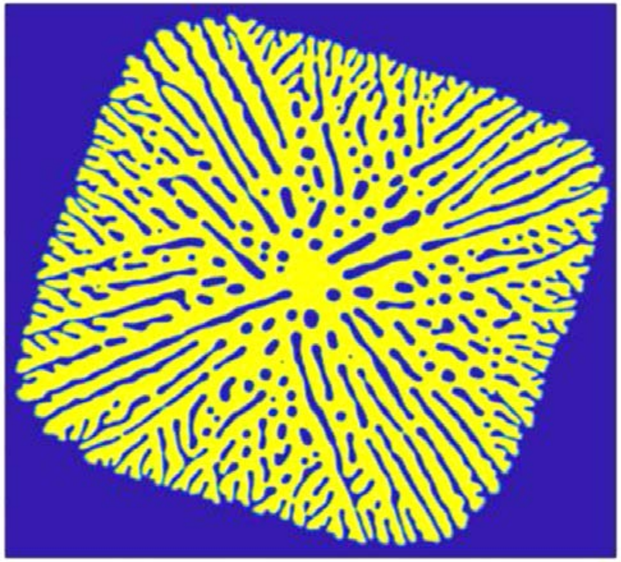
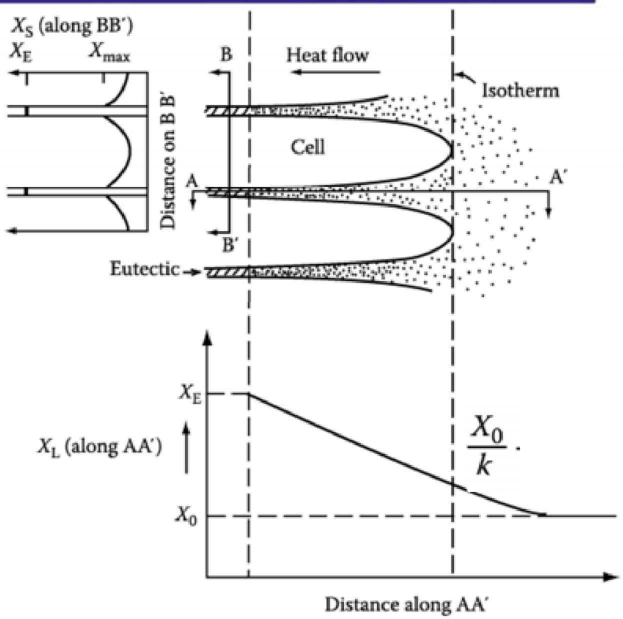
Grain Boundary Segregation Engineering
:A pathway to the design of interfaces

MIN SEOK KIM

18MAY2020

Solute segregation in alloys





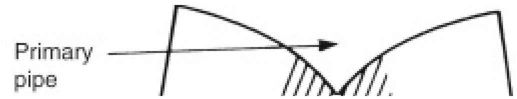
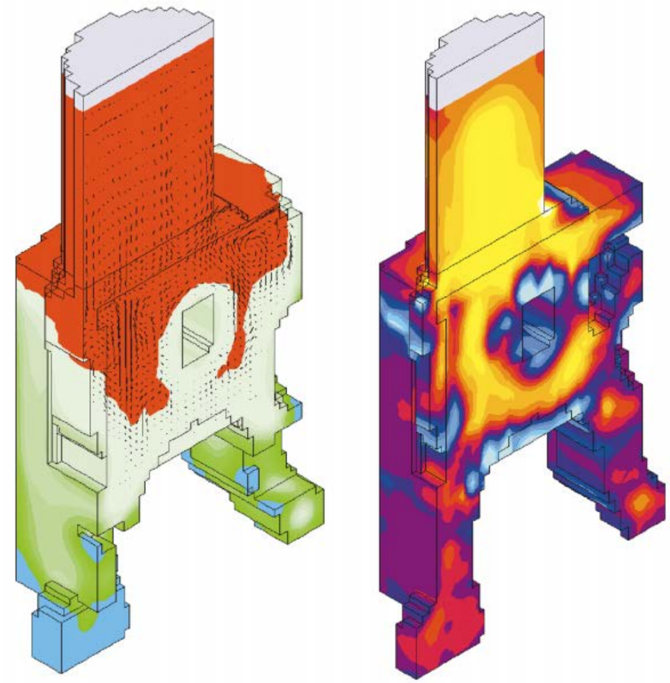
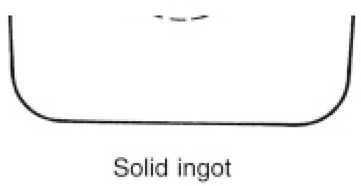
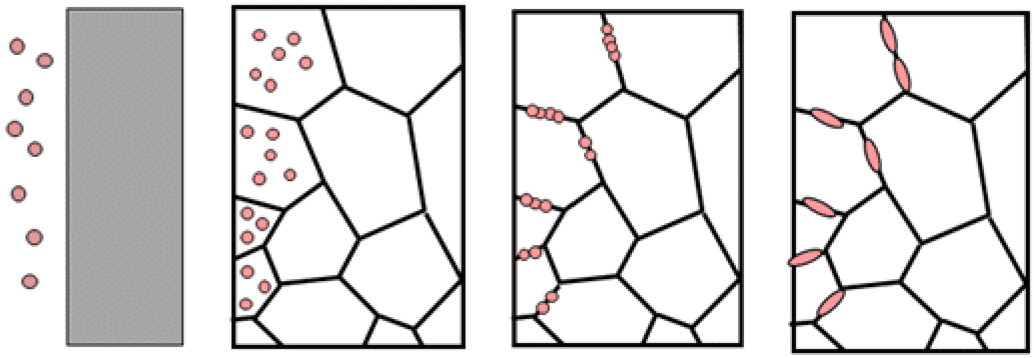


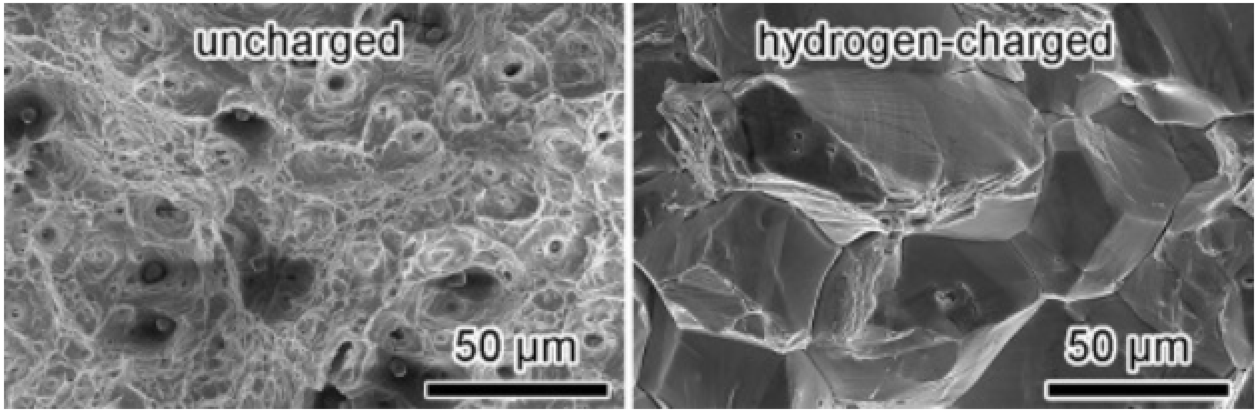
Fig. Simulation of macrosegregation formation in a large steel casting, showing liquid velocity vectors during solidification (left) and final carbon macrosegregation pattern (right).

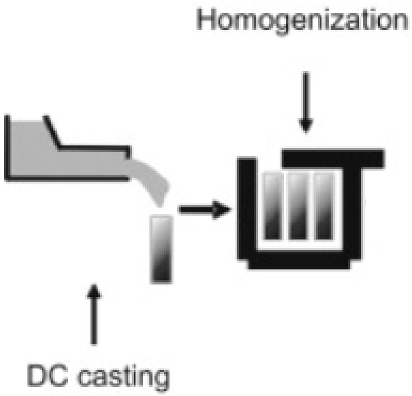




Hydrogen embrittlement in compositionally complex FeNiCoCrMn FCC solid solution alloy







Thermodynamic origin of segregation phenomenon

Gibbs isotherm

$$-\mathrm{d}\gamma = \Gamma_1 \mathrm{d}\mu_1 + \Gamma_2 \mathrm{d}\mu_2 \,,$$

where

γ is the surface tension,

Γ_i is the surface excess of component i,

μ_i is the chemical potential of component i.

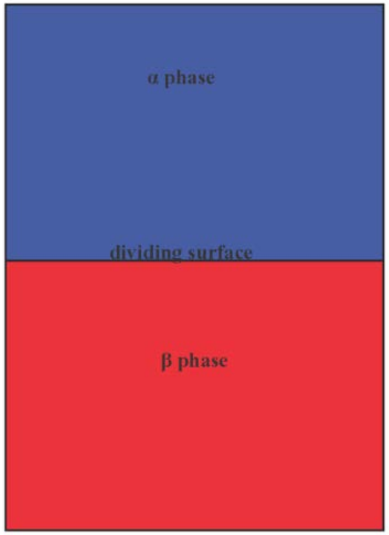
$$G = G^{\alpha} + G^{\beta} + G^{S}$$

$$G = U + pV - TS + \sum_{i=1}^{k} \mu_i \, \mathrm{n}_i \,,$$

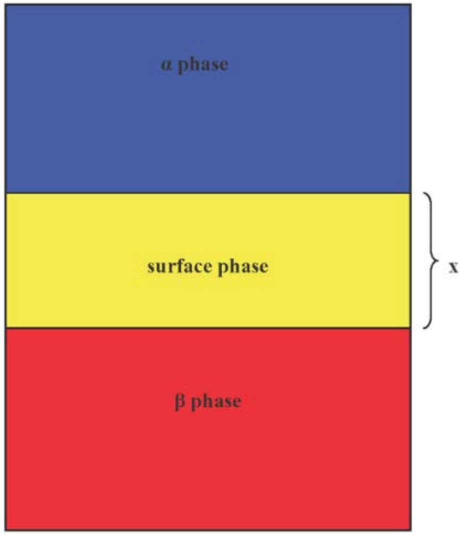
$$\mathrm{d}G = V\mathrm{d}p - S\mathrm{d}T + \sum_{i=1}^{k} \mu_i \, \mathrm{d}n_i \,.$$

$$\sum_{i=1}^{k} \mathrm{n_i}^{\alpha} \, \mathrm{d}\mu_i + \sum_{i=1}^{k} \mathrm{n_i}^{\beta} \, \mathrm{d}\mu_i + \sum_{i=1}^{k} \mathrm{n_i}^{S} \, \mathrm{d}\mu_i + A\mathrm{d}\gamma = 0 \,.$$

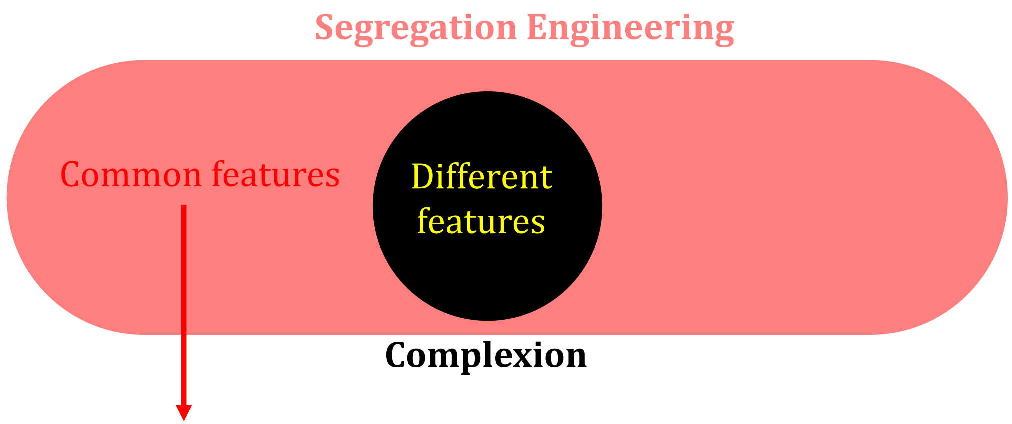
$$\sum_{i=1}^{k} \mathrm{n_i}^{S} \, \mathrm{d}\mu_i + A\mathrm{d}\gamma = 0 \,.$$



IDEAL SYSTEM



REAL SYSTEM

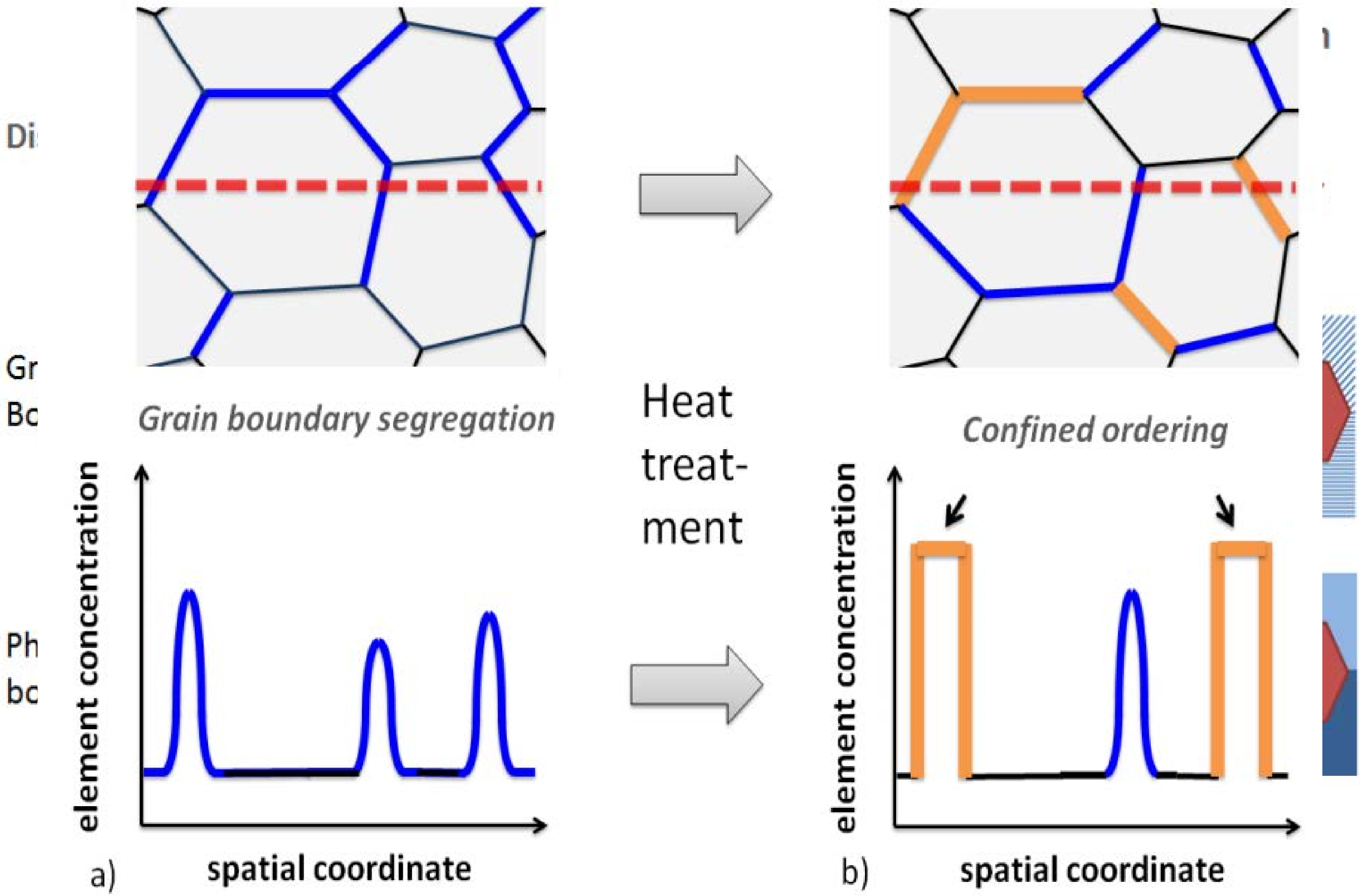


Interface designing utilizing segregation at **defects(GB, dislocations …)** **, constituting new phase**

Phase transformation =Nucleation & Growth

Nucleation
- **Thermodynamically : Can change G free energy(strain field, Surface energy…)**
- **Kinetically : High Diffusivity , Can act as heterogeneous nucleation site**

Segregation Engineering



Q. How to applicate grain boundary segregation engineering?

Important factors for segregation engineering

Considering effect of Segregated solution in GB local area
(Phase stability, GB cohesion…)

Grain boundary segregation tendency

↓

Solute element, fraction…

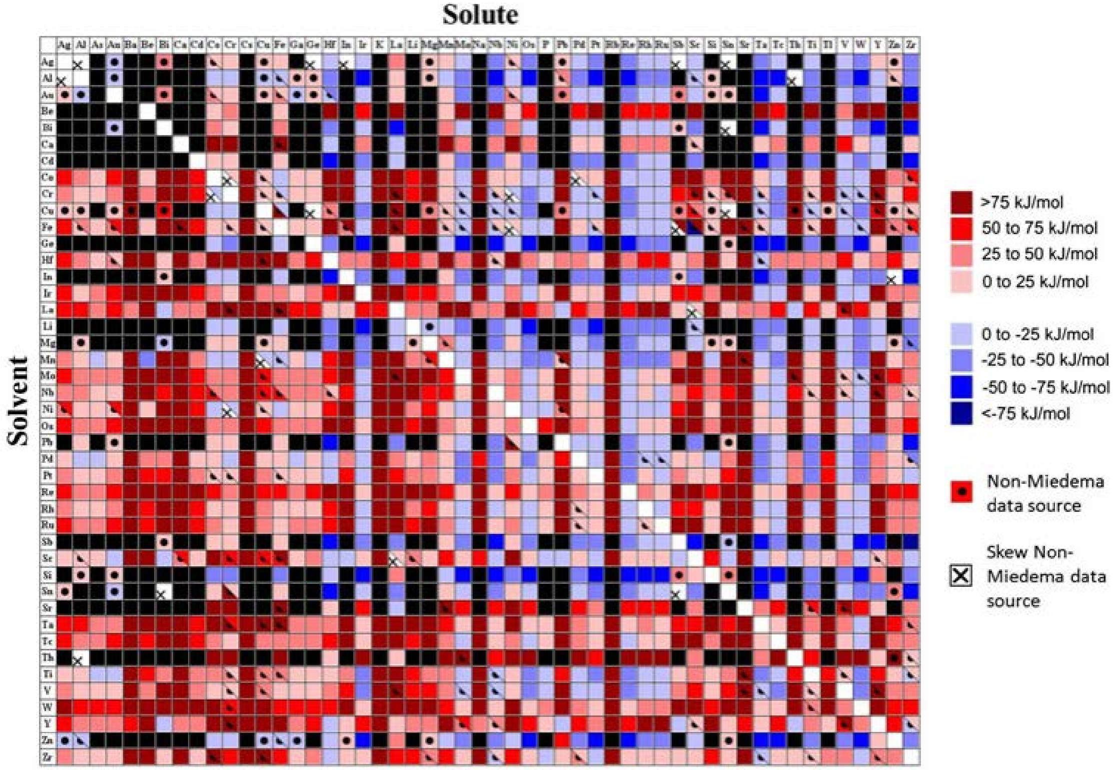
Annealing condition (time, temperature…)

Estimation of Grain boundary Segregation tendency

Journal of Materials Research

Estimation of grain boundary segregation enthalpy and its role in stable nanocrystalline alloy design

Heather A. Murdoch and Christopher A. Schuh[a)]
Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139



$$\Delta H^{seg}_{0,M} = -0.71 \times \frac{1}{3} \times \nu \times \left[-\Delta H^{int}_{BinA} - c_0 \gamma^S_A V^{2/3}_A + c_0 \gamma^S_B V^{2/3}_B \right] + \Delta E_{el} \quad .$$

Enhancing mechanical property of Martensitic steel

Phase nucleation through confined spinodal fluctuations at crystal defects evidenced in Fe-Mn alloys

A. Kwiatkowski da Silva[1], D. Ponge[1], Z. Peng[1], G. Inden[1], Y. Lu[2], A. Breen[1], B. Gault[1] & D. Raabe[1]

nature COMMUNICATIONS

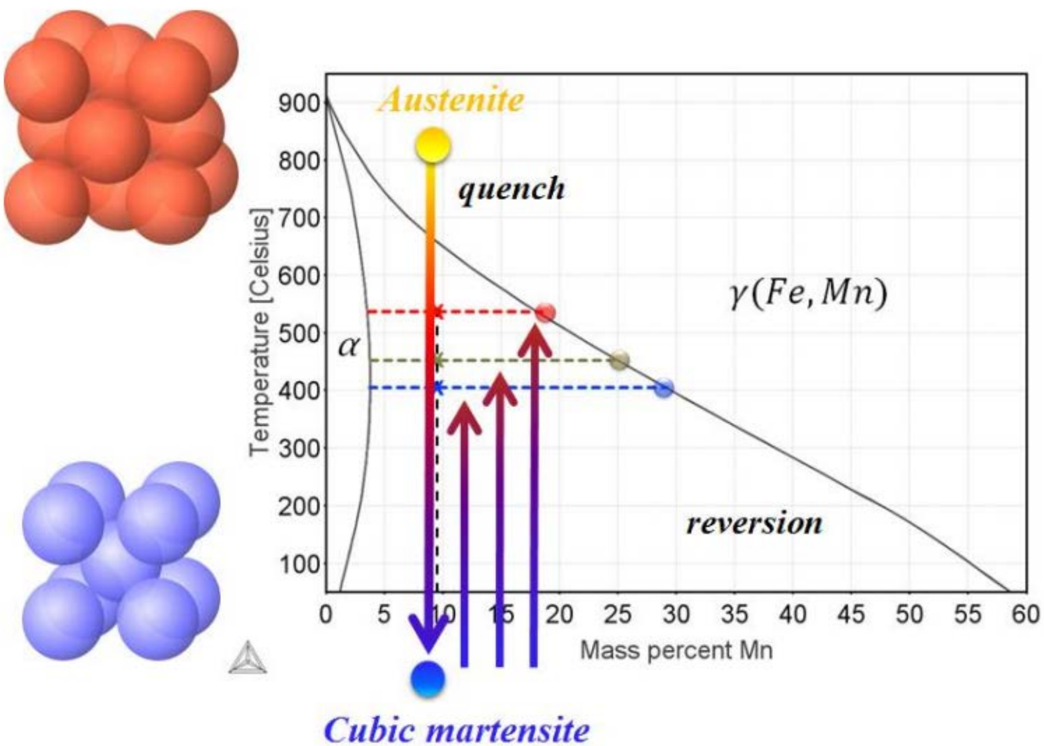
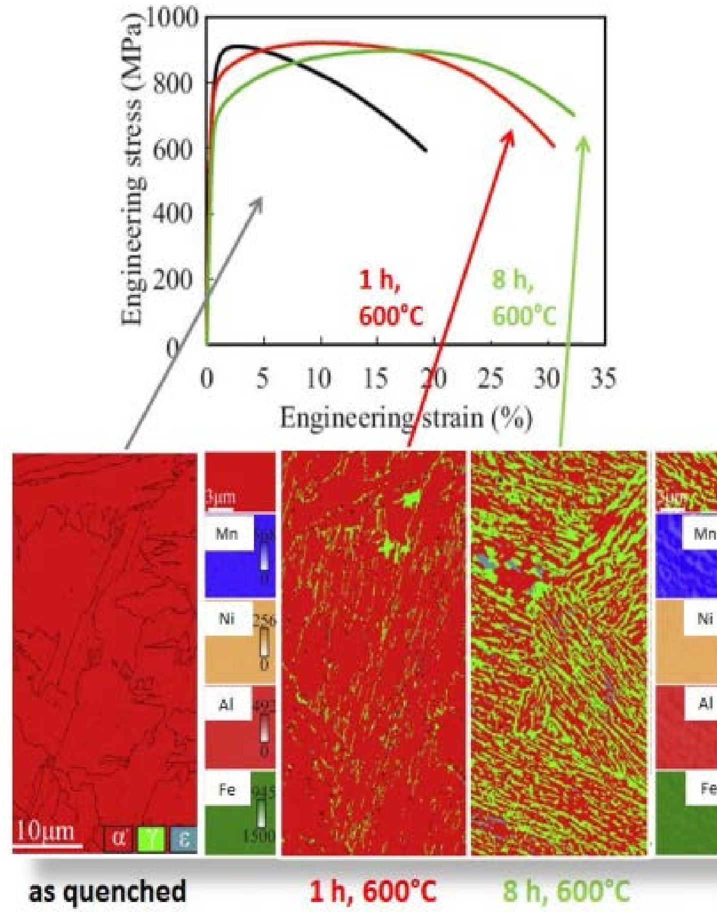


Figure 5. Martensite-to-austenite reversion heat treatment [1,3,4].

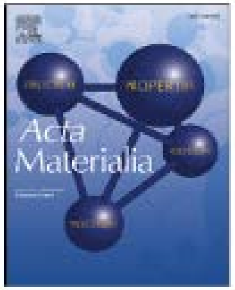


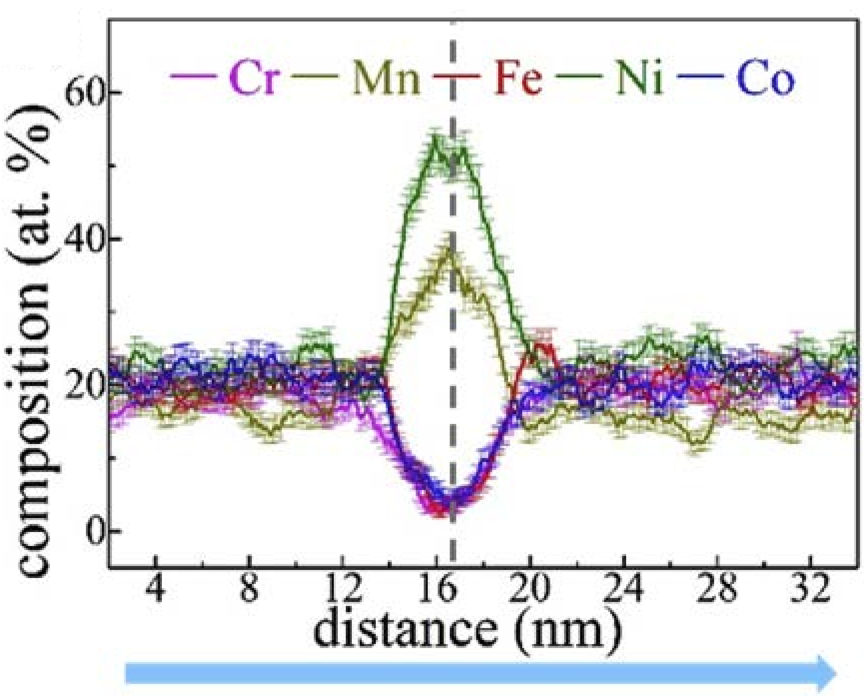
Segregation-driven grain boundary spinodal decomposition as a pathway for phase nucleation in a high-entropy alloy

Segregation-driven grain boundary spinodal decomposition as a pathway for phase nucleation in a high-entropy alloy

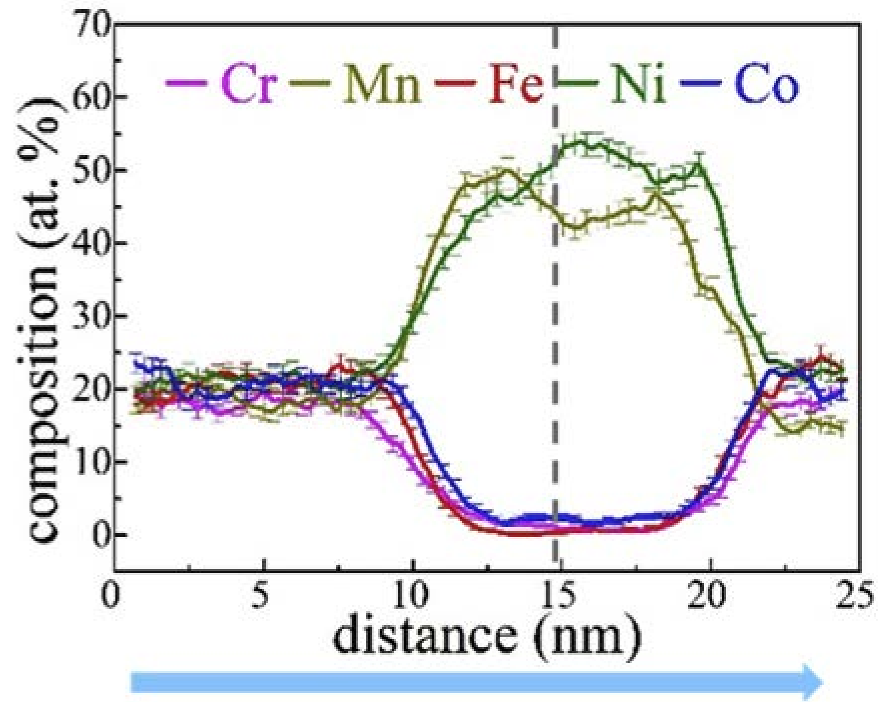
Linlin Li [a, b, *], Zhiming Li [a], Alisson Kwiatkowski da Silva [a], Zirong Peng [a], Huan Zhao [a], Baptiste Gault [a, c], Dierk Raabe [a, **]

[a] Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 40237, Düsseldorf, Germany
[b] Institute of Metal Research, Chinese Academy of Science, Wenhua Road 72, Shenyang, 110016, PR China
[c] Department of Materials, Royal School of Mine, Imperial College London, London, SW7 2AZ, UK





450°C, 6hr



450°C, 18hr

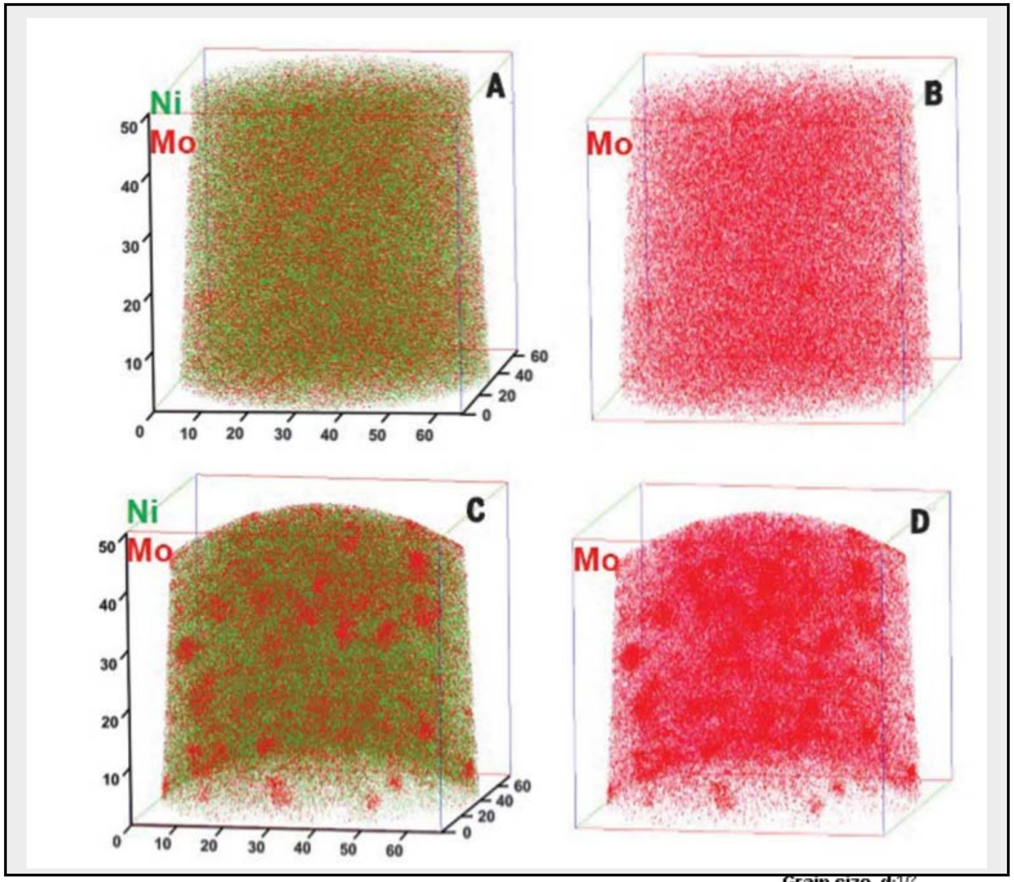
Grain boundary stability governs hardening and softening in extremely fine nano grained metals

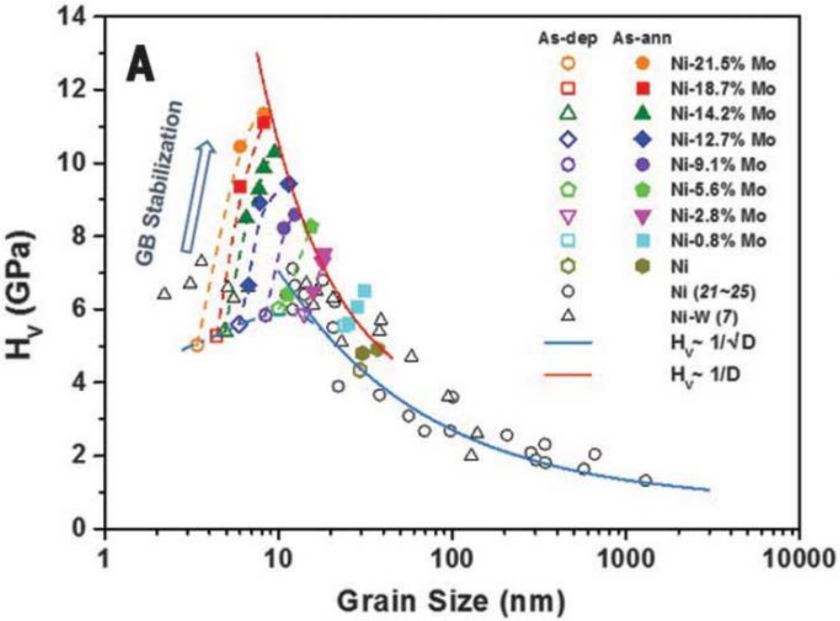
METALLURGY

Grain boundary stability governs hardening and softening in extremely fine nanograined metals

J. Hu,[1*] Y. N. Shi,[1*] X. Sauvage,[2] G. Sha,[3] K. Lu[1,3]†

500°C, 1hr





Stability criteria for nano crystalline alloys

Full length article

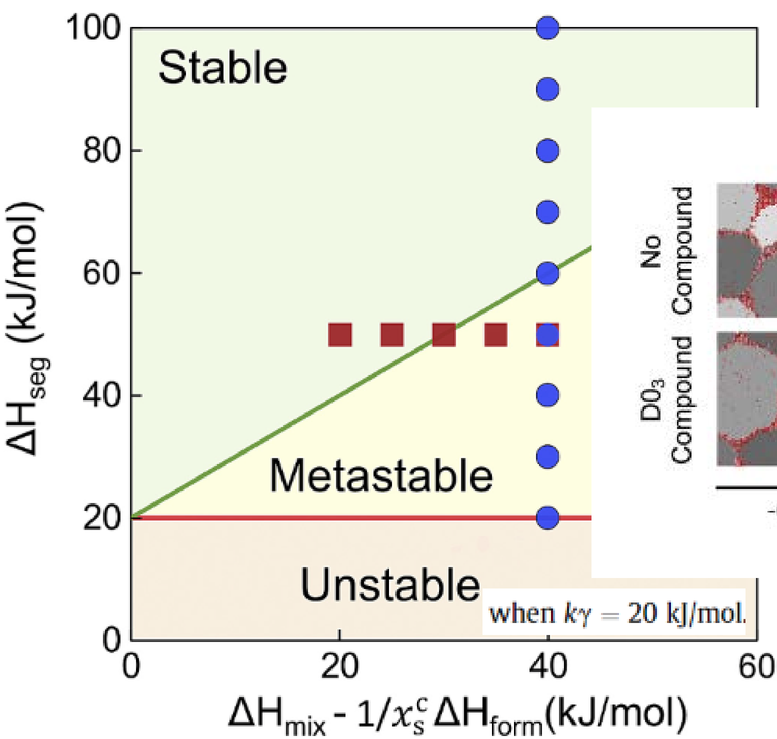
Stability criteria for nanocrystalline alloys

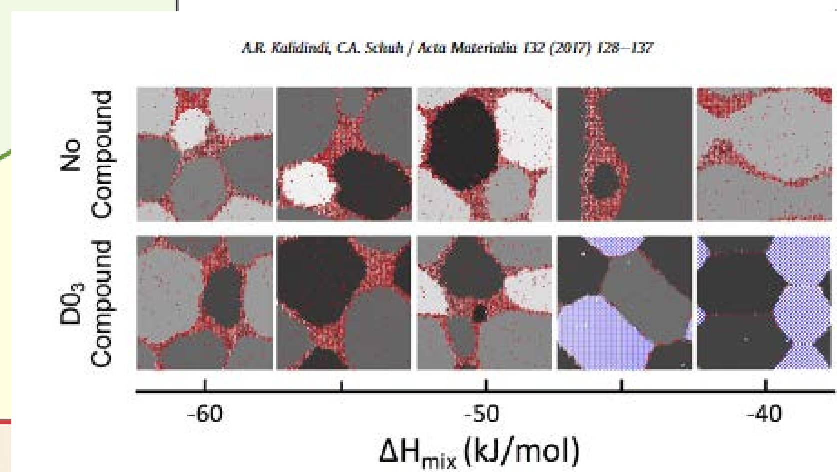
Arvind R. Kalidindi, Christopher A. Schuh*

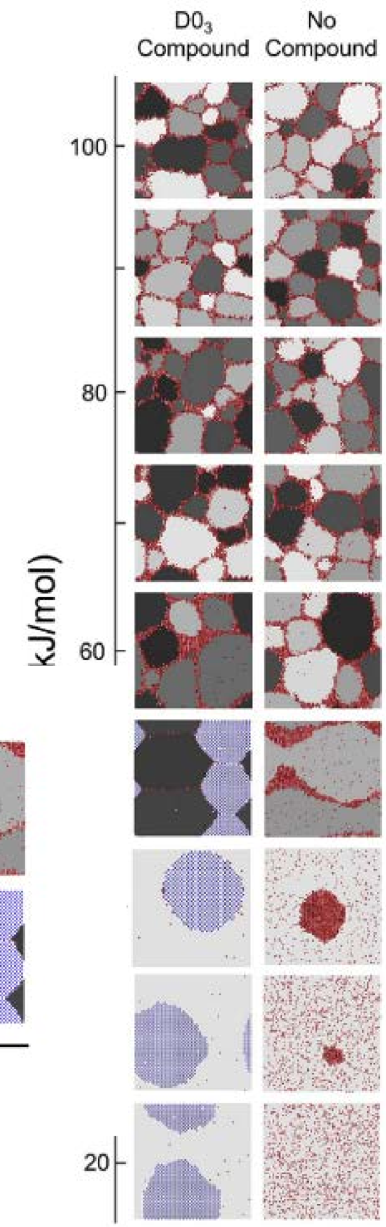
Department of Materials Science and Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA, 02139, USA

$$\Delta H_{\mathrm{seg}} > \Delta H_{\mathrm{mix}} - \frac{1}{x_s^c}\Delta H_{\mathrm{form}} + k\gamma$$

Compound formation **Grain growth**







Summary

Segregation has been accepted as a phenomenon to be avoided, which adversely affects the properties of the alloy.

However, it can be used as a methodology for interface design by controlling the segregation phenomenon in nanoscale.

Indeed, studies such as improving the physical properties of TRIP -assisted maraging steel or improving the phase stability of nano crystalline have recently attracted attention, and through this, th ere is a possibility that the existing alloy design method will overc ome limitations that cannot be overcome.

THANK YOU FOR YOUR KIND ATTENTION

ivy94@snu.ac.kr | http://espark.snu.ac.kr