



EVROPSKÁ UNIE  
Evropské strukturální a investiční fondy  
Operační program Výzkum, vývoj a vzdělávání



Audio test:



# C8965 Equilibrium States and Phase Transformations of Materials



Lecturer: Prof. RNDr. Jiří Sopoušek, CSc.

E-mail: [sopousek@mail.muni.cz](mailto:sopousek@mail.muni.cz), tel.: 549497138

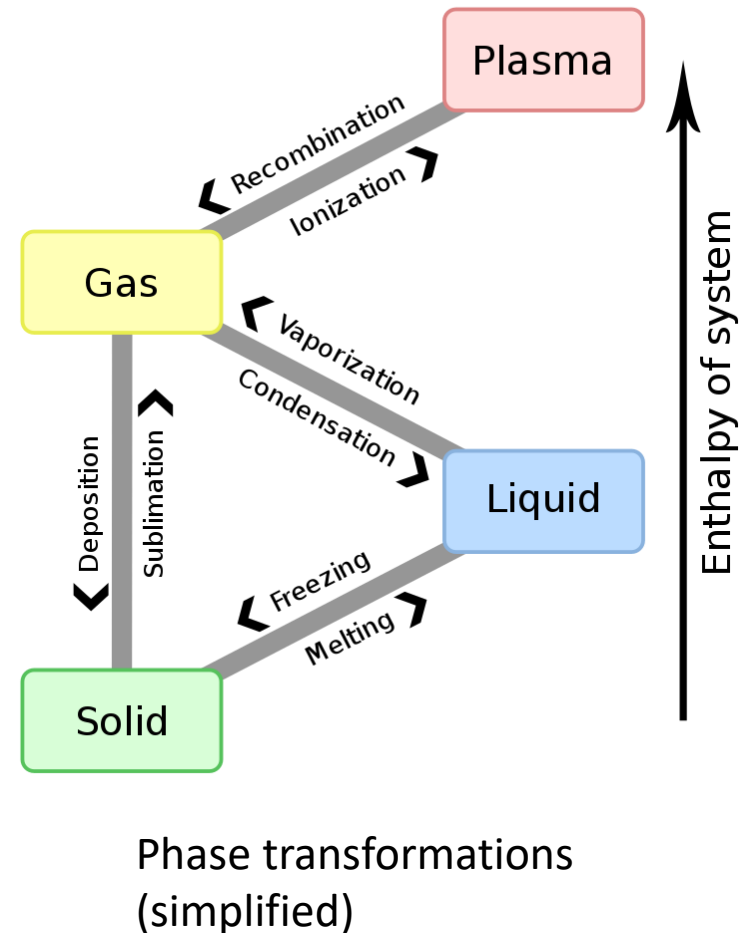
Office: UKB A12/M231

Department of Chemistry: <http://ustavchemie.sci.muni.cz/>

## Brno, PS

# Anotation

- Advanced equilibrium Thermodynamics of materials. The conditions of phase equilibria. The Gibbs energy and chemical potential of the system.
- The application of computational thermodynamics on the description of the equilibrium in the materials. Stable and metastable phase diagrams of multicomponent systems.
- Phase transformations, diffusion less phase transformations. Diffusion and nucleation mechanisms of phase transformations.
- Simulation of diffusion controlled phase transformations.
- Transformation diagrams of the materials.
- Advanced methods of study of phase transformations. Methods of thermal analysis of materials.



# Subject administration

- 2hrs/week
- Use of: **Interactive syllabi of the subject**
- (2+2) credits requirements: short presentation, passing the exam.

Teaching time:

Class UKB A12/M311

Study materials:

[Information system of Masaryk University](#)

# Interactive syllabi (IS MU)

The screenshot displays the IS MU web application interface. At the top, the browser address bar shows the URL <https://is.muni.cz/auth/el/1431/podzim2018/C8965/index.qwarp>. The page header includes the MU logo and the text "INFORMATION SYSTEM". The main content area is titled "C8965 Equilibrium states and phase transformation..." and lists three study weeks with their respective topics and teacher recommendations. A sidebar on the left lists "MY APPLICATIONS" including My Mail, Calendar, Guarantor, Teacher, Supervisor, and Publications. A sidebar on the right lists the course title and the three study weeks. The bottom of the screen shows the Windows taskbar with various application icons and the system clock indicating 13:26 on 22.1.2019.

**Study week 1: Introduction and basic thermodynamics of mixtures of materials.**  
Teacher recommends to study from 18/2/2019 to 24/2/2019.

**Study week 2: Phase equilibrium conditions inside multicomponent systems.**  
Teacher recommends to study from 25/2/2019 to 3/3/2019.

**Study week 3: Stable and metastable phase equilibria, calculation and prediction of phase diagrams. CALPHAD Method**

**C8965 Equilibrium states and phase transformation of materials**

- Study week 1: Introduction and basic thermodynamics of mixtures of materials.
- Study week 2: Phase equilibrium conditions inside multicomponent systems.
- Study week 3: Stable and metastable phase equilibria, calculation and prediction of phase diagrams. CALPHAD Method

# Interactive syllabi (content):

- Lectures (compressed file)
- Study materials (recommended pages)
- Movies
- Solution examples
- Testing

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CS

prof. RNDr. Jiří Sopoušek, CSc., učo 2405

🔌

C8965 Equilibrium states and phase transformation...

Home 🏠

MY APPLICATIONS

My Mail

Calendar

Guarantor

Teacher

Supervisor

Publications

Study week 1: Introduction and basic thermodynamics of mixtures of materials.

Lectures (compressed file):

📁

01L\_Introduction.zip

Study materials:

D.A. Porter: Phase Transformations in metals and Alloys, extent of study: pp. 0-xxx

M. Hiller: Phase Equilibria Phase Diagrams Phase Transformations, extent of study: pp. 0-yyy

Educative movies: (-)

Study test: (-)

⬅ Previous

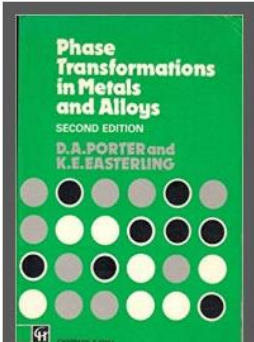
Next ➡

📖

Phase Transformations in Metals and Alloys

SECOND EDITION

D.A. PORTER and K.E. EASTERLING



☰ C8965 Equilibrium states and phase transformation of materials

➡ [Study week 1: Introduction and basic thermodynamics of mixtures of materials.](#)

🔒 Study week 2: Phase equilibrium conditions inside multicomponent systems.

🔒 Study week 3: Stable and metastable phase equilibria, calculation and prediction of phase diagrams. CALPHAD Method.

🔒 Study week 4: Diffusion and kinetic phenomena in materials. Nucleation. Interfaces and microstructure.

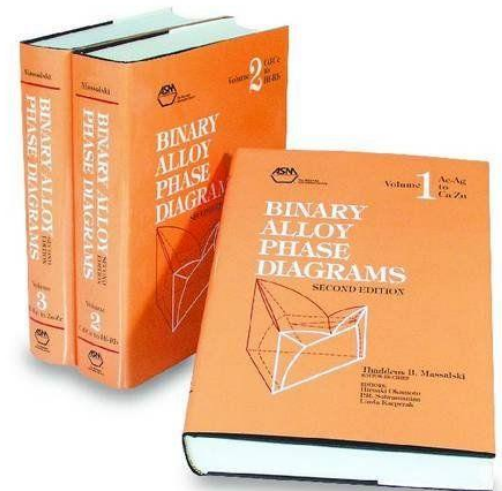
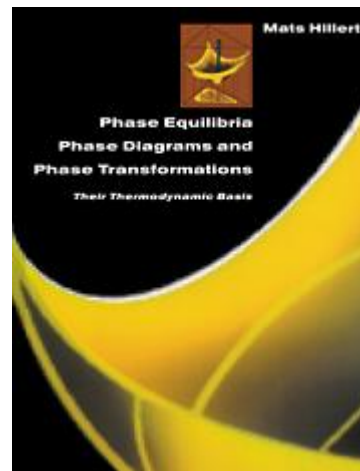
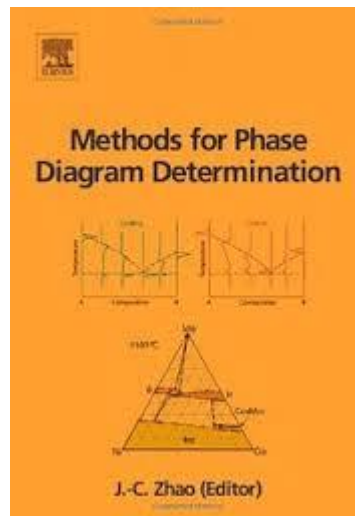
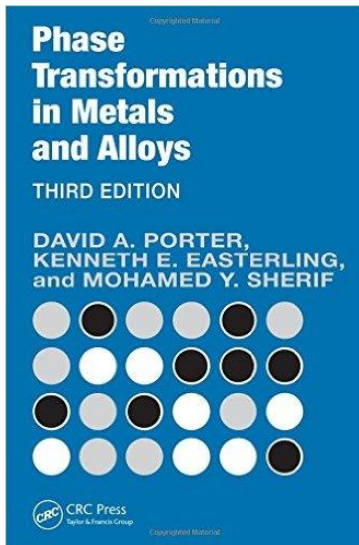
# Time shedule

Study week	Lecture	Study week	Program
1.	Introduction and basic thermodynamics of mixtures.of materials.	8.	Crystallization and melting.
2.	Phase equilibrium conditions inside multicomponent systems.	9.	Diffusion controlled phase transformation(DICTRA), massive transformation.
3.	Stable and metastable phase equilibria, calculation and prediction of phase diagrams. CALPHAD Method.	10.	Non-diffusion phase transformations. Simulations of phase transformations controlled by diffusion.
4.	Diffusion and kinetic phenomena in materials. Nucleation . Interfaces and microstructure.	11.	Non-diffusion phase transformations. Simulations of phase transformations controlled by diffusion.
5.	Transformation diagrams of materials (TTT and CCT diagrams).	12.	Non-ferrous alloys and special materials.
6.	Heat treatment of materials.	13.	Short student`s presentation
7	Experimental methods . Thermal analysis (TGA, DTA, DSC, ...). Electron microscopy, diffraction methods, etc.	14.	SW Presentations (ThermoCalc, DICTRA)



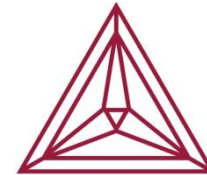
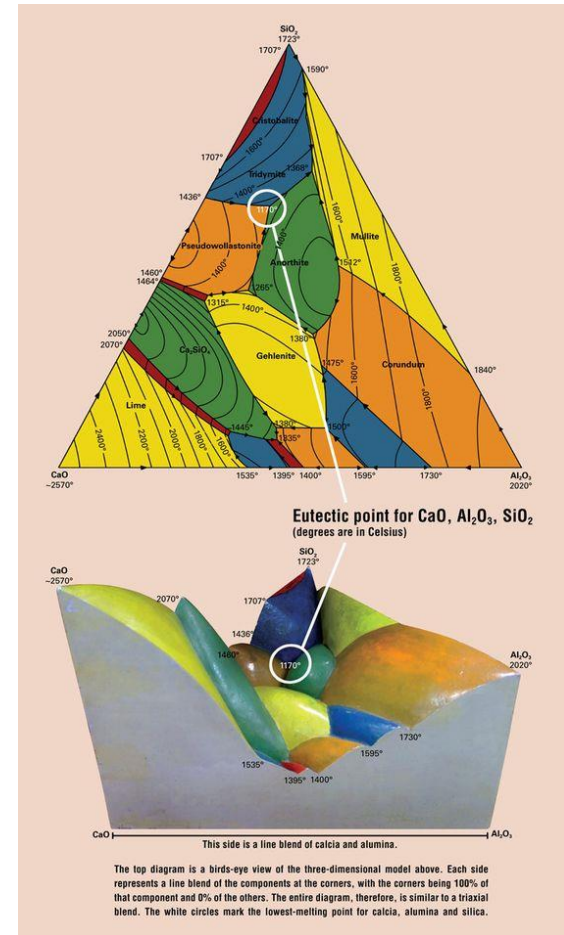
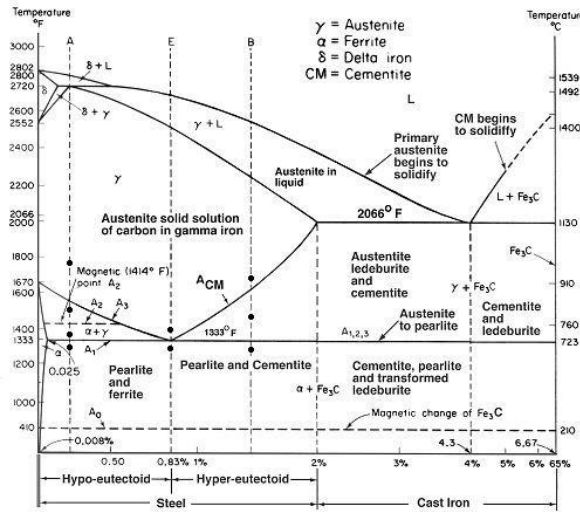
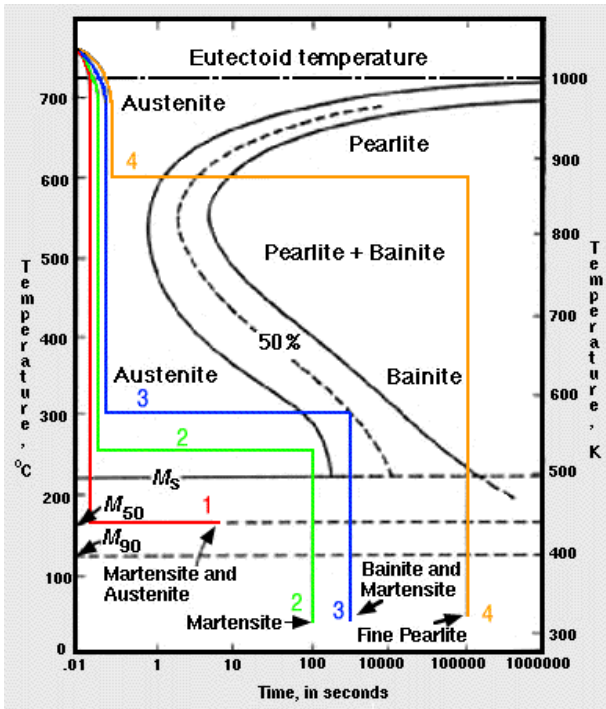
# Recommended literature

- PORTER, David A. Phase Transformations in Metal and Alloys. New York: Van Nostrand Reinhold, 1981. 445 s. ISBN 0-442-30439-0. [info](#) (<http://ebooks.bfwpub.com/pchemoup.php>, user: knihovna, password: uzivatell)
- SAUNDERS, Nigel a Peter A. MIODOWNIK. *Calphad : calculation of phase diagrams : a comprehensive guide*. Oxford: Pergamon, 1998. xvi, 479 s. ISBN 0-08-042129-6. [info](#)
- Mats Hillert: Phase Equilibria, Phase Diagrams and Phase Transformations (Their Thermodynamic Basis), 2nd Edition, ISBN: 9780521853514



## Learning Outcomes

- Phase diagram reading
- TTT and CCT reading
- Knowledge of transformations of common material
- SW: ThermoCalc, DICTRA





# Selected application of phase transformations

Videos:

[In Situ Electron Microscopy | Thermo Fisher Scientific - CZ](#)

[In-Situ Austenite-Ferrite Phase Transformation - YouTube](#)

[in situ phase transformation - Hledat Googlem](#)

Videos (insitu microscopy):

[In situ | Gatan, Inc.](#)

# Phase transformations for energy saving

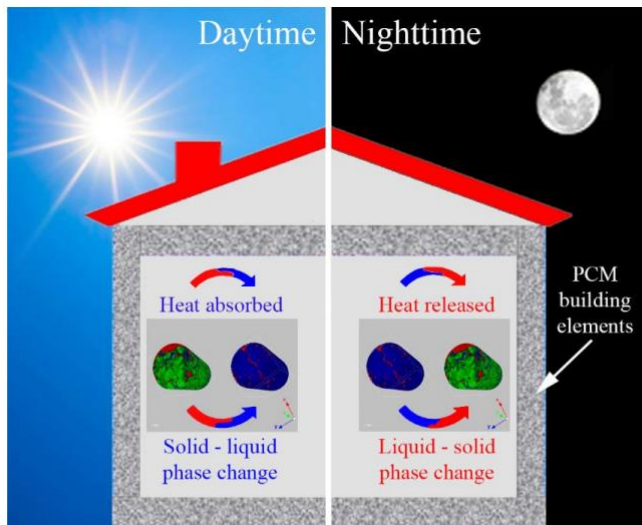


Figure 4. Charging process (working of PCM during daytime) and discharging process (working of PCM during nighttime).

	Material	Melting Temperature (°C)	Melting Enthalpy (J/g)
Fatty acids	Capric Acid	30.2	142.7
	Capric Acid	32	152.7
	Lauric acid	43.05	172.3
	Myristic acid	51.80	178.14
	Palmitic acid	60.42	233.24
	Stearic acid	54.29	188.28
Fatty acids esters	Butyl stearate	19	140
	Propyl palmitate	19	186
	Methyl palmitate	29	205
	Methyl eicosanate	45	230
	Methyl behenate	52	234
Alcohols	1-dodecanol	26	200
	Phenol	41	120
	Cetyl alcohol	49.3	141
Polyethylene glycol (PEG)	PEG 400	3.2	91.4
	PEG 600	22.2	108.4
	PEG800	25.39	133.6
	PEG 1000	34.89	143.62
	PEG 2000	52.63	180.70
	PEG 4000	48.95	183.10

[applsci-11-01490-v2.pdf](#)

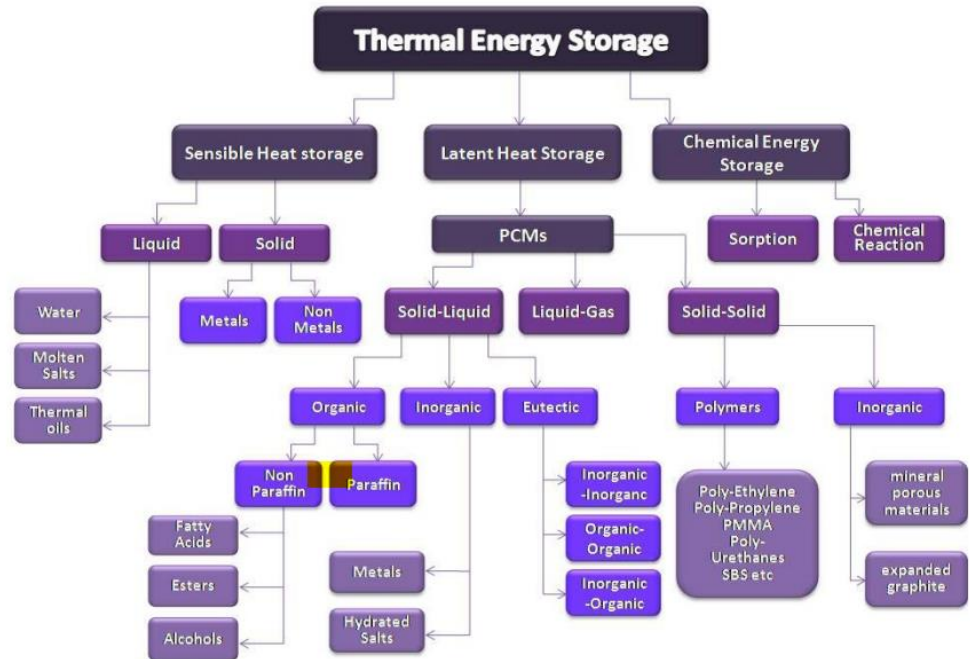


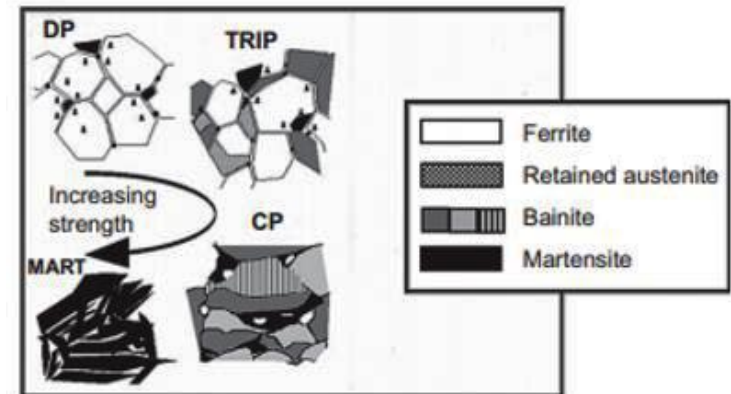
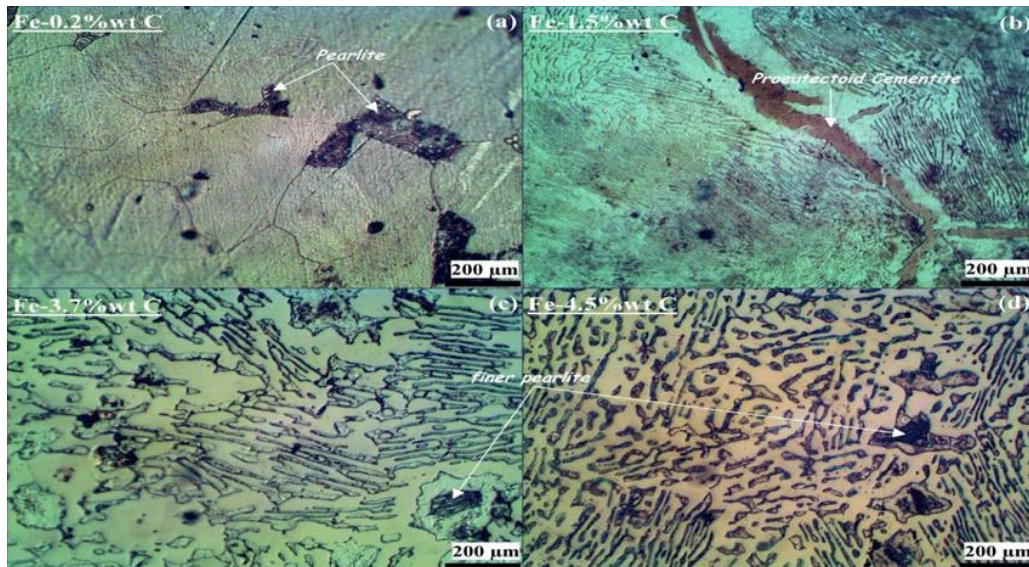
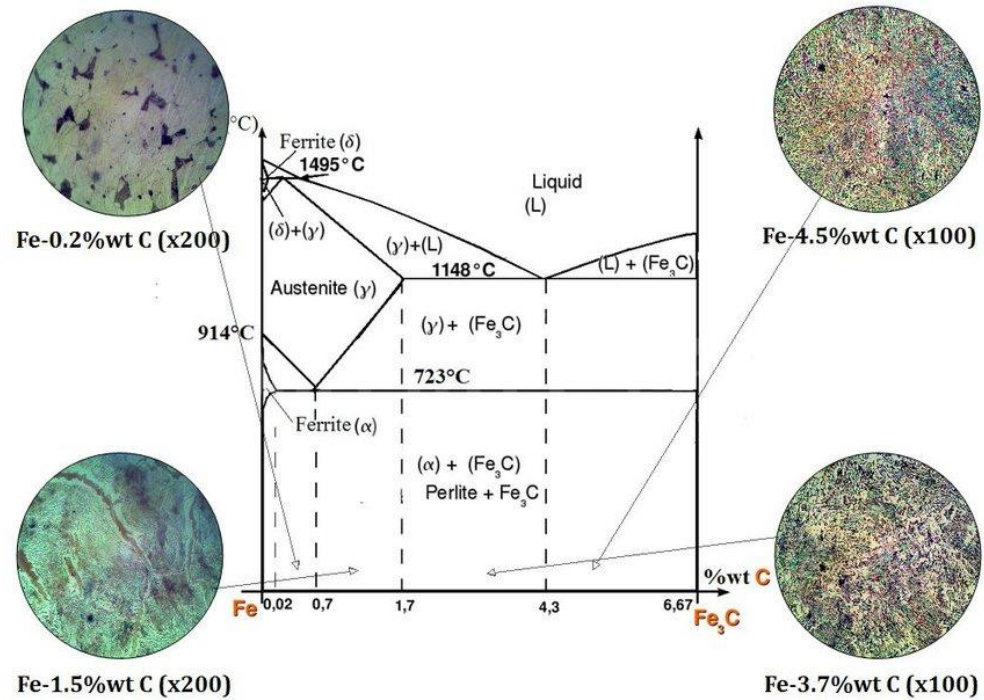
Figure 1. Classification of thermal energy storage types and materials.

Encapsulation needed

Latent heat of H<sub>2</sub>O: 333J/g

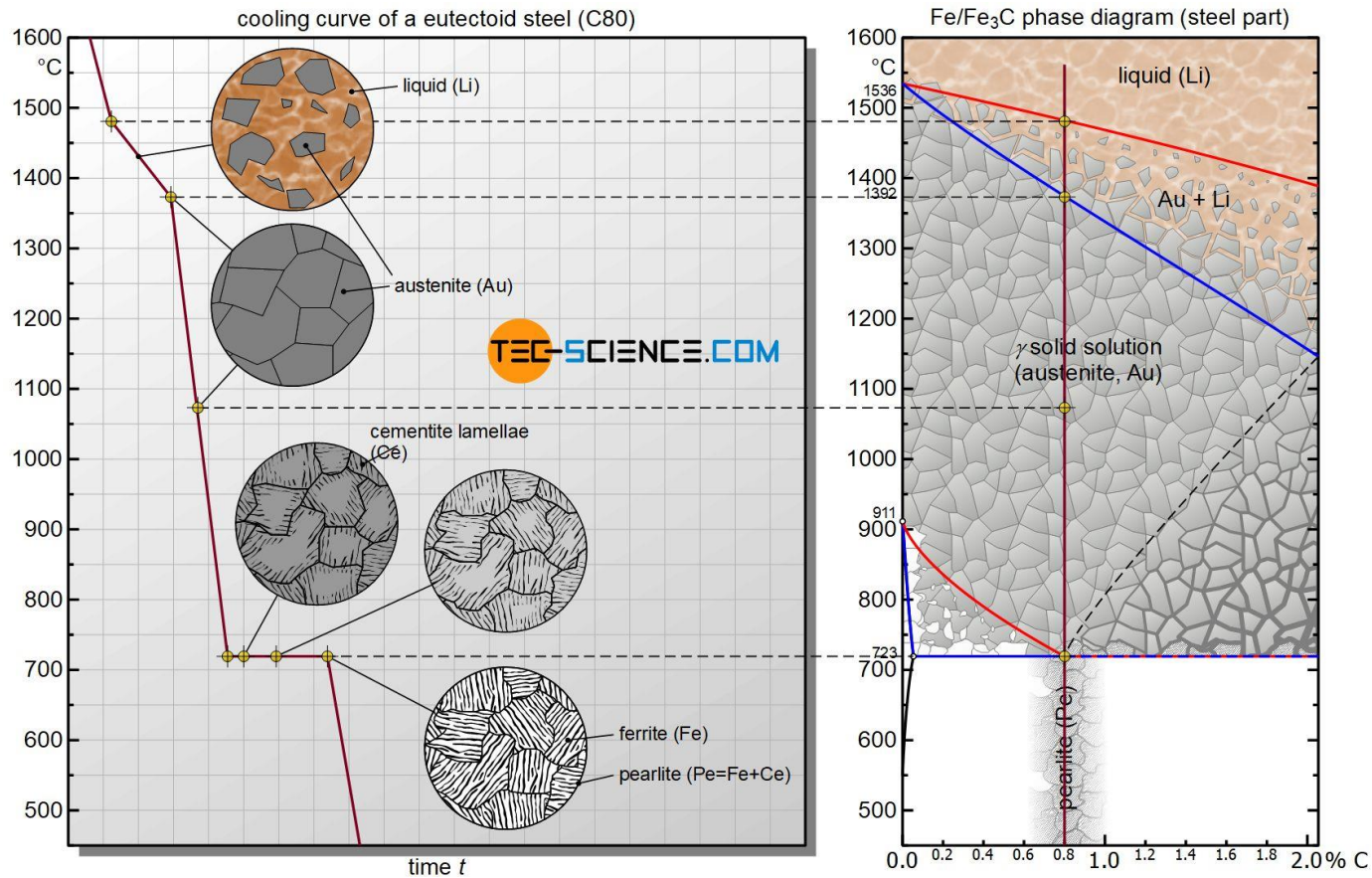
# Phase transformations and microstructure

[Optical micrograph of Fe-xC alloys, etched with 4% Nital](#) | [Download Scientific Diagram \(researchgate.net\)](#)





# Heat induced microstructure (eu.Fe-C)



[Phase transformations of steels in solidified state \(metastable system\) - tec-science](https://tec-science.com)

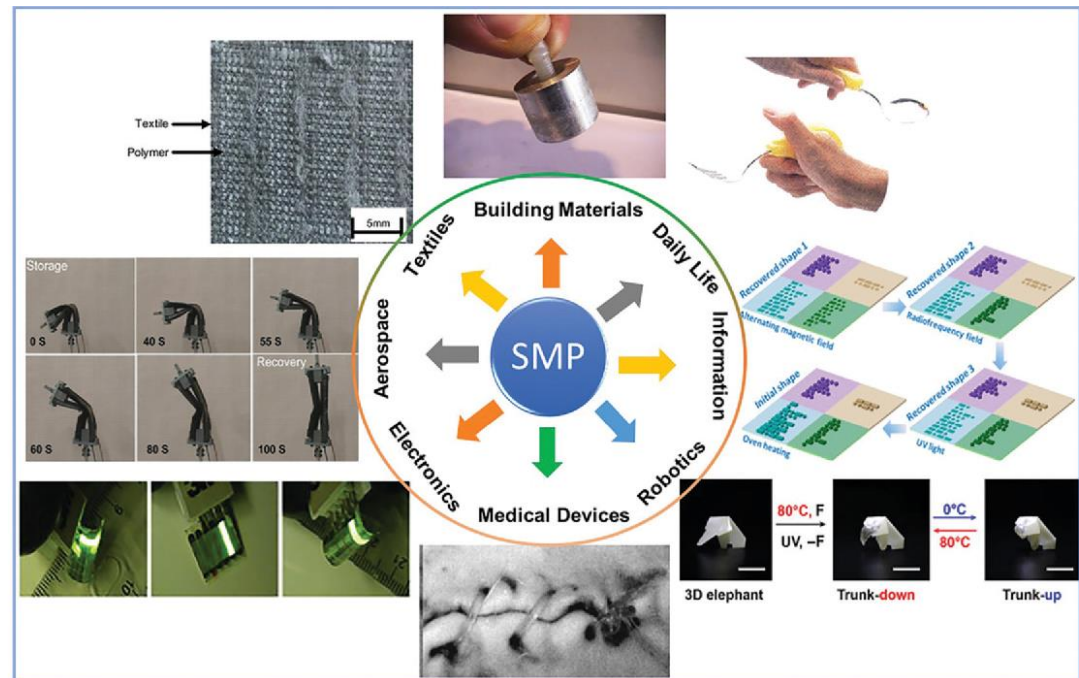
# Shape memory alloys

Videos:

[A shape memory alloy: why nitinol items return to their initial state - YouTube](#)

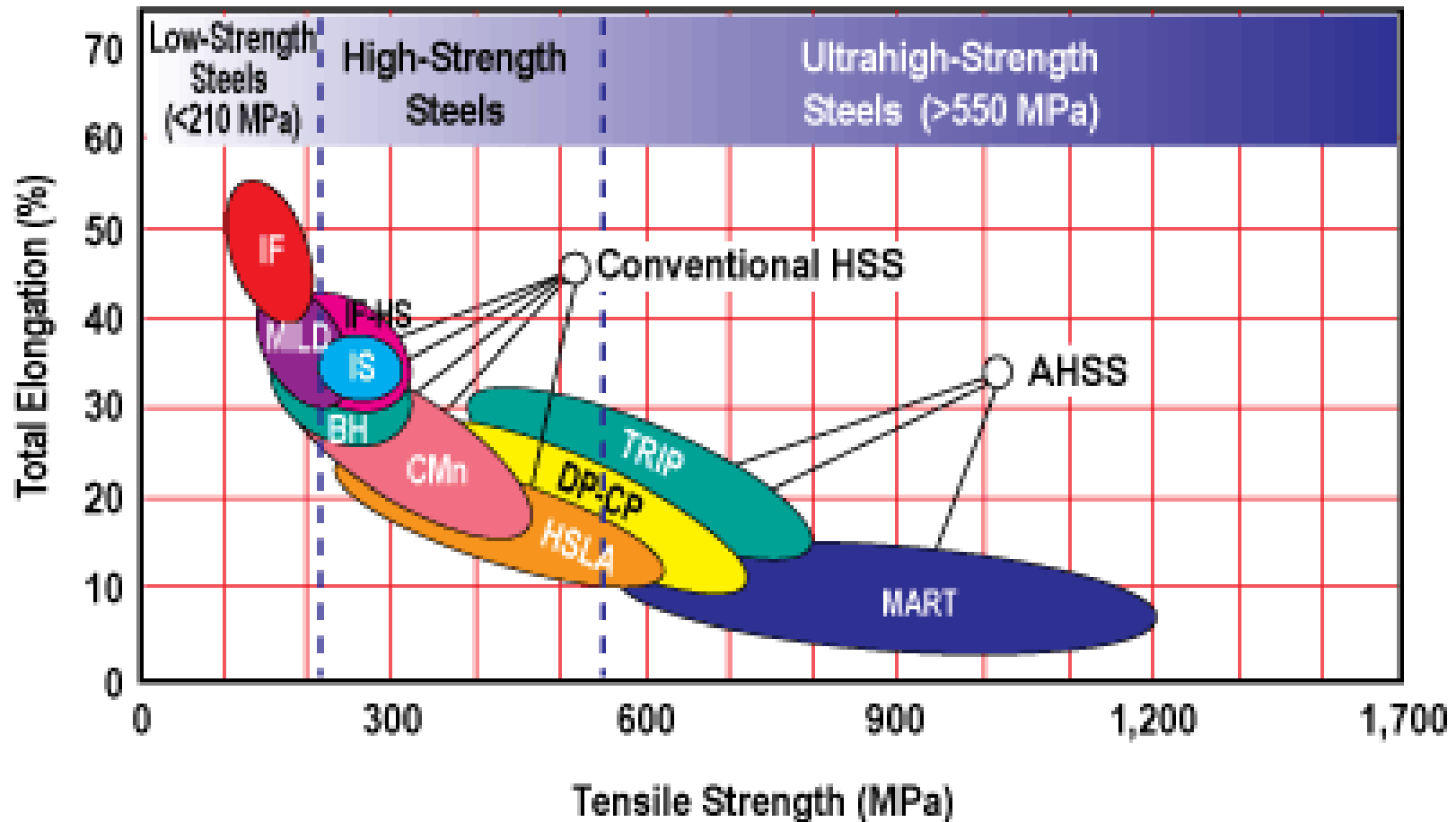
[Mini Lesson 5: What is a Shape Memory Alloy? - YouTube](#)

[Figure 1 from The research status and challenges of shape memory polymer-based flexible electronics | Semantic Scholar](#)



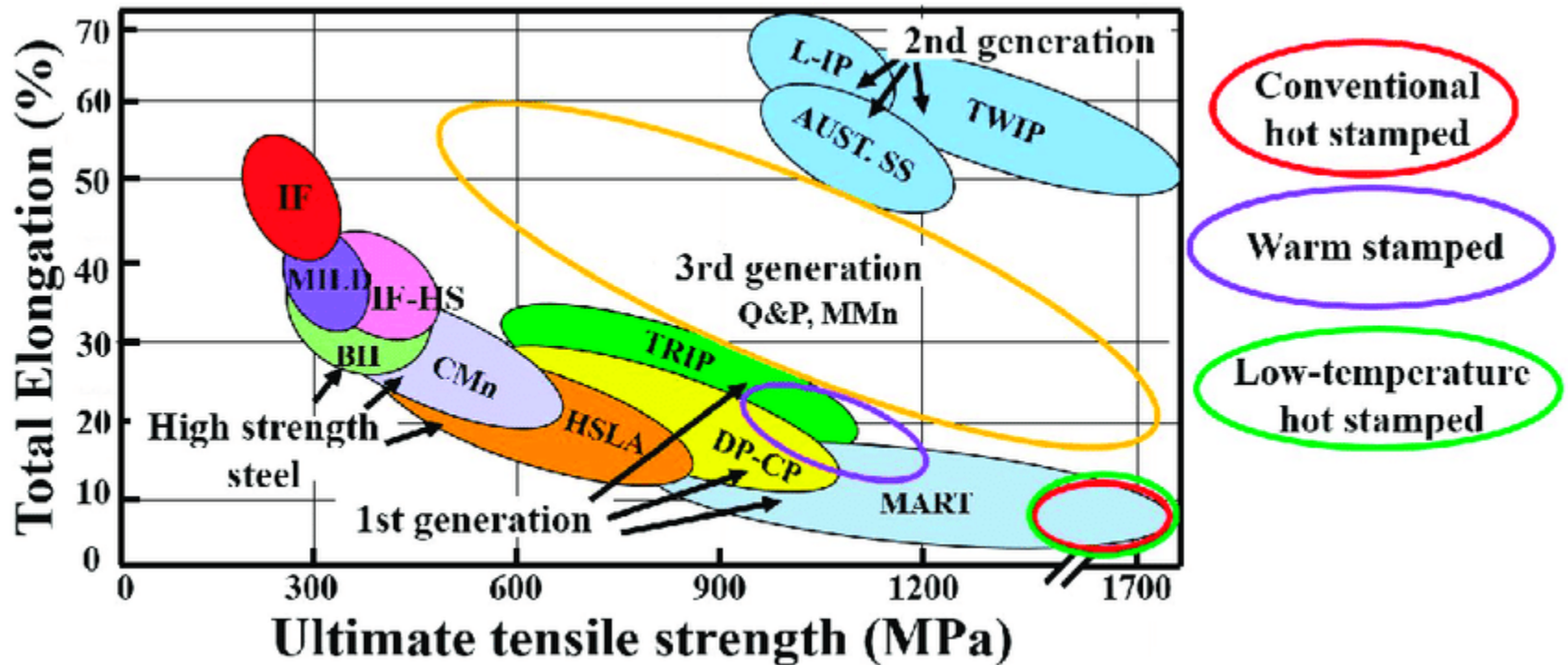
applications of SMPs in the areas of medical devices,<sup>43</sup> textiles,<sup>70</sup> aerospace,<sup>71</sup> building materials,<sup>72</sup> robotics,<sup>73</sup> daily life,<sup>74</sup> elec

# High strength materials - steels



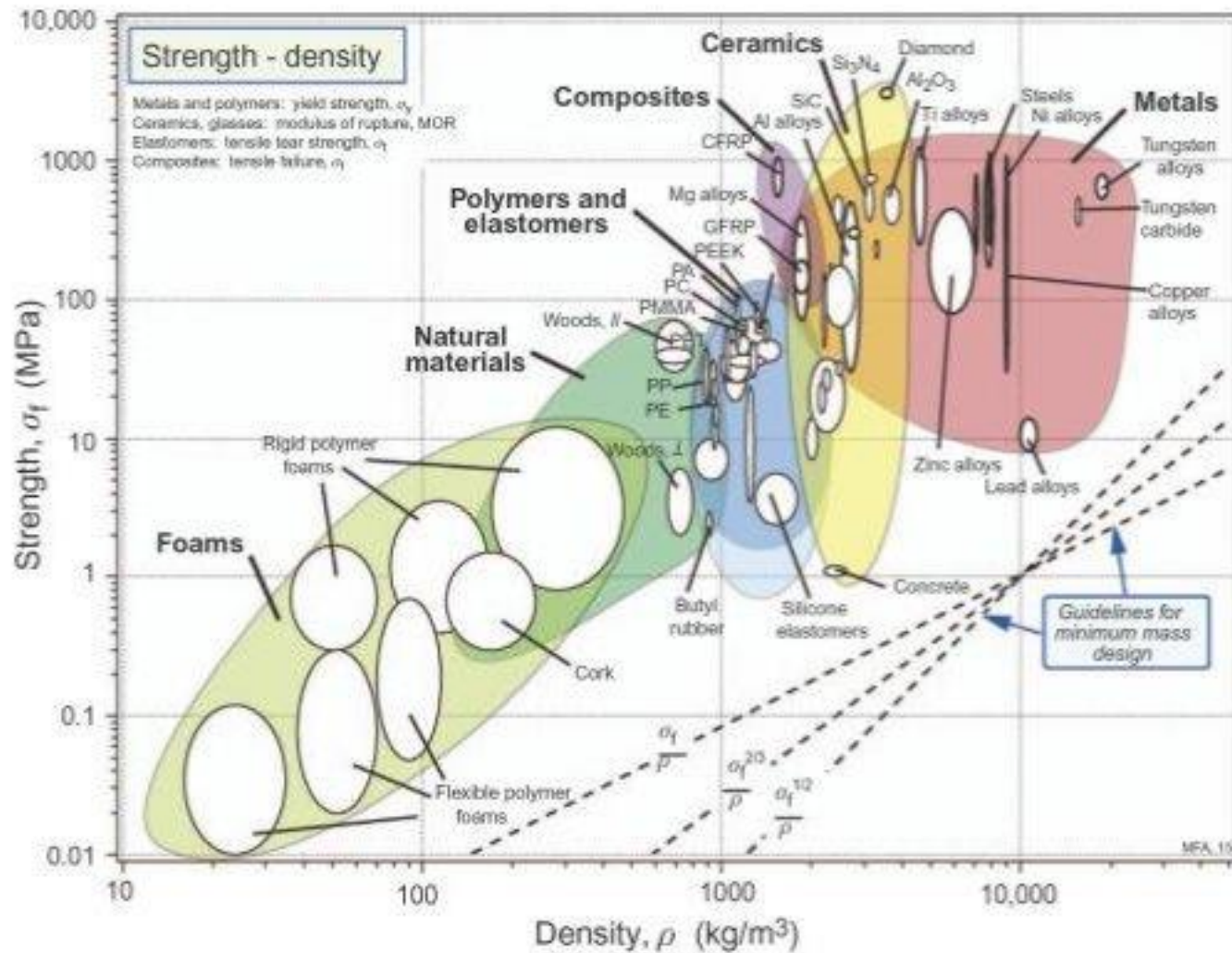


# High strength materials - steels



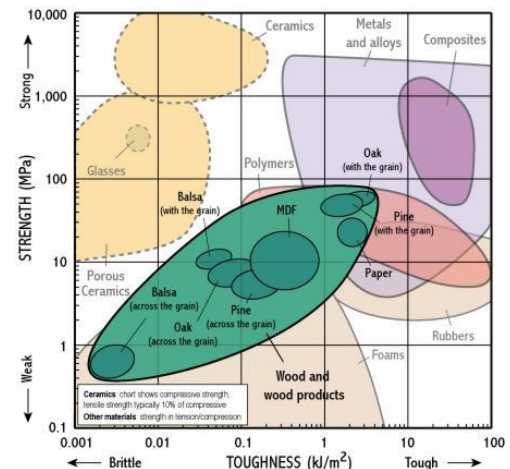
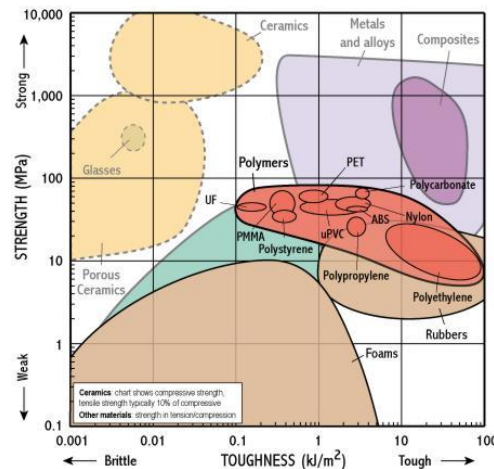
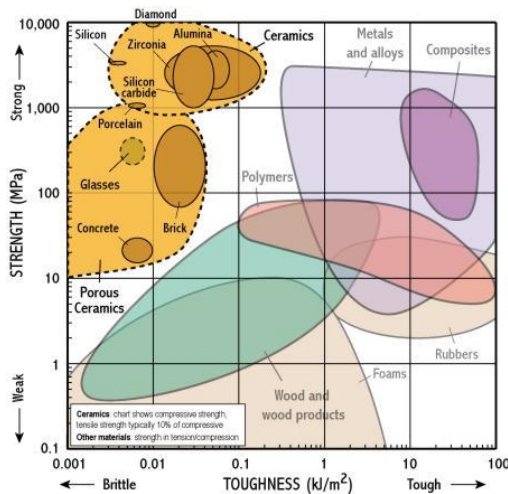
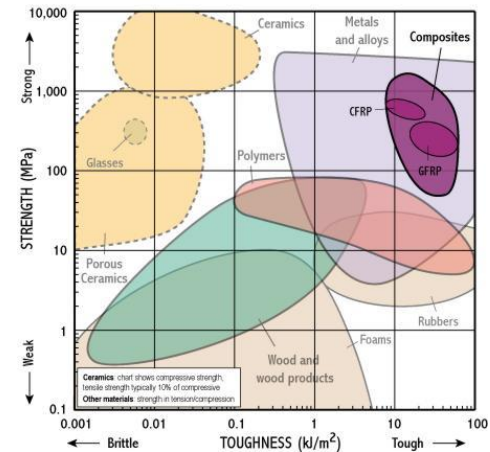
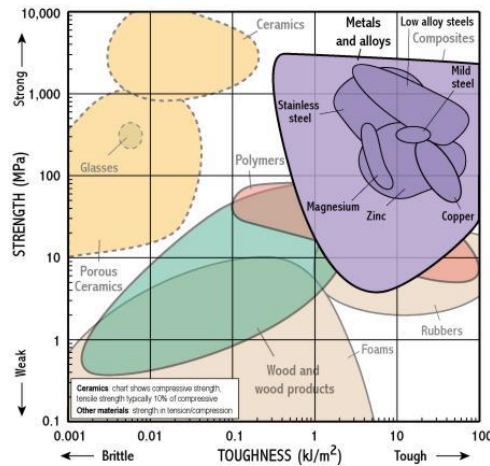
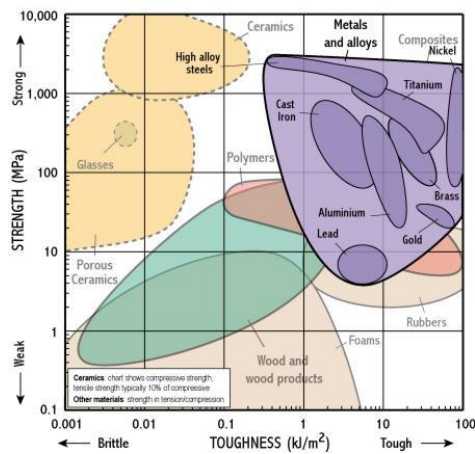
Comparison between mechanical properties of various types of industrially manufactured steel grades and of parts produced by various hot stamping processes. Q&P: quenching and partitioning; TRIP: transformation induced plasticity. IF: interstitial-free steels; MILD: mild steels; IF-HS: interstitial-free high-strength steels; BH: bake hardening steels; CMn: carbon-manganese steels; HSLA: high-strength low-alloy steels; TRIP: transformation induced plasticity steels; DP-CP: dual phase and complex phase steels; MART: martensitic steels; Q&P: quenching and partitioning steels; MMn: medium-Mn steels; AUST. SS: austenitic stainless steel; L-IP: lightweight steels with induced plasticity; TWIP: twinning-induced plasticity steels.

# Strength

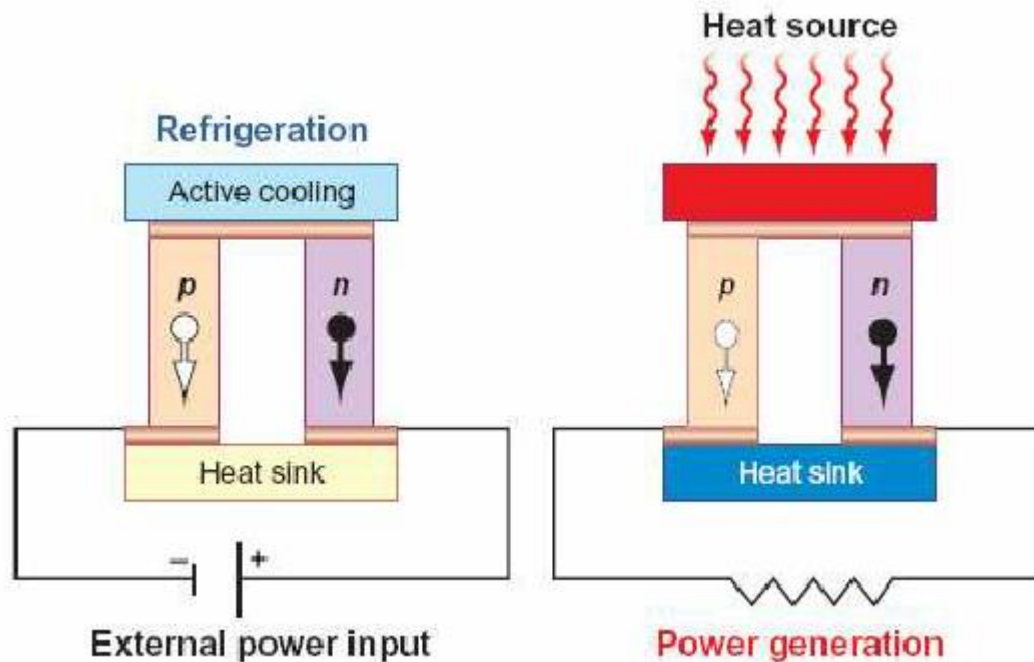


# Strength vs. toughness

- Strength measures the resistance of a material to failure, given by the applied stress (or load per unit area)
- The chart shows yield strength in tension for all materials, except for ceramics for which compressive strength is shown (their tensile strength being much lower)
- Toughness measures the energy required to crack a material; it is important for things which suffer impact
- There are many cases where strength is no good without toughness, e.g. a car engine, a hammer
- Increasing strength usually leads to decreased toughness
- Tempered steel is tougher but less strong than after quenching.

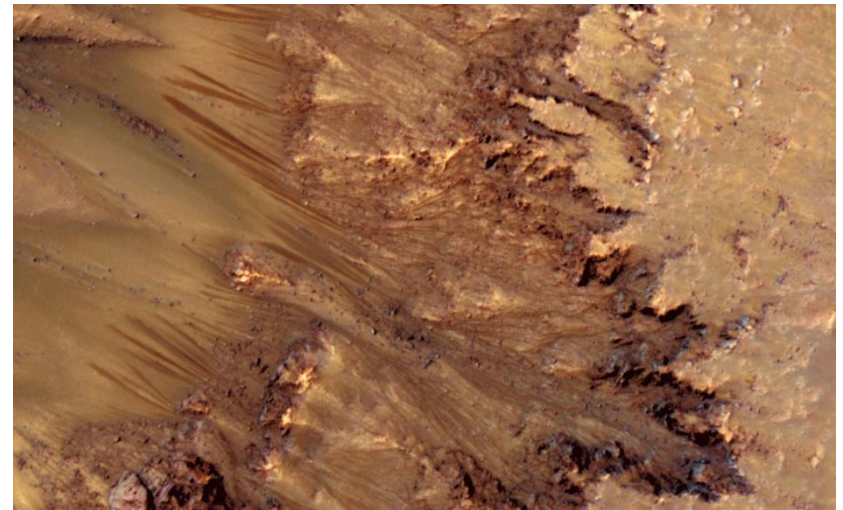
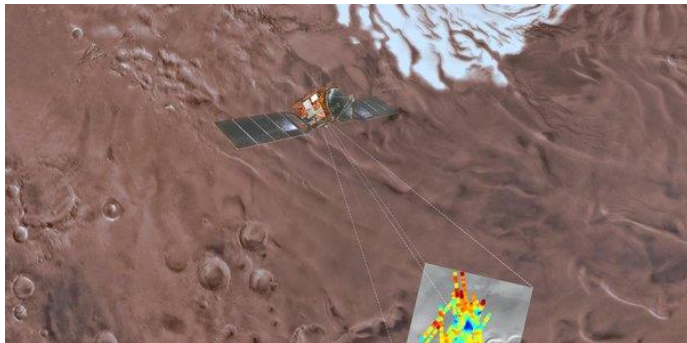
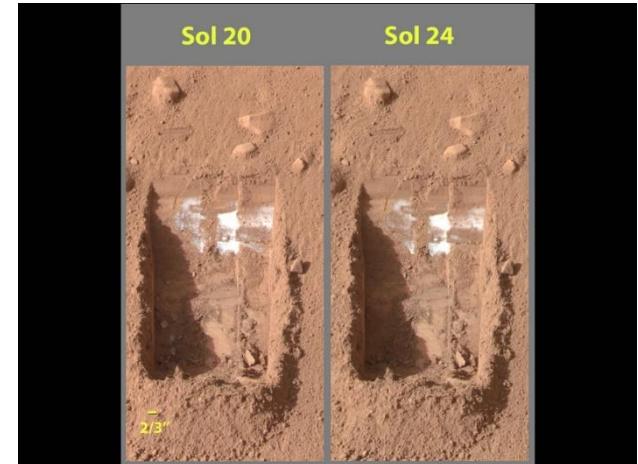
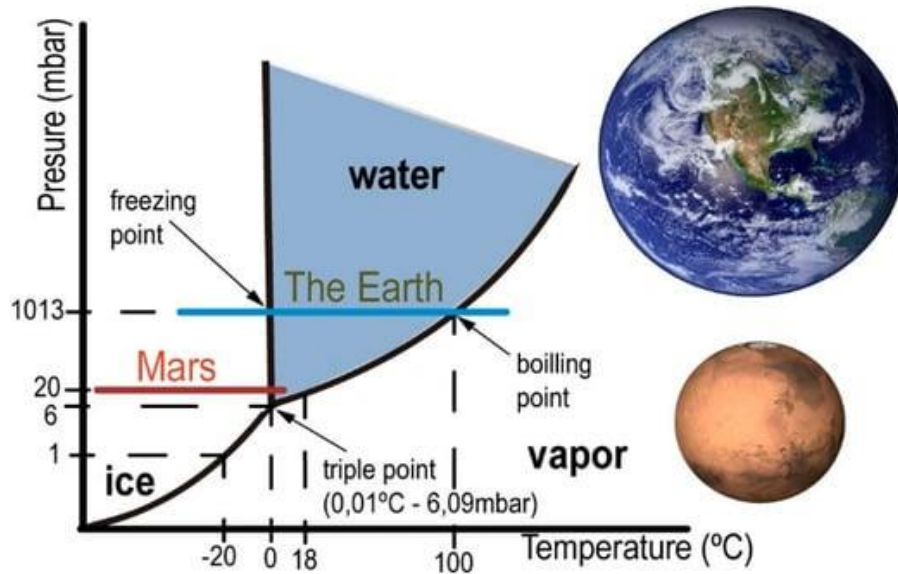


2017-2019, GA17-12844S: **Thermal and phase stability of advanced thermoelectric materials** (Investigator: P. Brož). Focused also on nanostructured thermoelectric materials.





# Phase transformations outside the Earth



[Water, Water Everywhere, but Not All Drops Have Life \(phys.org\)](http://phys.org)

# Discussion



**CEITEC:**

<http://www.ceitec.muni.cz/index.php>



**Department of Chemistry:**

<http://ustavchemie.sci.muni.cz/>

