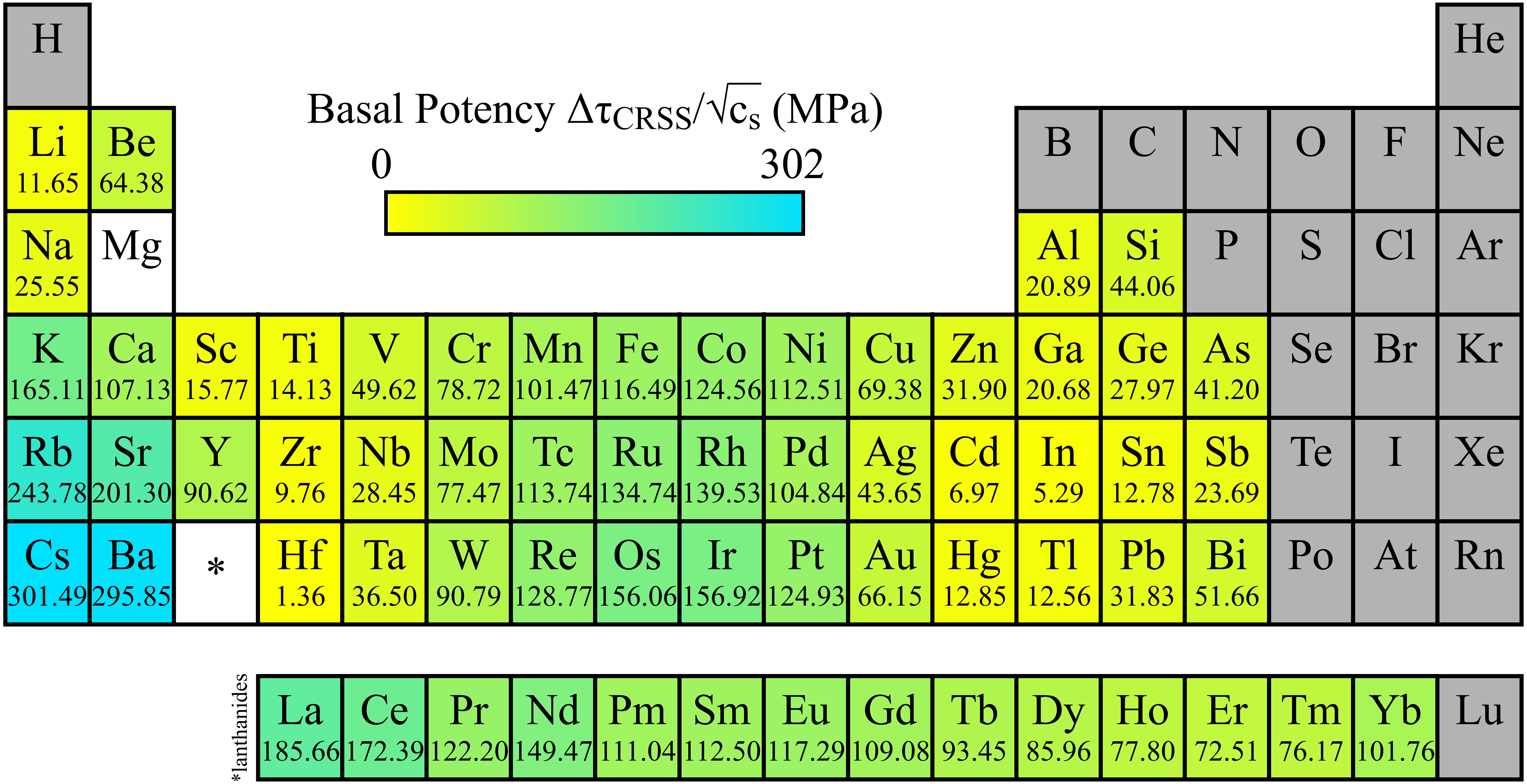
Solute trends in Mg alloys: basal strengthening

Basal potency: increase in basal CRSS with concentration

- correlated with size and basal stacking fault energy change
- derived for dilute limit, zero temperature pinning



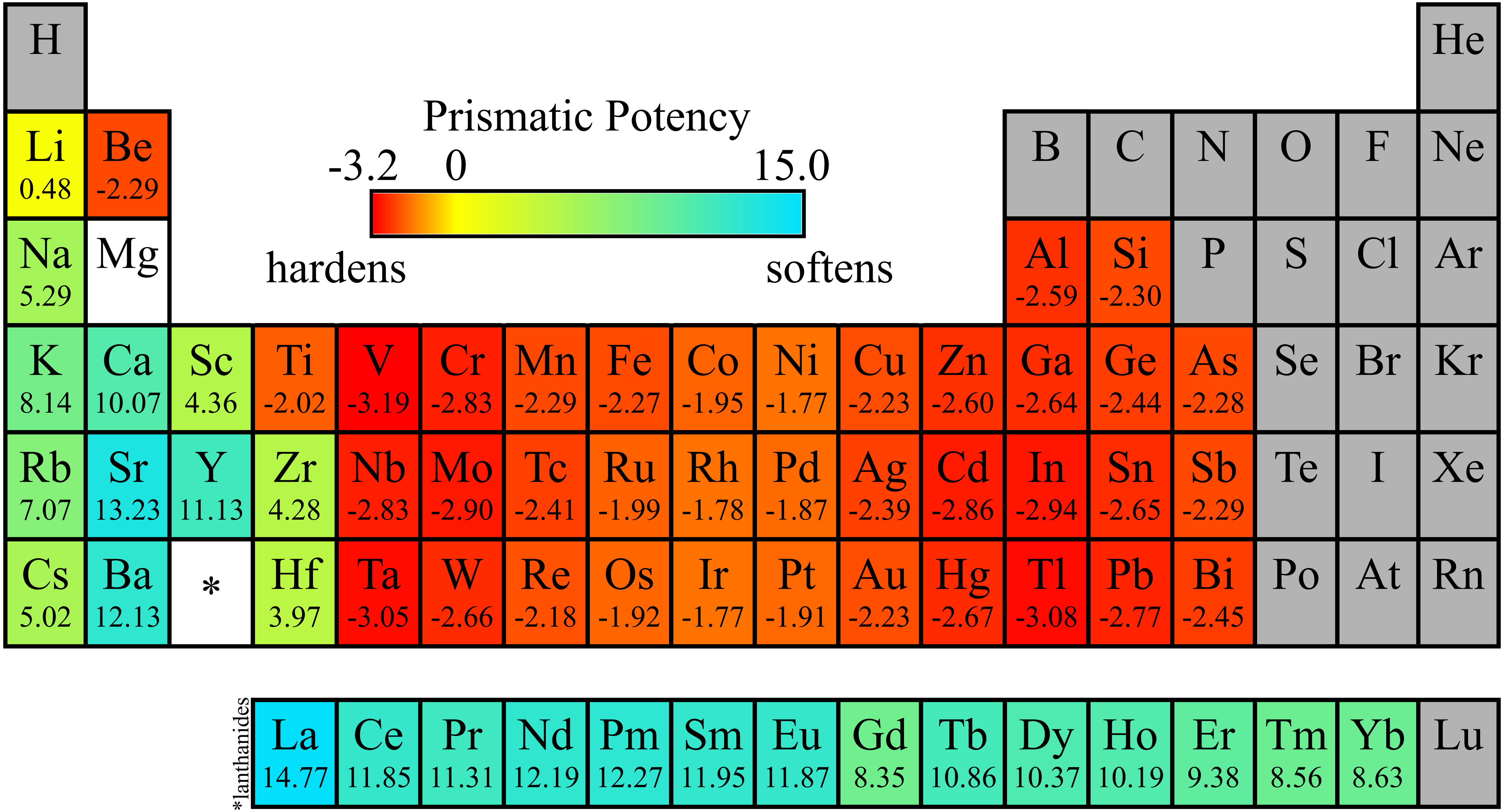
Basal Potency $\Delta\tau_{CRSS}/\sqrt{c_s}$ (MPa)

H																	He
Li 11.65	Be 64.38											B	C	N	O	F	Ne
Na 25.55	Mg											Al 20.89	Si 44.06	P	S	Cl	Ar
K 165.11	Ca 107.13	Sc 15.77	Ti 14.13	V 49.62	Cr 78.72	Mn 101.47	Fe 116.49	Co 124.56	Ni 112.51	Cu 69.38	Zn 31.90	Ga 20.68	Ge 27.97	As 41.20	Se	Br	Kr
Rb 243.78	Sr 201.30	Y 90.62	Zr 9.76	Nb 28.45	Mo 77.47	Tc 113.74	Ru 134.74	Rh 139.53	Pd 104.84	Ag 43.65	Cd 6.97	In 5.29	Sn 12.78	Sb 23.69	Te	I	Xe
Cs 301.49	Ba 295.85	*	Hf 1.36	Ta 36.50	W 90.79	Re 128.77	Os 156.06	Ir 156.92	Pt 124.93	Au 66.15	Hg 12.85	Tl 12.56	Pb 31.83	Bi 51.66	Po	At	Rn
		*lanthanides	La 185.66	Ce 172.39	Pr 122.20	Nd 149.47	Pm 111.04	Sm 112.50	Eu 117.29	Gd 109.08	Tb 93.45	Dy 85.96	Ho 77.80	Er 72.51	Tm 76.17	Yb 101.76	Lu

Solute trends in Mg alloys: prismatic softening

Prismatic potency: maximum possible cross-slip softening

- correlated with prismatic stacking fault energy reduction (except Li)
- strictly for **random binary** solute distribution



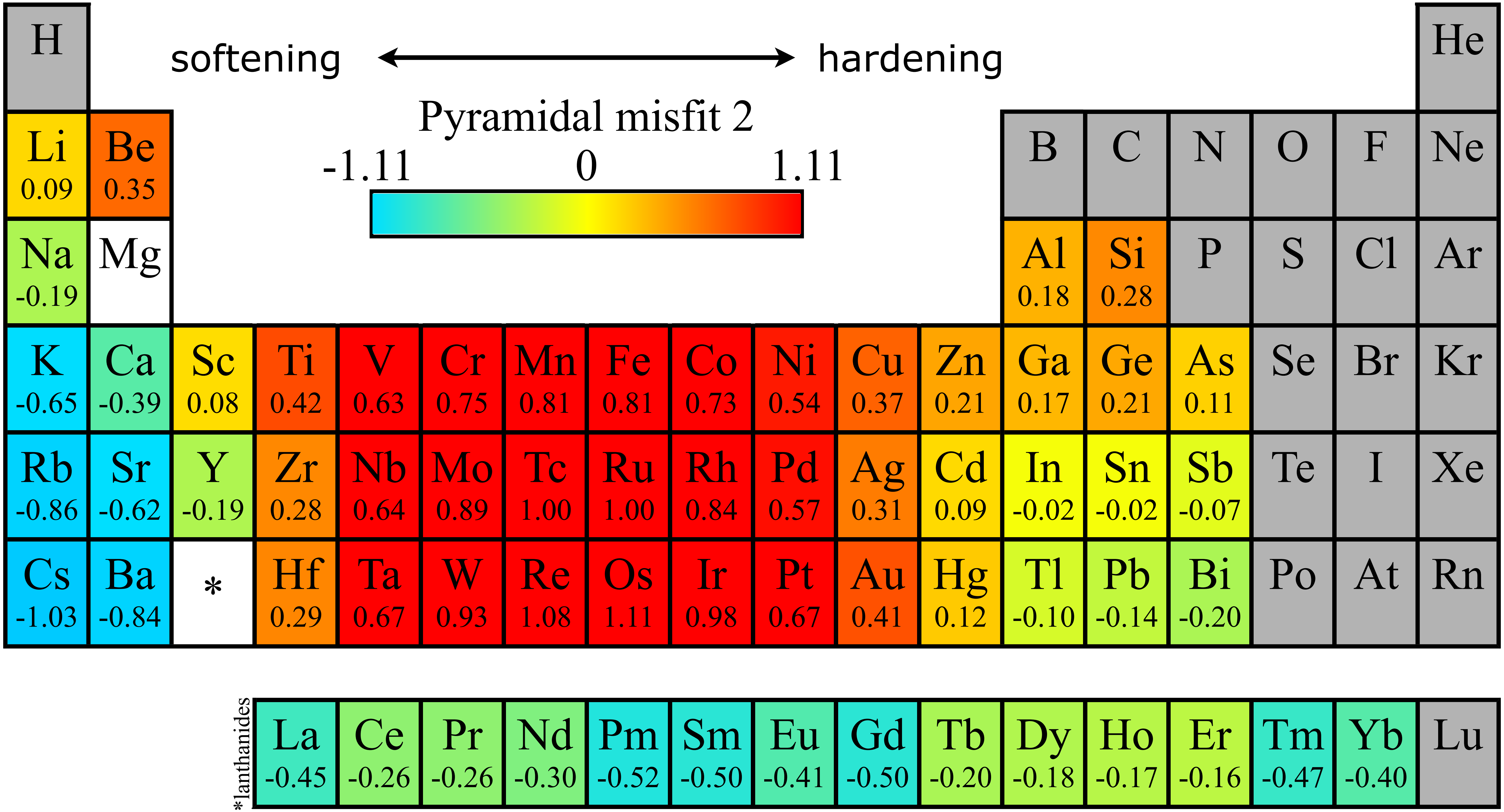
H																	He
Li 0.48	Be -2.29											B	C	N	O	F	Ne
Na 5.29	Mg											Al -2.59	Si -2.30	P	S	Cl	Ar
K 8.14	Ca 10.07	Sc 4.36	Ti -2.02	V -3.19	Cr -2.83	Mn -2.29	Fe -2.27	Co -1.95	Ni -1.77	Cu -2.23	Zn -2.60	Ga -2.64	Ge -2.44	As -2.28	Se	Br	Kr
Rb 7.07	Sr 13.23	Y 11.13	Zr 4.28	Nb -2.83	Mo -2.90	Tc -2.41	Ru -1.99	Rh -1.78	Pd -1.87	Ag -2.39	Cd -2.86	In -2.94	Sn -2.65	Sb -2.29	Te	I	Xe
Cs 5.02	Ba 12.13	*	Hf 3.97	Ta -3.05	W -2.66	Re -2.18	Os -1.92	Ir -1.77	Pt -1.91	Au -2.23	Hg -2.67	Tl -3.08	Pb -2.77	Bi -2.45	Po	At	Rn
		*lanthanides	La 14.77	Ce 11.85	Pr 11.31	Nd 12.19	Pm 12.27	Sm 11.95	Eu 11.87	Gd 8.35	Tb 10.86	Dy 10.37	Ho 10.19	Er 9.38	Tm 8.56	Yb 8.63	Lu

magnesium.matse.illinois.edu

Solute trends in Mg alloys: c+a softening

Change in pyramidal $(1\bar{1}01)$ stacking fault with addition of solute

- size, valency change, localization / delocalization of orbitals
- changes to Mg local electronic structure (3s and 2p)



H																	He
Li 0.09	Be 0.35											B	C	N	O	F	Ne
Na -0.19	Mg											Al 0.18	Si 0.28	P	S	Cl	Ar
K -0.65	Ca -0.39	Sc 0.08	Ti 0.42	V 0.63	Cr 0.75	Mn 0.81	Fe 0.81	Co 0.73	Ni 0.54	Cu 0.37	Zn 0.21	Ga 0.17	Ge 0.21	As 0.11	Se	Br	Kr
Rb -0.86	Sr -0.62	Y -0.19	Zr 0.28	Nb 0.64	Mo 0.89	Tc 1.00	Ru 1.00	Rh 0.84	Pd 0.57	Ag 0.31	Cd 0.09	In -0.02	Sn -0.02	Sb -0.07	Te	I	Xe
Cs -1.03	Ba -0.84	*	Hf 0.29	Ta 0.67	W 0.93	Re 1.08	Os 1.11	Ir 0.98	Pt 0.67	Au 0.41	Hg 0.12	Tl -0.10	Pb -0.14	Bi -0.20	Po	At	Rn
		*lanthanides	La -0.45	Ce -0.26	Pr -0.26	Nd -0.30	Pm -0.52	Sm -0.50	Eu -0.41	Gd -0.50	Tb -0.20	Dy -0.18	Ho -0.17	Er -0.16	Tm -0.47	Yb -0.40	Lu

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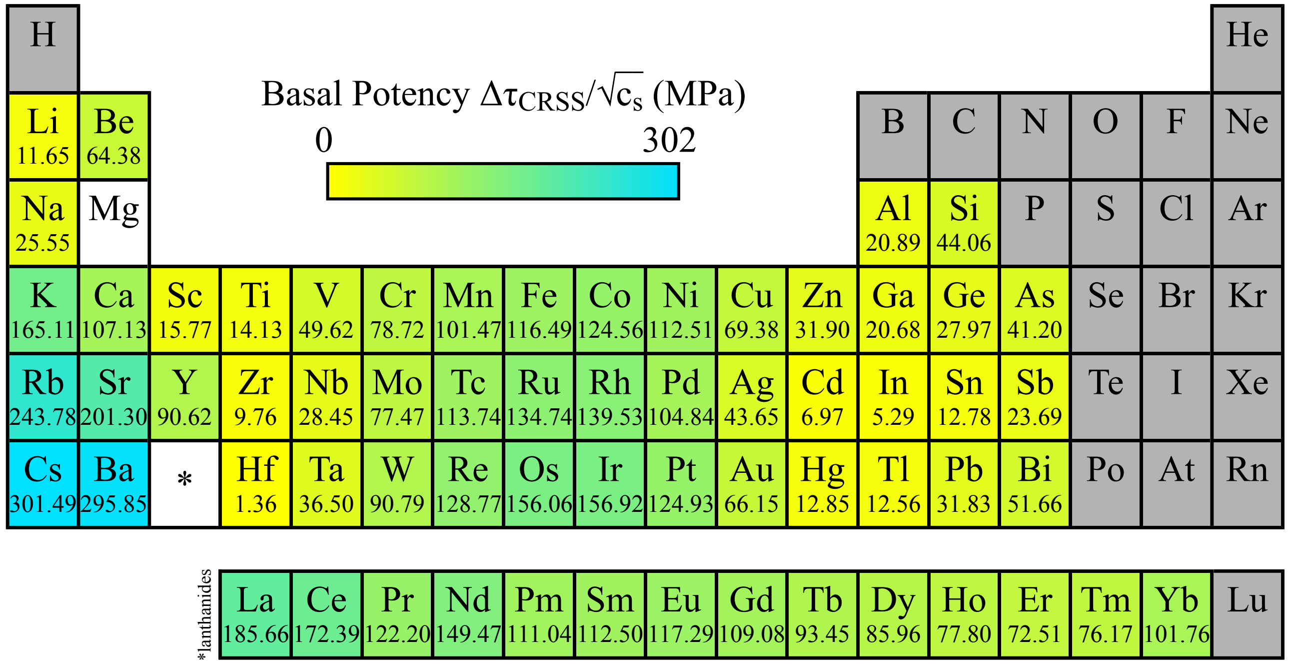
Solute trends in Mg alloys: effect on slip

Multiple misfits (changes in SFE) and potencies (changes in slip)

- pyramidal fault energies needed for ⟨c+a⟩ slip
- combined effects even more important



Basal Potency $\Delta\tau_{CRSS}/\sqrt{c_s}$ (MPa)

0 302

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Li 11.65	Be 64.38											B	C	N	O	F	Ne
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Cs 301.49	Ba 295.85	*	Hf 1.36	Ta 36.50	W 90.79	Re 128.77	Os 156.06	Ir 156.92	Pt 124.93	Au 66.15	Hg 12.85	Tl 12.56	Pb 31.83	Bi 51.66	Po	At	Rn
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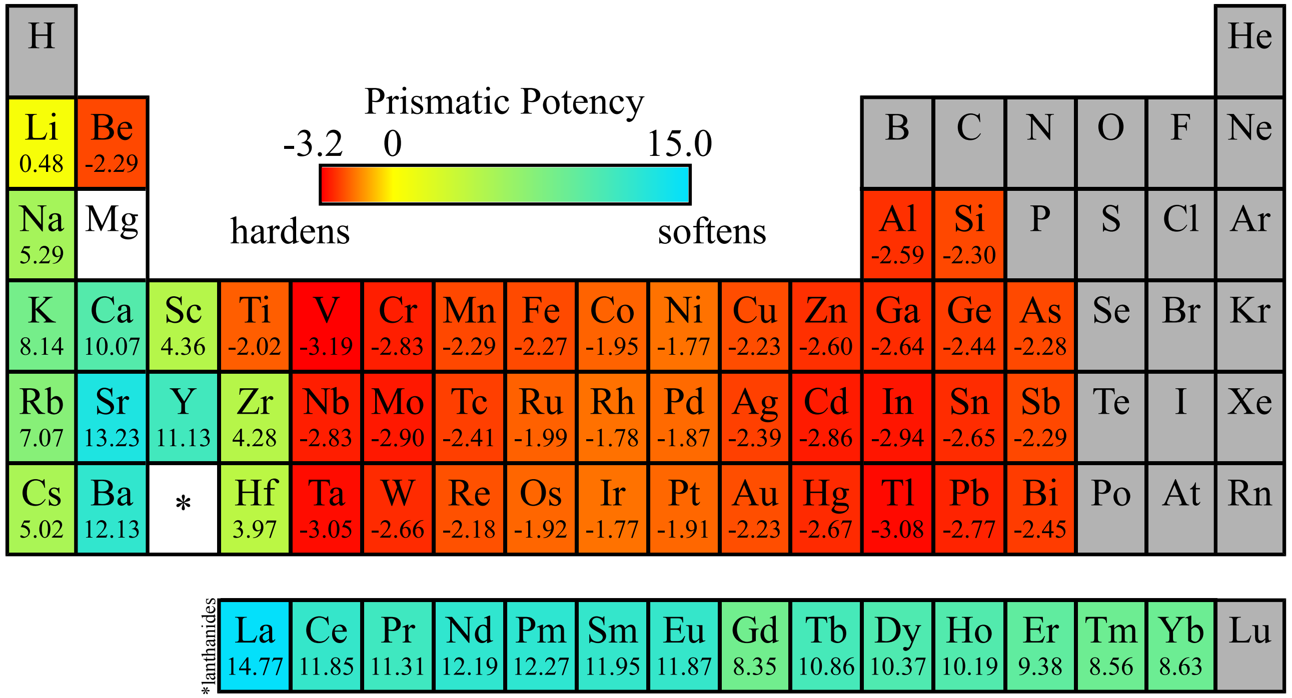

Prismatic Potency

-3.2 0 15.0

hardens softens

H																	He
Li 0.48	Be -2.29											B	C	N	O	F	Ne
Na 5.29	Mg											Al -2.59	Si -2.30	P	S	Cl	Ar
K 8.14	Ca 10.07	Sc 4.36	Ti -2.02	V -3.19	Cr -2.83	Mn -2.29	Fe -2.27	Co -1.95	Ni -1.77	Cu -2.23	Zn -2.60	Ga -2.64	Ge -2.44	As -2.28	Se	Br	Kr
Rb 7.07	Sr 13.23	Y 11.13	Zr 4.28	Nb -2.83	Mo -2.90	Tc -2.41	Ru -1.99	Rh -1.78	Pd -1.87	Ag -2.39	Cd -2.86	In -2.94	Sn -2.65	Sb -2.29	Te	I	Xe
Cs 5.02	Ba 12.13	*	Hf 3.97	Ta -3.05	W -2.66	Re -2.18	Os -1.92	Ir -1.77	Pt -1.91	Au -2.23	Hg -2.67	Tl -3.08	Pb -2.77	Bi -2.45	Po	At	Rn
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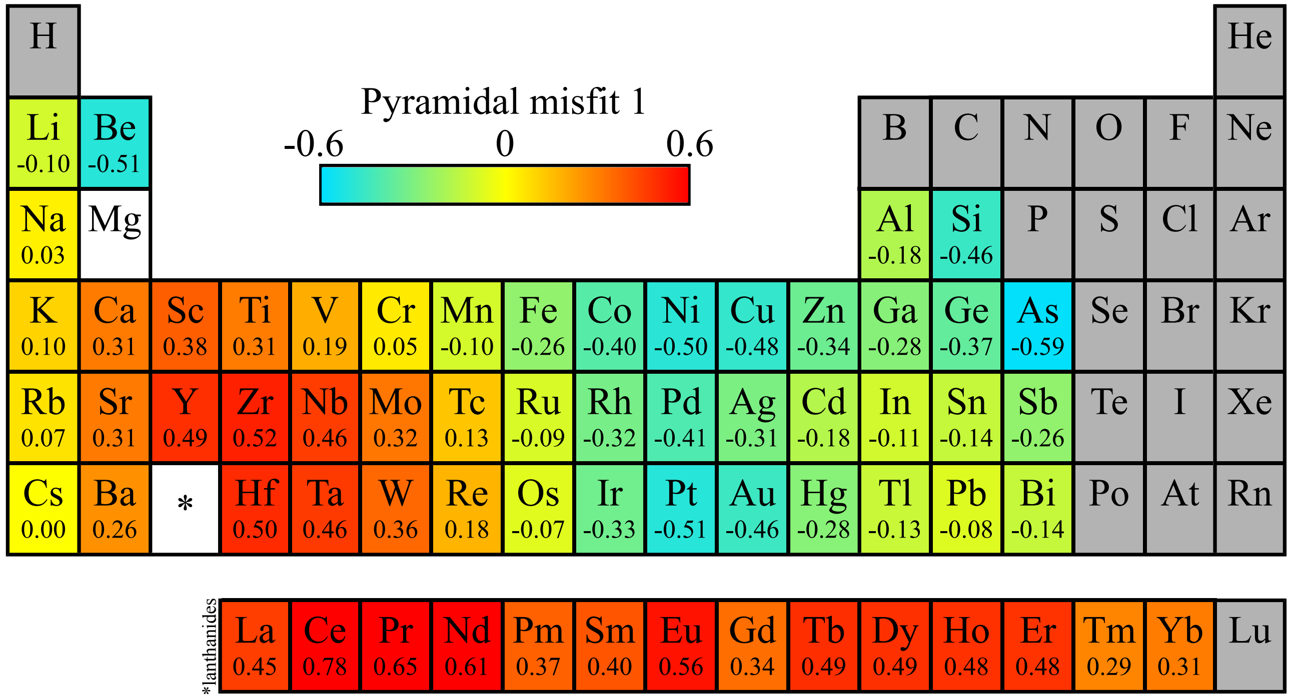
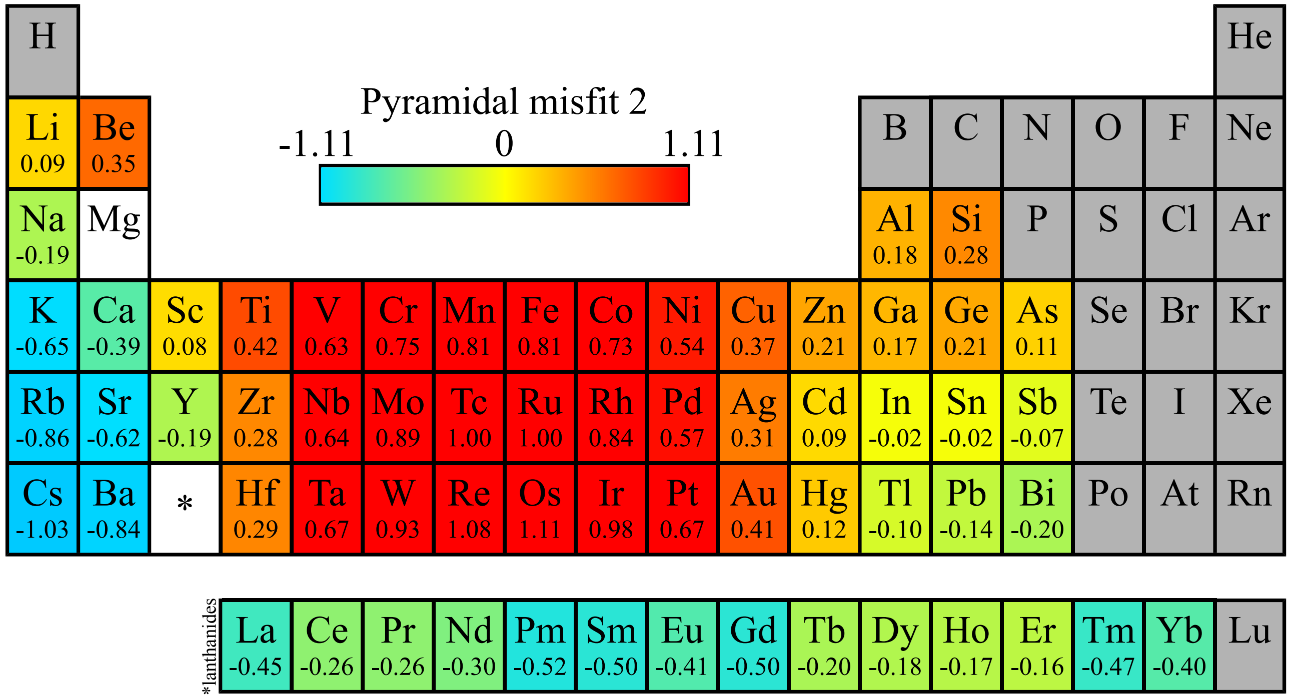


Pyramidal misfit 1

-0.6 0 0.6

H																	He
Li -0.10	Be -0.51											B	C	N	O	F	Ne
Na 0.03	Mg											Al -0.18	Si -0.46	P	S	Cl	Ar
K 0.10	Ca 0.31	Sc 0.38	Ti 0.31	V 0.19	Cr 0.05	Mn -0.10	Fe -0.26	Co -0.40	Ni -0.50	Cu -0.48	Zn -0.34	Ga -0.28	Ge -0.37	As -0.59	Se	Br	Kr
Rb 0.07	Sr 0.31	Y 0.49	Zr 0.52	Nb 0.46	Mo 0.32	Tc 0.13	Ru -0.09	Rh -0.32	Pd -0.41	Ag -0.31	Cd -0.18	In -0.11	Sn -0.14	Sb -0.26	Te	I	Xe
Cs 0.00	Ba 0.26	*	Hf 0.50	Ta 0.46	W 0.36	Re 0.18	Os -0.07	Ir -0.33	Pt -0.51	Au -0.46	Hg -0.28	Tl -0.13	Pb -0.08	Bi -0.14	Po	At	Rn
		*lanthanides	La 0.45	Ce 0.78	Pr 0.65	Nd 0.61	Pm 0.37	Sm 0.40	Eu 0.56	Gd 0.34	Tb 0.49	Dy 0.49	Ho 0.48	Er 0.48	Tm 0.29	Yb 0.31	Lu



Pyramidal misfit 2

-1.11 0 1.11

H																	He
Li 0.09	Be 0.35											B	C	N	O	F	Ne
Na -0.19	Mg											Al 0.18	Si 0.28	P	S	Cl	Ar
K -0.65	Ca -0.39	Sc 0.08	Ti 0.42	V 0.63	Cr 0.75	Mn 0.81	Fe 0.81	Co 0.73	Ni 0.54	Cu 0.37	Zn 0.21	Ga 0.17	Ge 0.21	As 0.11	Se	Br	Kr
Rb -0.86	Sr -0.62	Y -0.19	Zr 0.28	Nb 0.64	Mo 0.89	Tc 1.00	Ru 1.00	Rh 0.84	Pd 0.57	Ag 0.31	Cd 0.09	In -0.02	Sn -0.02	Sb -0.07	Te	I	Xe
Cs -1.03	Ba -0.84	*	Hf 0.29	Ta 0.67	W 0.93	Re 1.08	Os 1.11	Ir 0.98	Pt 0.67	Au 0.41	Hg 0.12	Tl -0.10	Pb -0.14	Bi -0.20	Po	At	Rn
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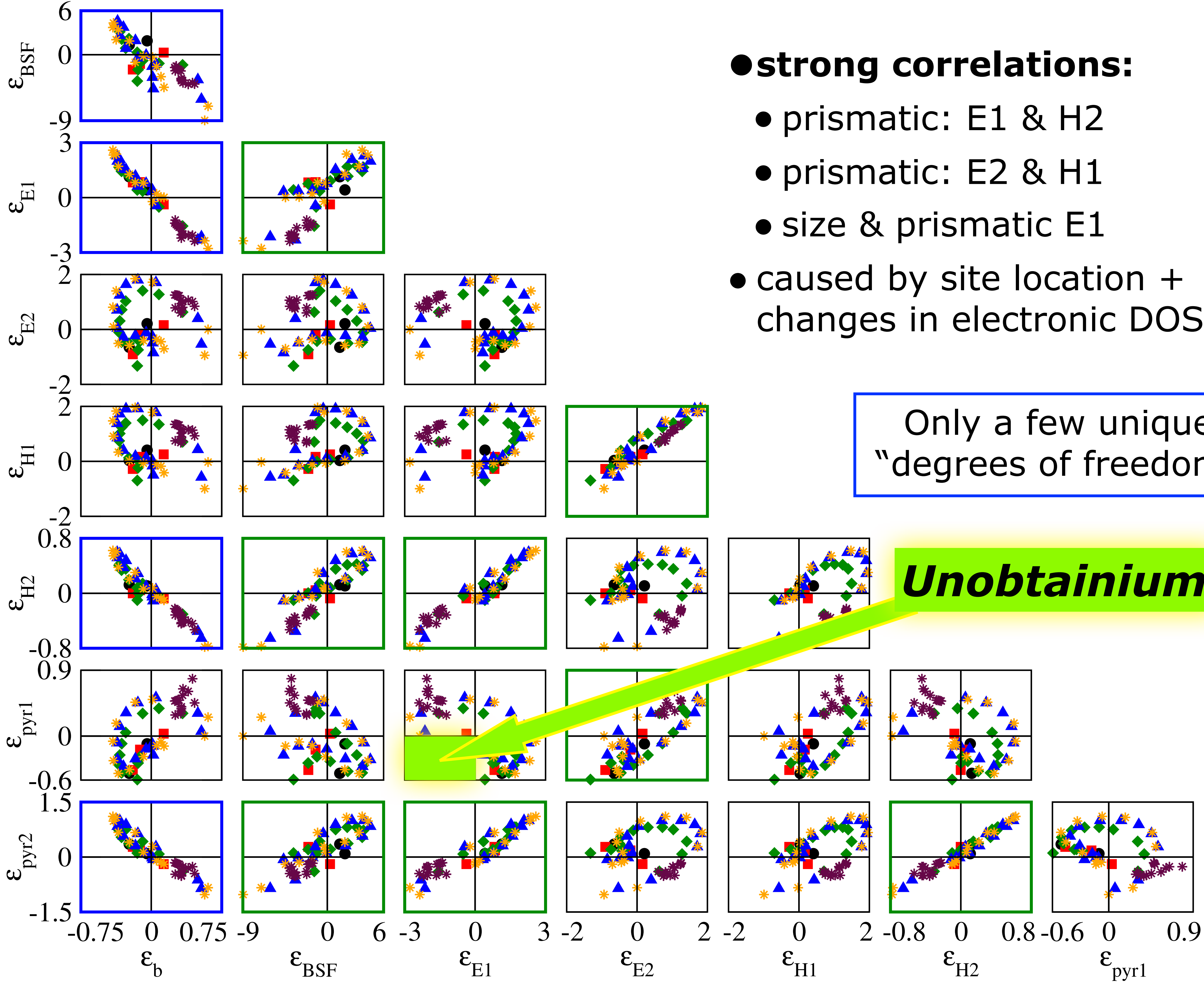
Solute misfits in magnesium: misfit correlations

- **strong correlations:**
  - prismatic: E1 & H2
  - prismatic: E2 & H1
  - size & prismatic E1
- caused by site location + changes in electronic DOS

Only a few unique “degrees of freedom”

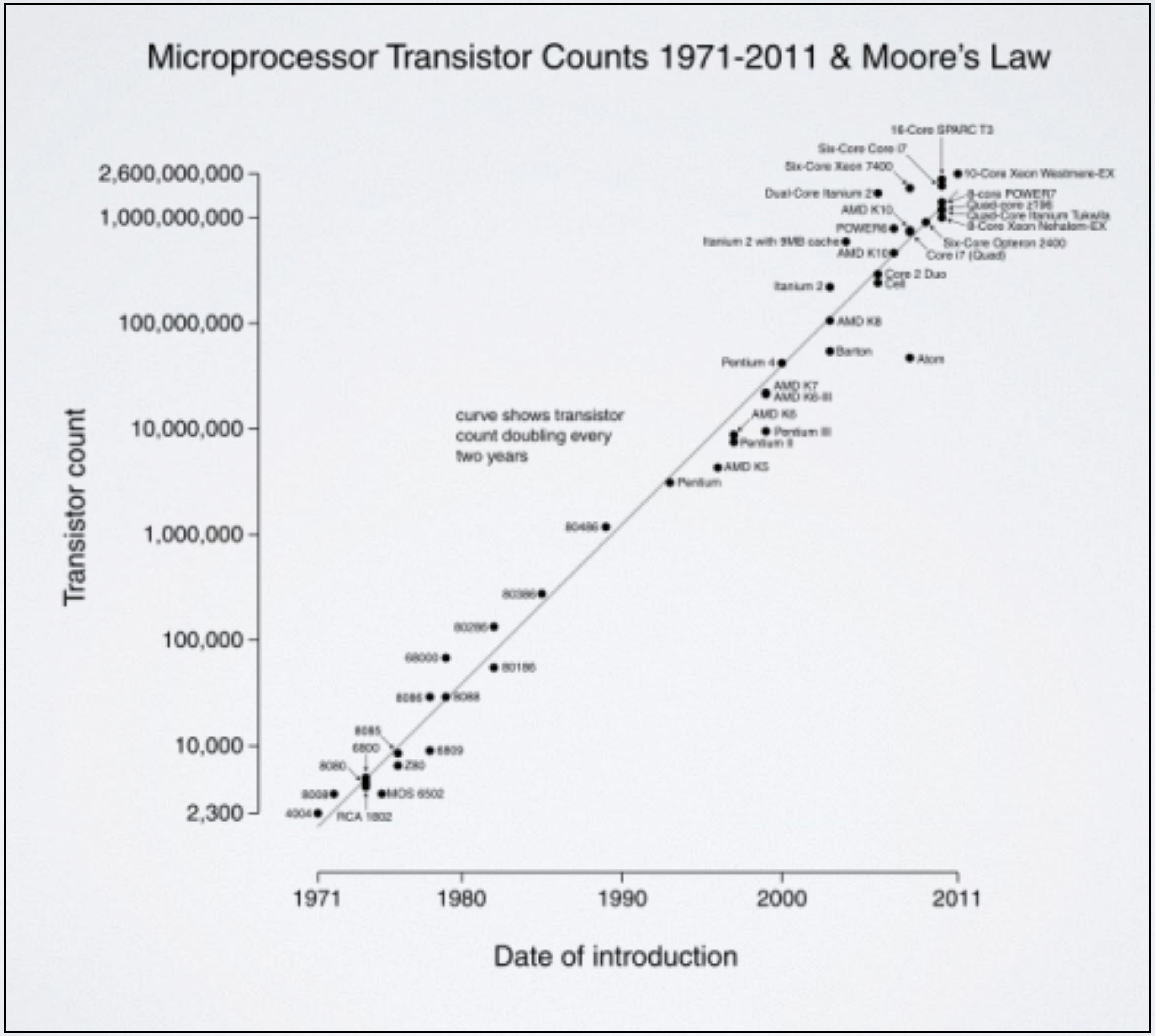


Unobtainium

II. Why CMSE / ICME?

Moore's Law

- Gordon Moore's 1965 prediction (just) continues to hold
- Modern computation is **cheap** and **powerful**



Microprocessor Transistor Counts 1971-2011 & Moore's Law

http://www.eeweb.com/blog/alex_toombs/the-potential-for-the-end-of-moores-law

What is driving CMSE?

- Industry, government, and academia are united (!)
- CMSE will **drive innovation and discovery**
- Critical to:

address national goals

(mineral security, military hardware, biomedicine)

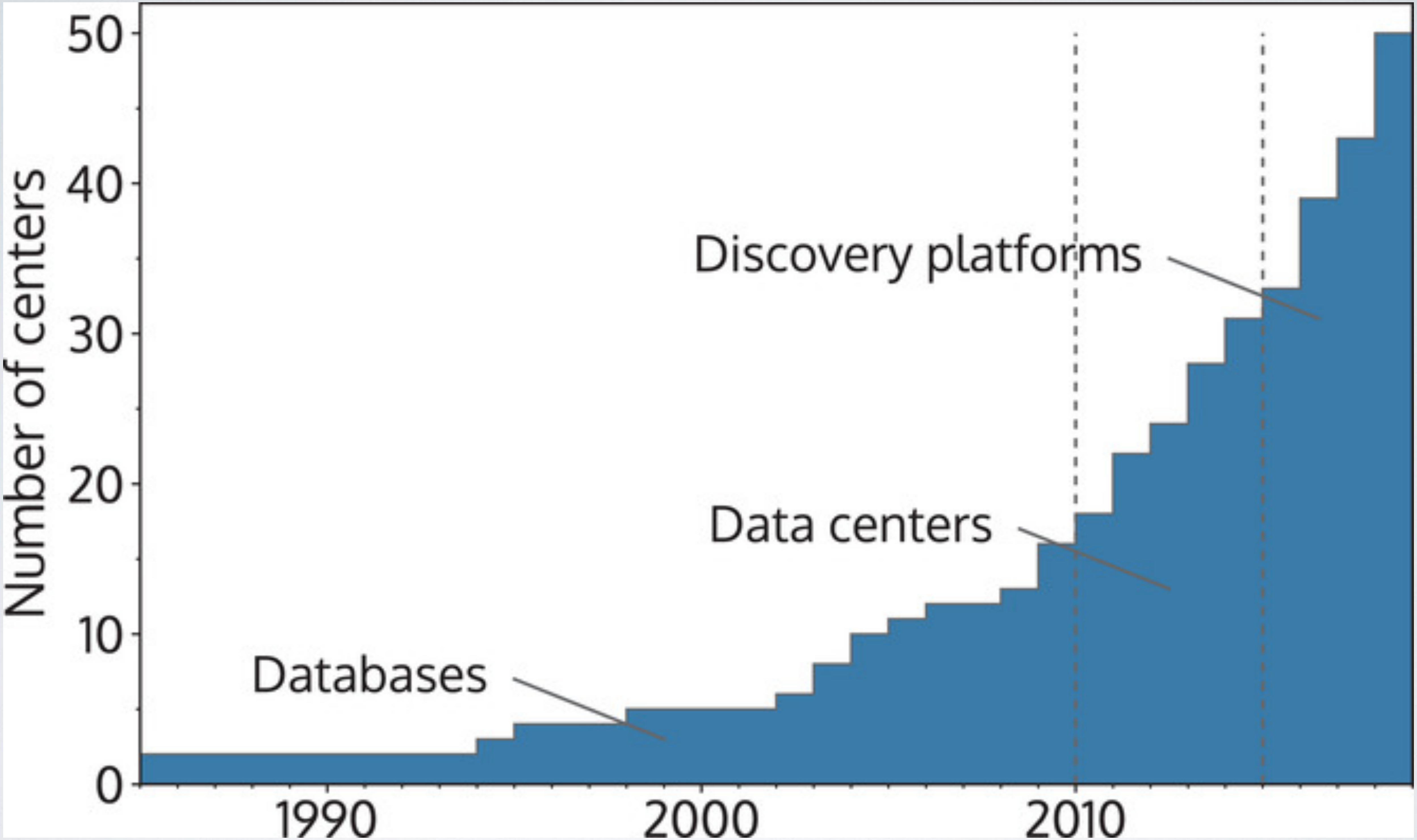
bring new products to market

(renewable energy, advanced electronics, prosthetics)

train next-generation workforce

(knowledge economy, domestic competitiveness)

Growth of data



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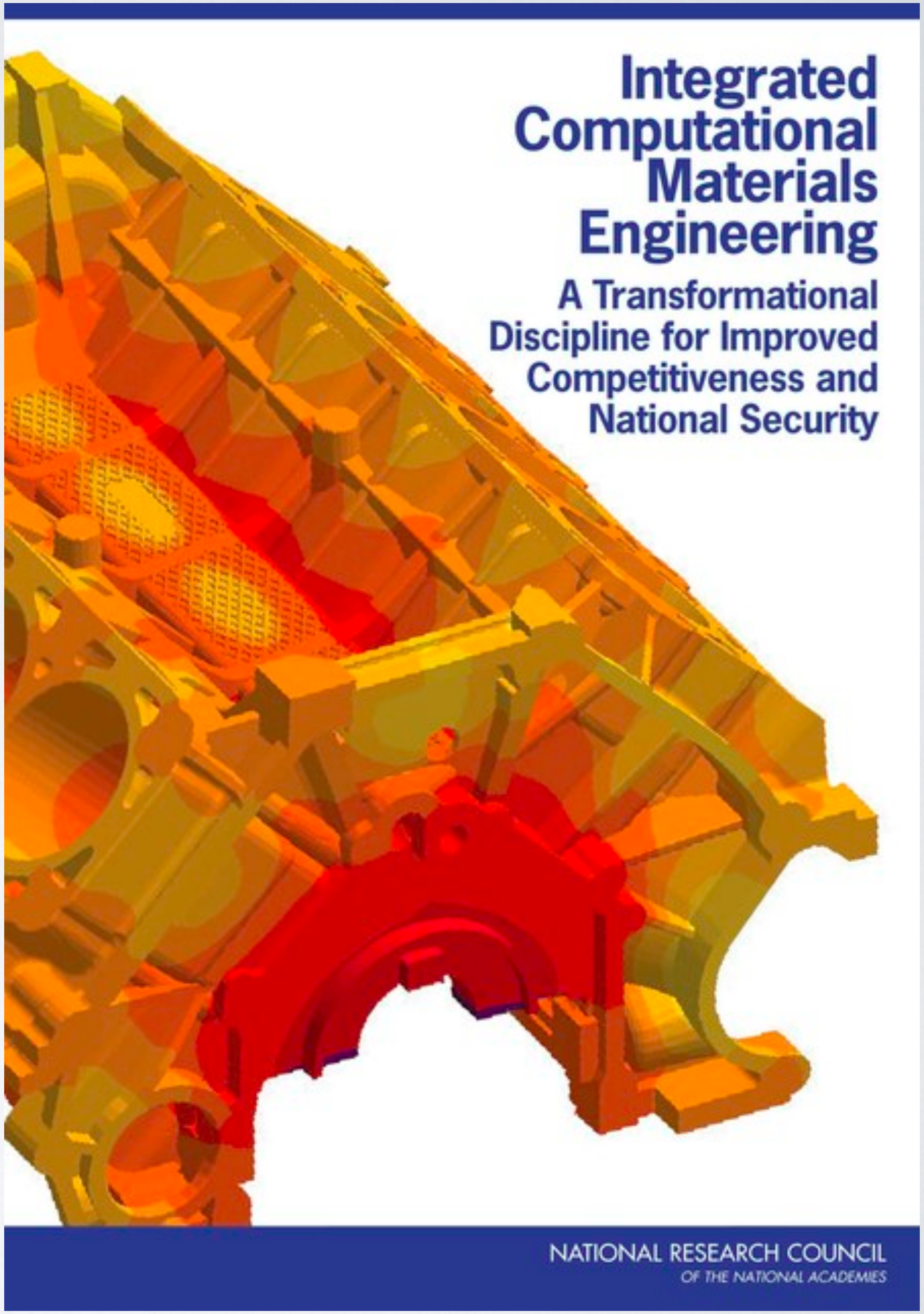
Public policy

Materials Genome Initiative
for Global Competitiveness

June 2011



Integrated Computational Materials Engineering

A Transformational Discipline for Improved Competitiveness and National Security

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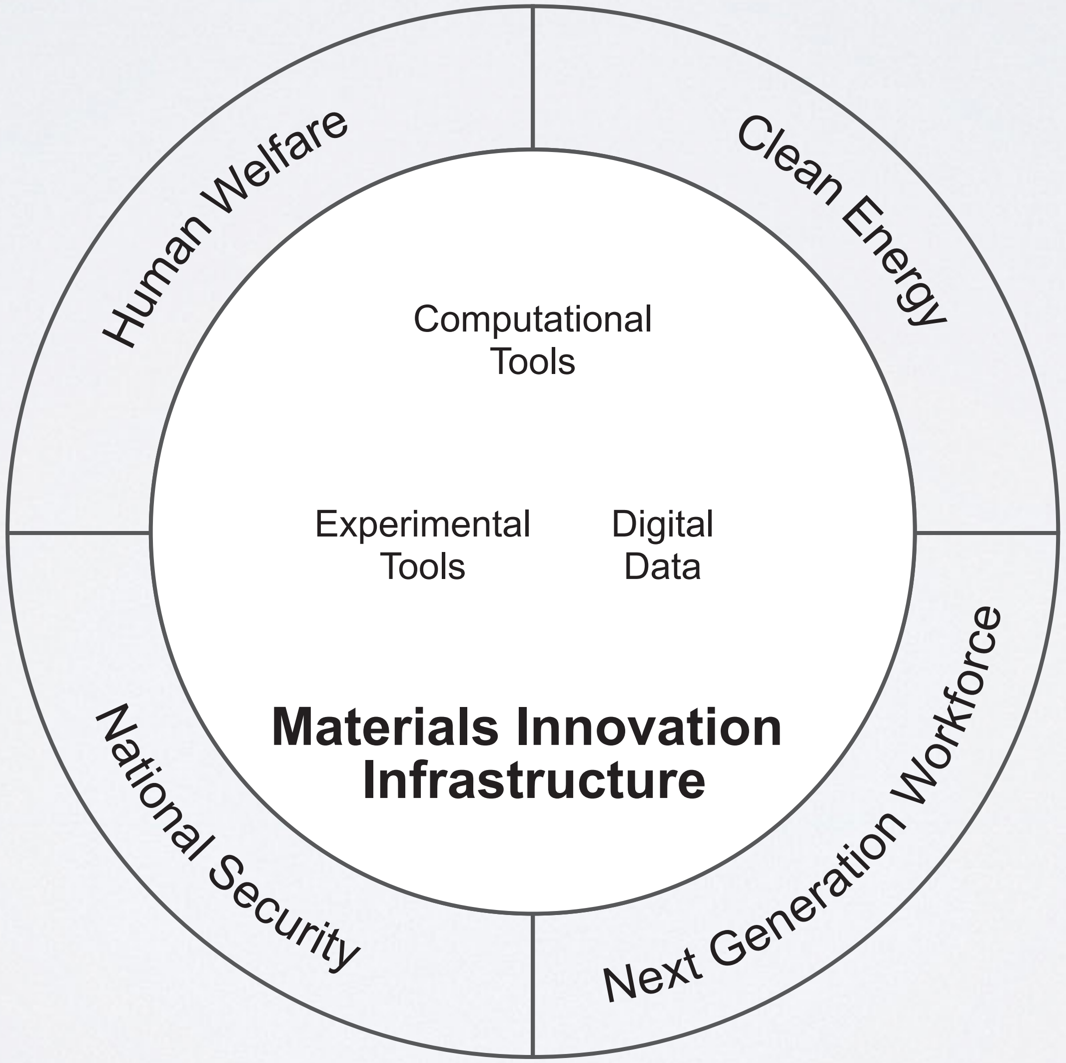
Public policy

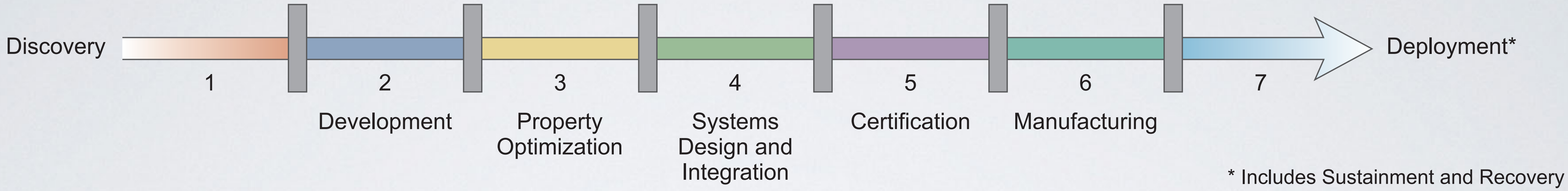
In summary, advanced materials are essential to human well-being and are the cornerstone for emerging industries. Yet, the time frame for incorporating advanced materials into applications is remarkably long, often taking 10 to 20 years from initial research to first use. The Materials Genome Initiative is an effort that will address this problem through the dedicated involvement of stakeholders in government, education, professional societies, and industry, to deliver: (1) the creation of a new materials-innovation infrastructure, (2) the achievement of national goals with advanced materials, and (3) the preparation of a next-generation materials workforce to sustain this progress. Such a set of objectives will serve a more competitive domestic manufacturing presence — one in which the United States will develop, manufacture, and deploy advanced materials at least two times faster than is possible today, at a fraction of the cost.



White House Materials Genome Initiative for Global Competitiveness (June, 2011)

Industry

- Global competitiveness of manufacturing firms requires accelerated materials development and deployment



- CMSE can compress development pipeline by eliminating laborious, costly, and lengthy experimental "trial and error"

- Validated computational models to perform:

prototyping	screening	materials selection
materials design	failure analysis	forensics
virtual analysis	optimization	reliability testing

White House Materials Genome Initiative for Global Competitiveness (June, 2011)

Industry

- Case Study: Ford Motor - Virtual Aluminum Casting (VAC)

- Integrated computational tools for design of Al powertrain

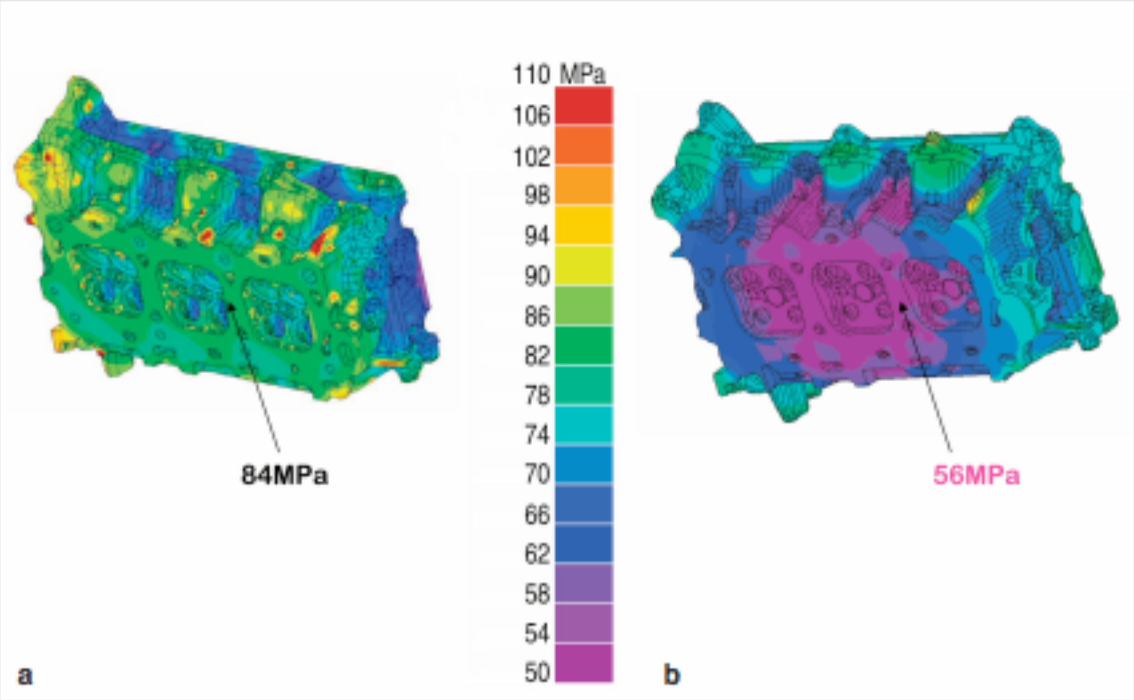


Figure 6. Using VAC predictions of local fatigue strengths in the selection of a manufacturing process for a cylinder head: (a) casting Process A, (b) casting Process B.

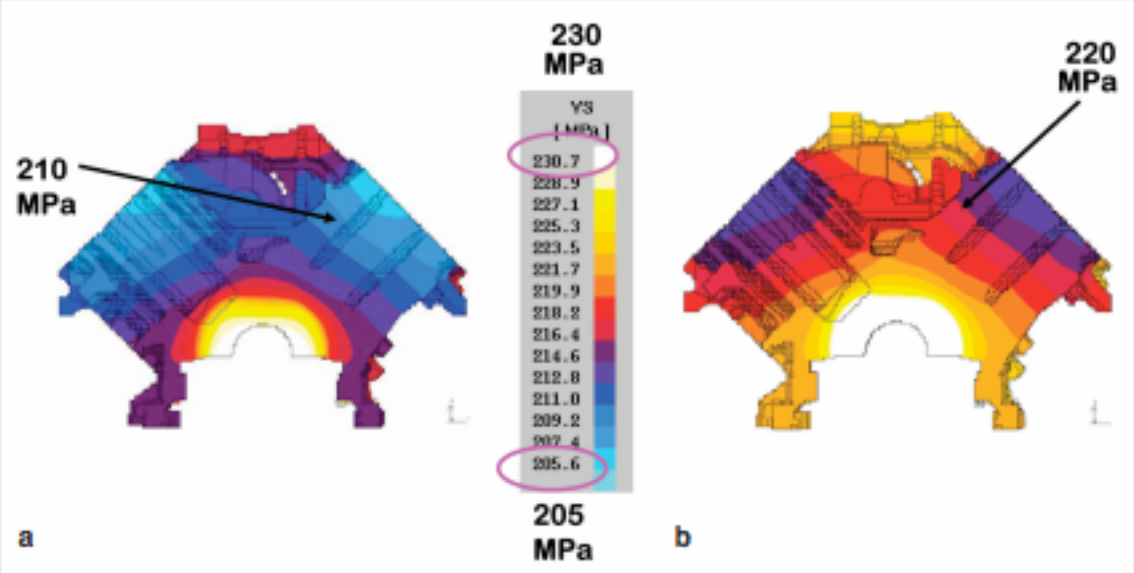


Figure 7. Using VAC predictions of the local yield strength in a hypothetical cylinder block to optimize the heat treatment process: (a) initial heat-treatment process for 5 h age at 240°C, (b) optimized heat-treatment process for 3 h age at 250°C. (Note: Property target in bolt boss area indicated by arrow is 220 MPa.)

- Reduced experimental iterations and optimized processing
- Development time shortened by 15-20%

  Cost savings of $10-20M p.a.

J. Allison, M. Li, C. Wolverton, and X. Su Virtual Aluminum Castings: An Industrial Application of ICME JOM 11 28 (2011)

Academia

Computational Materials Science and Engineering Education: A Survey of Trends and Needs

K. Thornton, Samanthule Nola, R. Edwin Garcia, Mark Asta, and G.B. Olson

Enhanced for the Web

This article appears on the JOM web site ***(www.tms.org/jom.html)*** *in html format and includes links to additional on-line resources.*

Results from a recent reassessment of the state of computational materials science and engineering (CMSE) education are reported. Surveys were distributed to the chairs and heads of materials programs, faculty members engaged in computational research, and employers of materials scientists and engineers, mainly in the United States. The data was compiled to assess current course offerings related to CMSE, the general climate for introducing computational methods in MSE curricula, and the requirements from the employers' viewpoint. Furthermore, the available educational resources and their utilization by the community are examined. The surveys show a general support for integrating computational content into MSE education. However, they also reflect remaining issues with implementation, as well as a gap between the tools being taught in courses and those that are used by employers. Overall, the results suggest the necessity for a comprehensively developed vision and plans to further the integration of computational methods into MSE curricula.

INTRODUCTION

Materials science and engineering (MSE) encompasses metallurgy, semiconductors, ceramic engineering, and polymer science. It is a multidisciplinary field that enables new technologies required to address a wide variety of critical challenges facing society, such as clean energy production. While traditionally viewed as an experimental discipline, many researchers have begun to take advantage of rapidly growing computing resources and associated algorithmic and theoretical developments, and the capabilities of integrated computational approaches are increasingly being utilized to accelerate materials design and development. Recent National Research Council (NRC) reports[1,2] indicate that successful integration of computational tools has also begun to be demonstrated in industrial settings, comparing its potential impact to that of bioinfomatics. The reports summarized recommendations that include incorporation of computational modules into a broad range of materials science courses in order to train the next generations of materials engineers with the abilities required to exploit these tools. However, the degree to which such efforts are already under way, and what steps must still be taken to address these NRC recommendations remain unclear. Therefore, we have undertaken a survey of the field to assess the current status of computational materials science and engineering (CMSE) education. A summary is presented below, which serves as an update to a previously published report[3] based on similar surveys performed in 2003–2004. See the sidebars on page 13 for a survey description and the list of respondents.

UNDERGRADUATE EDUCATION IN CMSE

The status of undergraduate CMSE curriculum was assessed through five survey questions directed to department chairs, as well as corresponding questions included in the survey tar-

Figure 1. Survey results on the importance of two specific aspects of CMSE education from the computational faculty members' view and that of the department chairs and program heads.

Figure 2. Survey responses on how CMSE should be implemented into undergraduate MSE education, obtained from the same two groups. *"Equally useful" option was omitted for the computational faculty survey, but some respondents wrote in this option (shown in light red).

Institute of Physics Publishing Modelling and Simulation in Materials Science and Engineering

Modelling Simul. Mater. Sci. Eng. **13** (2005) R53–R69 doi:10.1088/0965-0393/13/2/R01

TOPICAL REVIEW

Current status and outlook of computational materials science education in the US

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Abstract

We examine the current state of computational materials science education based upon information compiled from top universities in materials science and engineering (MSE). We find that there is a large variation in the emphasis on computational modelling between universities. It is reported that a relatively large course offering is the result of changes in the curriculum made in the last five years, showing a rapid pace in the implementation of computational courses at these departments. We also collected information from industry and national labs regarding their current and future needs in MSE graduates, and the results are summarized. This paper also provides a list of resources that are currently used in computational materials science education.

1. Introduction

Materials science and engineering (MSE) is a discipline which has grown substantially from its original roots in metallurgy and ceramic and polymer engineering. Traditionally, significant research breakthroughs in this discipline have been driven mainly by advances in experimental techniques, rather than theory or modelling. However, recent advances in theoretical and numerical methods, coupled with an explosion in available computational resources, has led to enormous progress in the development and integration of modelling techniques applicable to the study of a wide range of materials systems and properties. Modelling and simulation tools are thus finding increasing applications not only in fundamental materials-science research, but also in real-world design and optimization of new materials. The relatively new field of computational materials science is continuing to find a growing number of practitioners not only in academia and national labs but also, increasingly, in industry.

The growing impact of computation in materials research is clear. In surveying the publications in *Acta Materialia* during 2003, one out of five articles included at least one of the two words 'simulat*' and 'comput*' in the key words (including the title and the abstract) [1].

0965-0393/05/020053+17$30.00

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- Role of academy to **develop CMSE tools** (research) and **train practitioners in their use** (education)

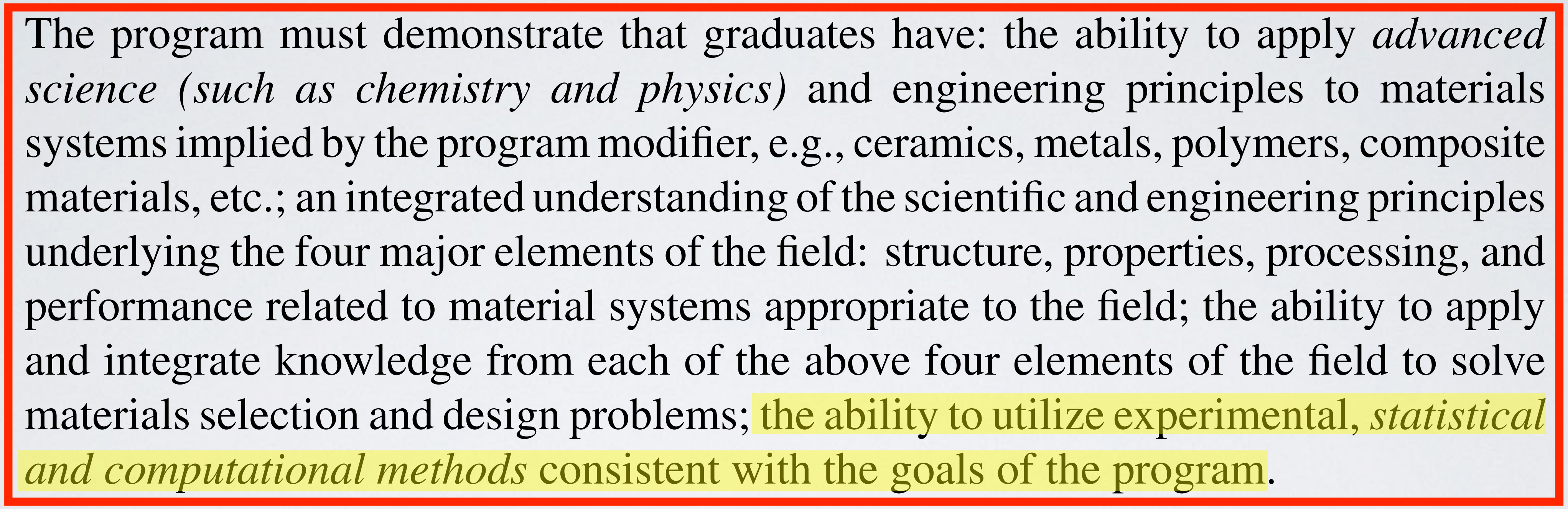
- Studies have identified a role for formal undergraduate and graduate CMSE training to support:
  - graduate placement in industry and national labs
  - improved employee productivity and expanded skill set
  - provision of expertise for post-graduate research

- Other key findings:
  - academic / industrial mismatch in software focus
  - industry privileges software skills, not programming
  - familiarity and competency with range of CMSE software
  - "hands-on" experimental labs, but not computational

K. Thornton and M. Asta Current status and outlook of computational materials science education in the US Modelling Simul. Mater. Sci. Eng. 13 R53 (2005)
K. Thornton, S. Nola, R.E. Garcia, M. Asta and G.B> Olson COmputational Materials Science and Engineering Education: A survey of trends and needs JOM 61 10 12 (2009)

Academia

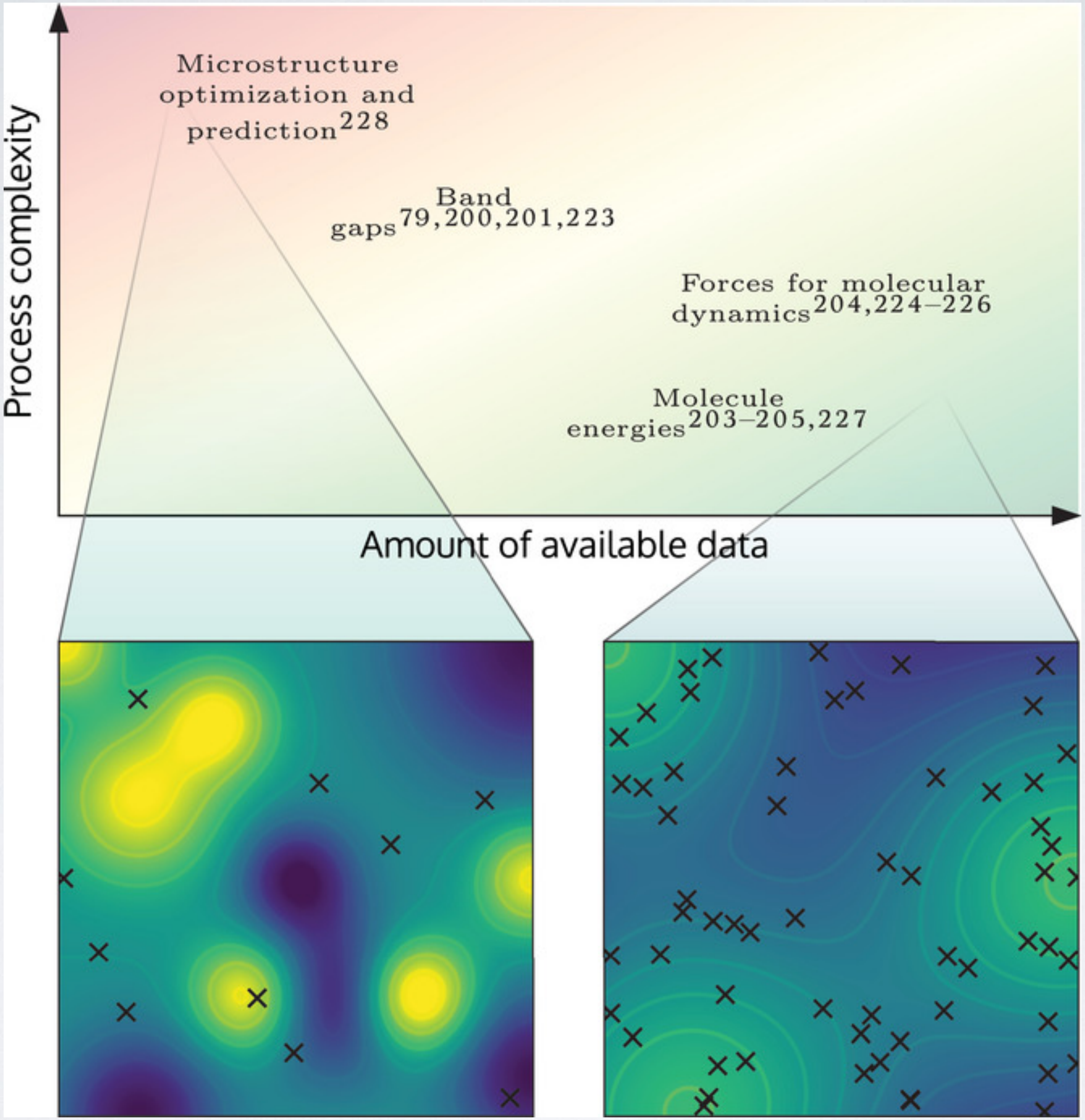
- ABET - Materials Engineering Programs:



The program must demonstrate that graduates have: the ability to apply *advanced science (such as chemistry and physics)* and engineering principles to materials systems implied by the program modifier, e.g., ceramics, metals, polymers, composite materials, etc.; an integrated understanding of the scientific and engineering principles underlying the four major elements of the field: structure, properties, processing, and performance related to material systems appropriate to the field; the ability to apply and integrate knowledge from each of the above four elements of the field to solve materials selection and design problems; the ability to utilize experimental, *statistical and computational methods* consistent with the goals of the program.

K. Thornton and M. Asta Current status and outlook of computational materials science education in the US Modelling Simul. Mater. Sci. Eng. 13 R53 (2005)

Challenge of data



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III. CMSE/ICME tools

CMSE/ICME resources

MATERIALS TECHNOLOGY @ TMS

Materials Education

http://iweb.tms.org/forum/

nanoHUB.org
an nCn project

ONLINE SIMULATION AND MORE FOR NANOTECHNOLOGY

http://nanohub.org/

4CeeD

http://4ceed.github.io/

AFLOW

Automatic - **FLOW for Materials Discovery**

http://aflowlib.org

MATERIALS DATA FACILITY

http://materialsdatafacility.org

http://materialsproject.org

http://mits.nims.go.jp

http://materialsdata.nist.gov

IV. Surveys

Entrance Survey

https://forms.illinois.edu/sec/1302183