Metals Research in 2040

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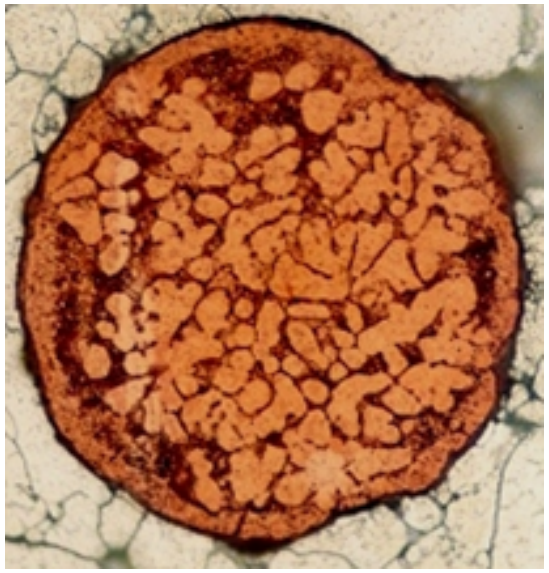
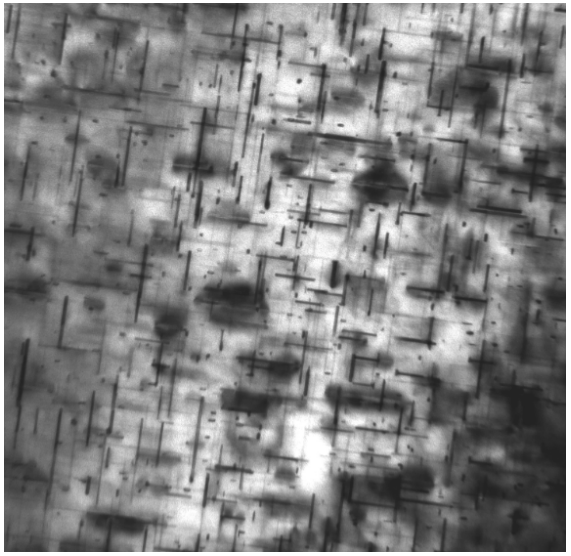
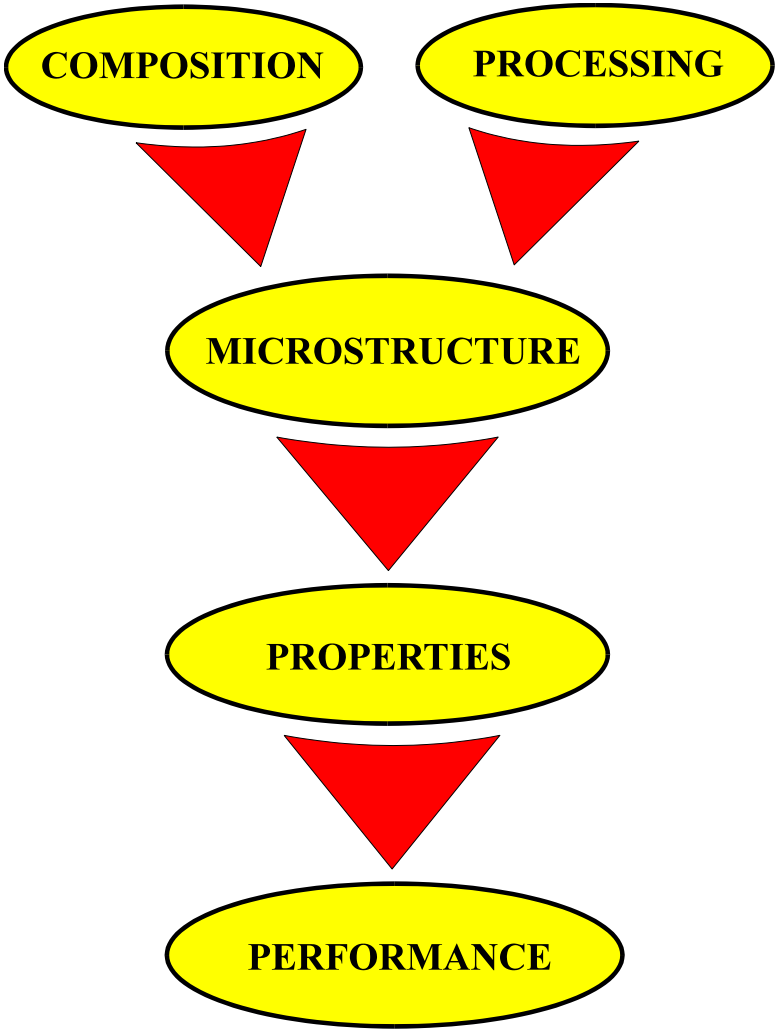
Outline

- Materials Science and Engineering
- Future directions for metals research
- Sustainability
- Computational materials design and engineering

The central materials paradigm







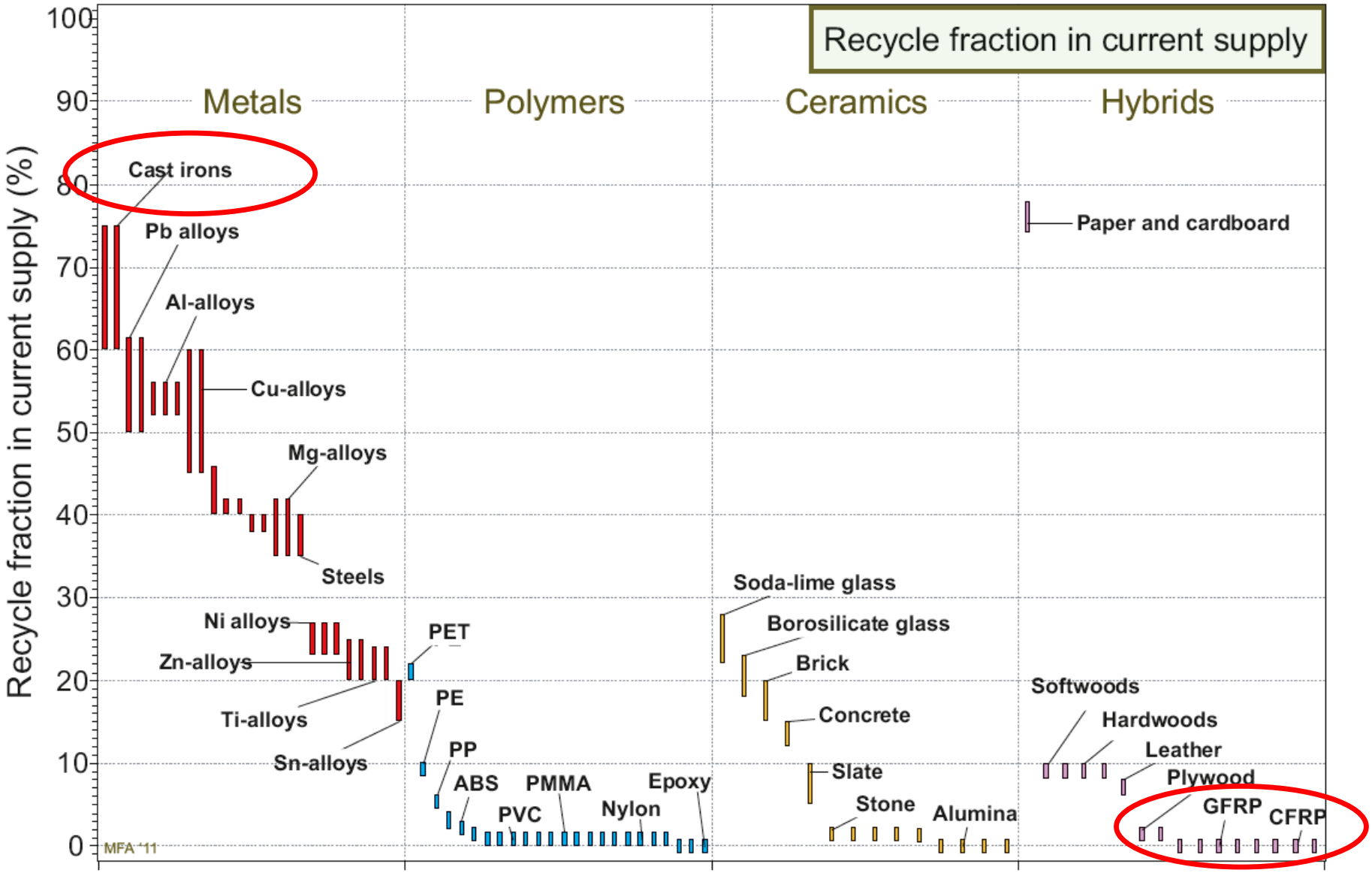
Classification of materials

Metals	**Ceramics**	**Polymers**	**Composites**	**Hybrids**	Nanomaterials

Structural	**Functional**
Mechanical	Chemical
	Biomedical
	Electrical
	Electronic
	Optical
	Magnetic

Quo Vadis Metalla?

- New alloys– eg high entropy alloys
- New metals for new processes – eg additive manufacturing
- Metals for a sustainable planet
- Computational materials design and engineering



Ashby, Shercliff and Cebon, Materials: Engineering Science Processing and Design, Elsevier, 2014

Which metals will become critical in which countries and when, and what will be the impact?

In future competition for land-use, which renewable materials will be constrained and what impact will this have?

Will it be possible to create a closed loop materials system?

Would we be better off with fewer materials?

Materials Design

Materials Design

Chocolate and cognac cake

This cake is so moreish. It's an elegant, indulgent way to finish a great meal. All this cake needs is a dollop of whipped cream.

SERVES 10–12

- 400 g (14 oz) good-quality dark chocolate (I use Valrhona 53% cocoa solids), broken up
- 6 free-range eggs, separated
- 150 g (5½ oz) caster (superfine) sugar
- 100 ml (3½ fl oz) good-quality cognac
- 300 ml (10½ fl oz) thin (pouring/whipping) cream
- unsweetened cocoa powder or icing (confectioners') sugar, to serve

+ Preheat the oven to 170°C (325°F/Gas 3). Cut a piece of baking paper to fit a 20 cm (8 inch) round cake tin, with a double layer for the side and a single layer for the base. Spray the tin with cooking oil and fit the baking paper snugly. Don't use a springform tin here — it needs to be solid.
+ Melt the chocolate in a stainless-steel bowl set over a saucepan of hot water ensuring the base of the bowl doesn't touch the water. Don't let the water boil, as you can scald the chocolate. Remove the chocolate from the heat and let it return to room temperature.
+ Using an electric mixer, beat the egg yolks and 100 g (3½ oz) of the caster sugar until pale and creamy. Add the cognac and continue to beat until well combined. Add the chocolate and stir until completely incorporated, then slowly stir in half the cream. Set aside.
+ Whip the remaining cream until soft peaks form. Set aside. Whisk the egg whites in a very clean bowl until soft peaks form, then slowly add the remaining caster sugar and whisk until very firm. Fold the whipped cream into the chocolate mixture, then gently fold in the egg whites.
+ Pour the cake mixture into the prepared tin, place the tin in a deep roasting tin and add enough hot water to come 2.5 cm (1 inch) up the side of the tin. Bake for 45 minutes, then turn the oven temperature down to 150°C (300°F/Gas 2) and bake for another 45 minutes. Turn the oven off and leave the cake in the oven for 40 minutes, then remove to a wire rack. Run a knife around the inside edge of the tin and turn it onto a plate or a board — the cake should slide out easily but be extremely careful as the cake is so soft and fragile. Sprinkle with cocoa powder or icing sugar. To slice the cake, use a knife dipped in hot water and clean the knife after each cut. You will only want a slither per person as this cake is so rich.

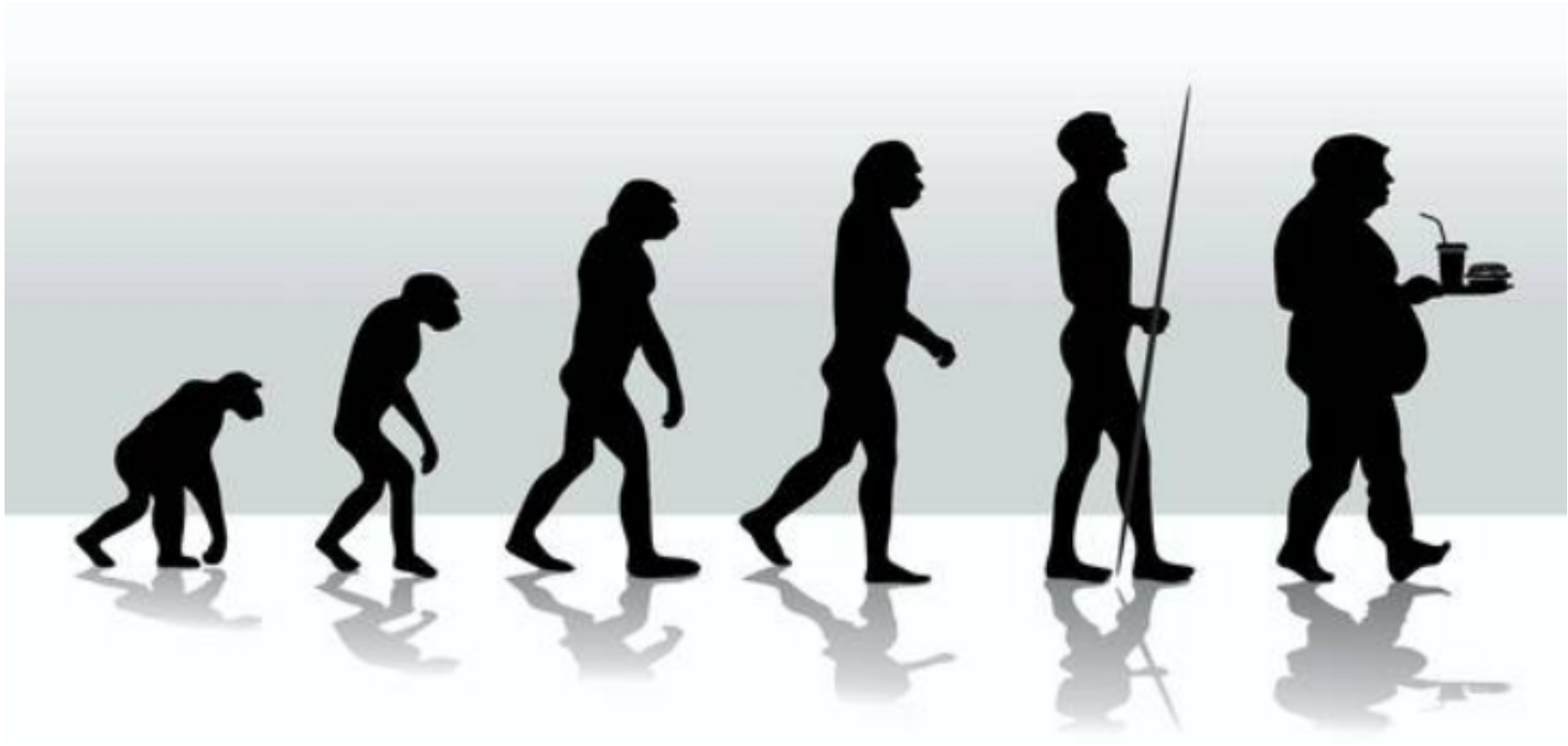
NOTES

The quality of the chocolate you use is directly proportional to the quality of the cake. This rule also applies to the cognac.

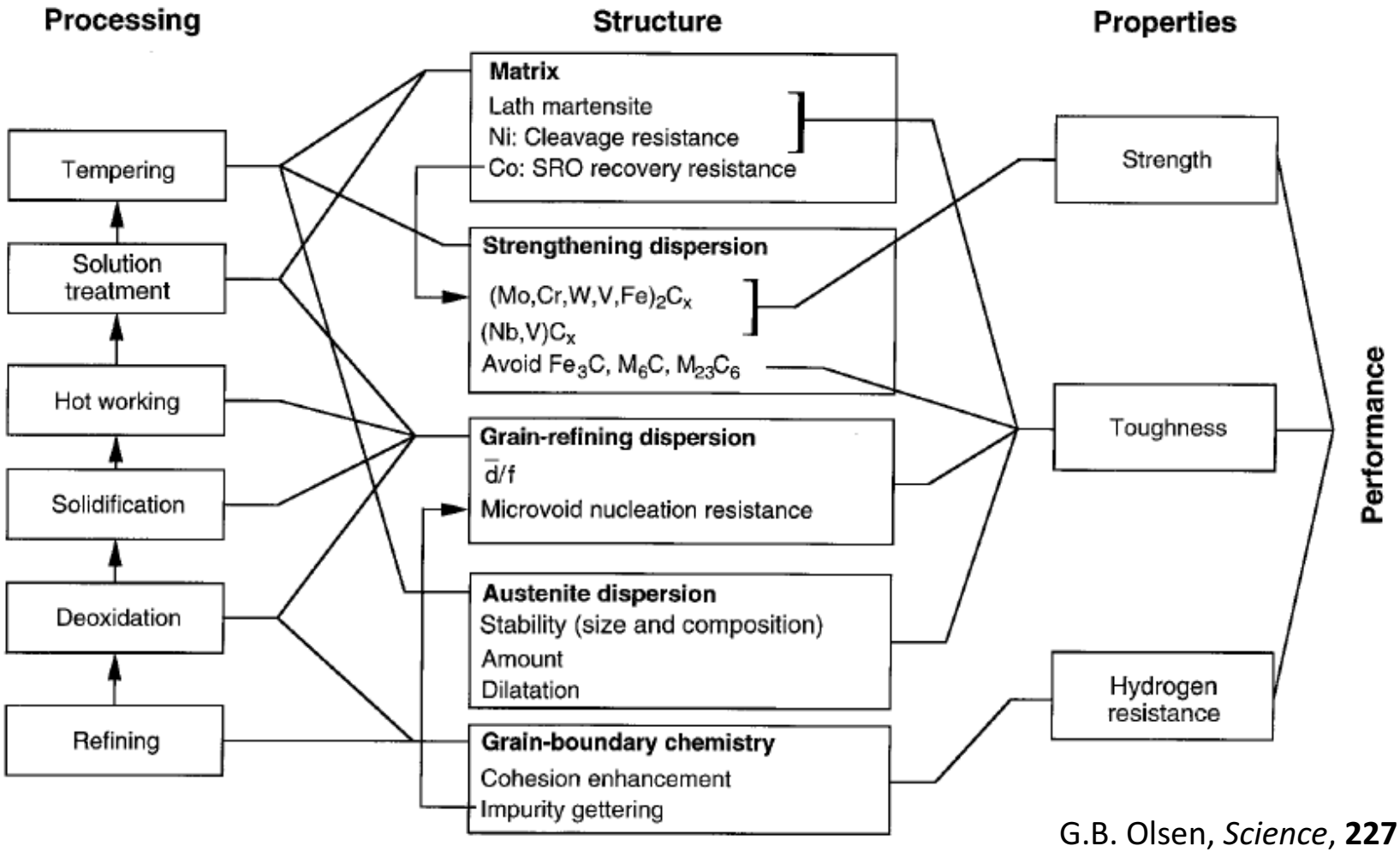
This cake rises like a soufflé, since that's really what it is. It will fall and set slowly in the oven as it cools, so don't be tempted to take it out too soon.

This cake will last for 3 days, covered, at room temperature. Don't refrigerate it: it will set like a brick!

Materials Design



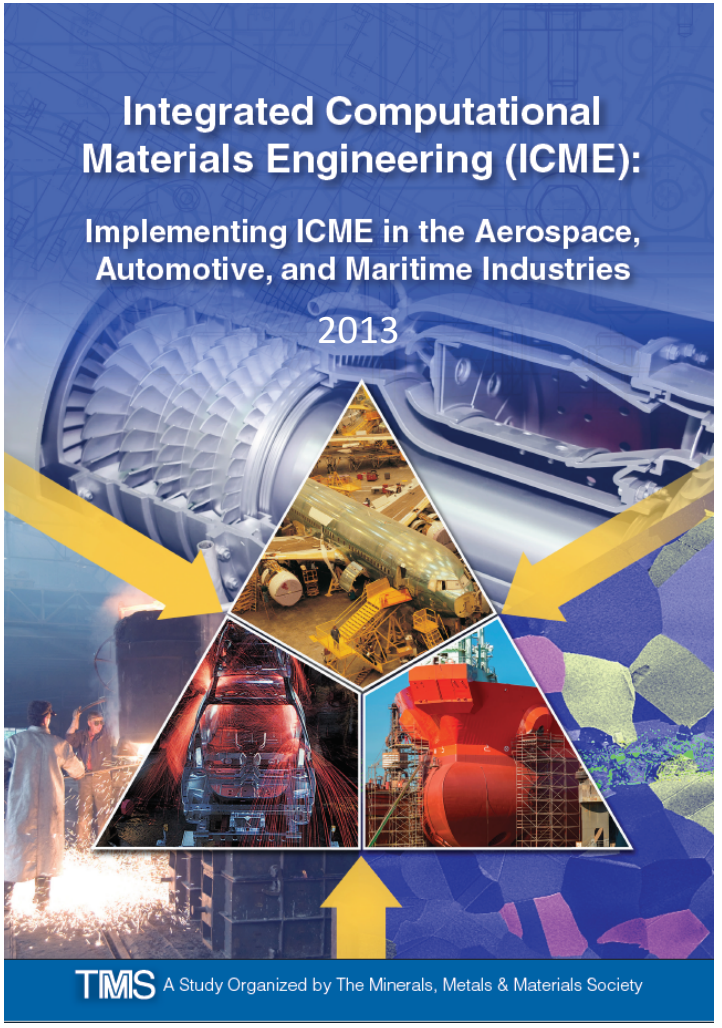
Materials Design



G.B. Olsen, *Science*, **227** (1997) p1237

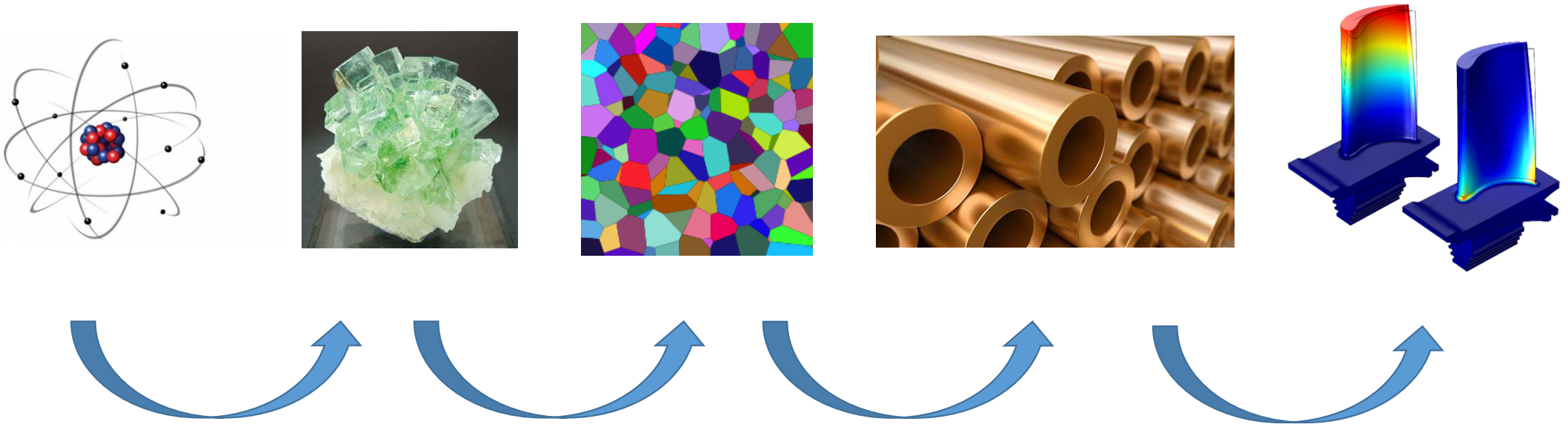

Integrated Computational Materials Engineering
A Transformational Discipline for Improved Competitiveness and National Security
2008
NATIONAL RESEARCH COUNCIL
OF THE NATIONAL ACADEMIES


Materials Genome Initiative
for Global Competitiveness
June 2011

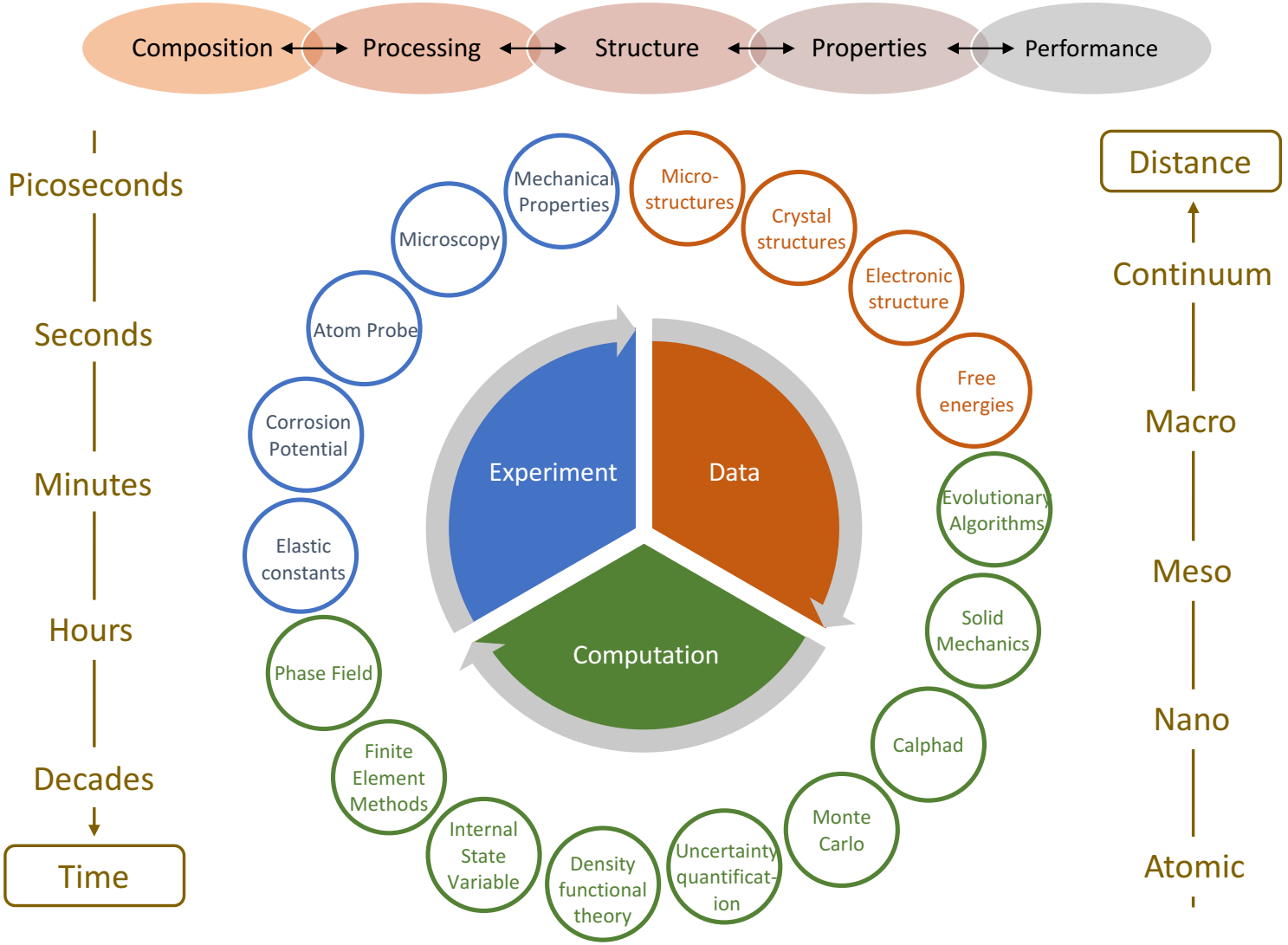

Integrated Computational Materials Engineering (ICME):
Implementing ICME in the Aerospace, Automotive, and Maritime Industries
2013
TMS A Study Organized by The Minerals, Metals & Materials Society

Integrated Computational Materials Engineering

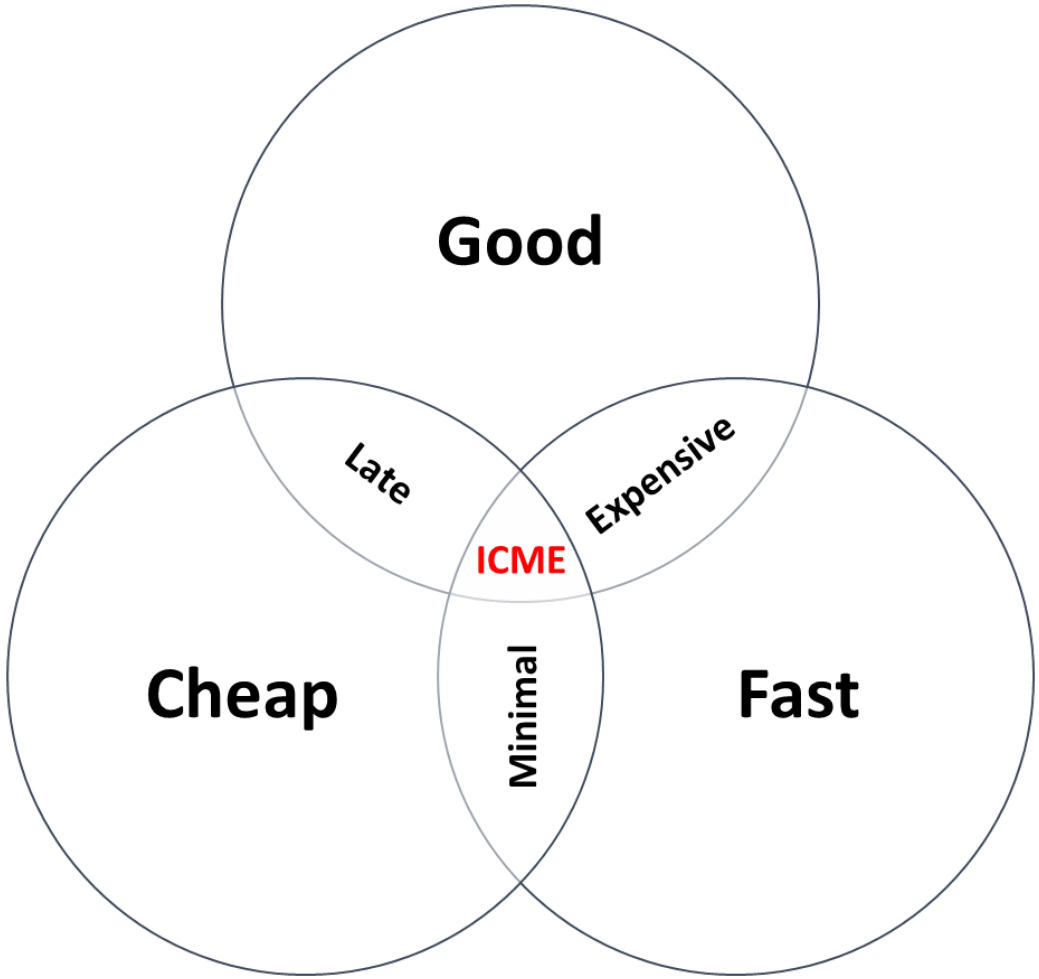
links composition with manufacturing process, the modelling of atomic interactions, the development of microstructure and the prediction of properties for the material and the component.



The Integrated Computational Materials Engineering Framework



The Holy Grail of Materials Design



ICME in Practice

- Ferrium S35 – QuesTek (from design to flight in 10 years, savings of approximately $50m)
- Ferrium M54 – QuesTek (from design to flight in 7 years)
- Virtual Aluminum Castings – Ford (20% reduction in time and 7:1 return on investment)
- High strength 18K gold watch – Apple
- Anodizable Aluminium watch and phone - Apple

ICME Research Needs

- Digital data infrastructure
- Materials informatics
- Models which link across scales and processes
- Uncertainty quantification
- Skilled workforce

ICME in the USA

Federal Agencies	Companies	Laboratories	Universities	Projects
DoE	GE	Naval Research Laboratory	Northwestern	Advanced high strength steels
DoD	Lockheed Martin	Army Research Laboratory	Michigan	Additive manufacturing of stainless steels
DARPA	Boeing	Air Force Research Laboratory	Ohio State	Cast aluminium alloys
Office of Naval Research	Ford Motor Co	Lawrence Livermore National Laboratory	MIT	Materials in extreme dynamic environments
Army Research Office	GM	Sandia National Laboratory	Georgia Tech	Electronic materials
Air Force Office of Scientific Research	Fiat-Chrysler	Argonne National Laboratory	UC Santa Barbara	Sheet forming of titanium
NIST	Caterpillar	Oak Ridge National Laboratory	Mississippi State	Magnesium
NSF	ArcelorMittal	Pacific Northwest National Laboratory	Tennessee	Carbon fibre composites for lightweight vehicles
	US Steel	Ames National Laboratory	Maryland	Nanosensors
	Dow Chemical		Clemson	
	John Deere		Colorado School of Mines	
	Cummins		Johns Hopkins	
	Mercury Marine		Utah	

ICME in Europe and Asia

- 7th European Framework Project, RWTH Aachen & KTH
- European Horizon 2020 Centres of Excellence (x3),
- Thermo-Calc Software, Sweden and Sente Software (JMatPro), UK
- Japan, National Centre for Materials Science (NIMS), Center for Materials Research by Information Integration
- Tohoku University, Center for Computational Materials Science
- Beijing Computational Science Research Center, Chinese Academy of Engineering Physics

ICME in Australia

National Australian Symposium on ICME, University of Melbourne, 19 February 2018

Plenary Speakers: Professor Tresa Pollock, UC Santa Barbara

Professor Dave McDowell, Georgia Tech

Google: UniMelb Hallmark ICME

Summary

- ICME will accelerate the insertion of new materials into products and systems.
- ICME will reduce the cost of materials and process development.
- ICME will transform materials research.
- ICME is a big opportunity but has many challenges….

Integrated Computational Materials Engineering

links composition with manufacturing process, the modelling of atomic interactions, the development of microstructure and the prediction of properties for the material and the component.