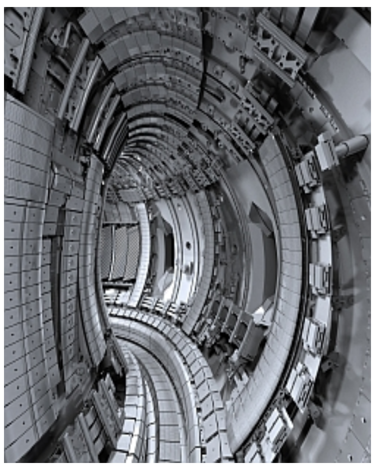
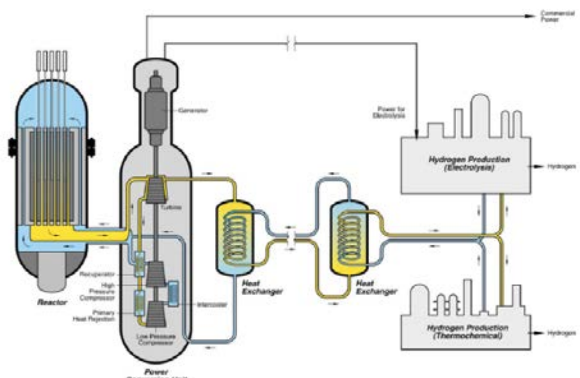
New alloys still necessary?

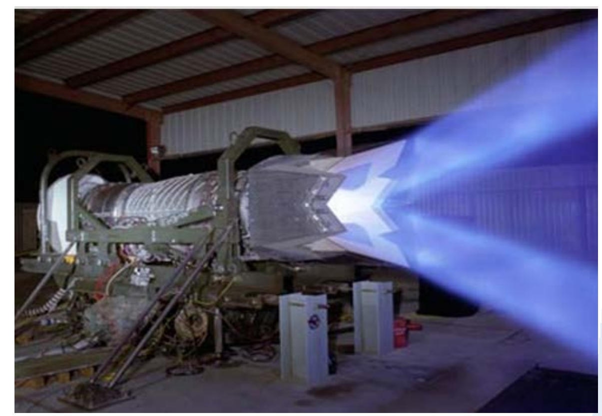
Fusion Plasma Facing Materials	Advanced Reactors	Aerospace Applications



- Plasma Resistance
- Thermal Shock Resistance

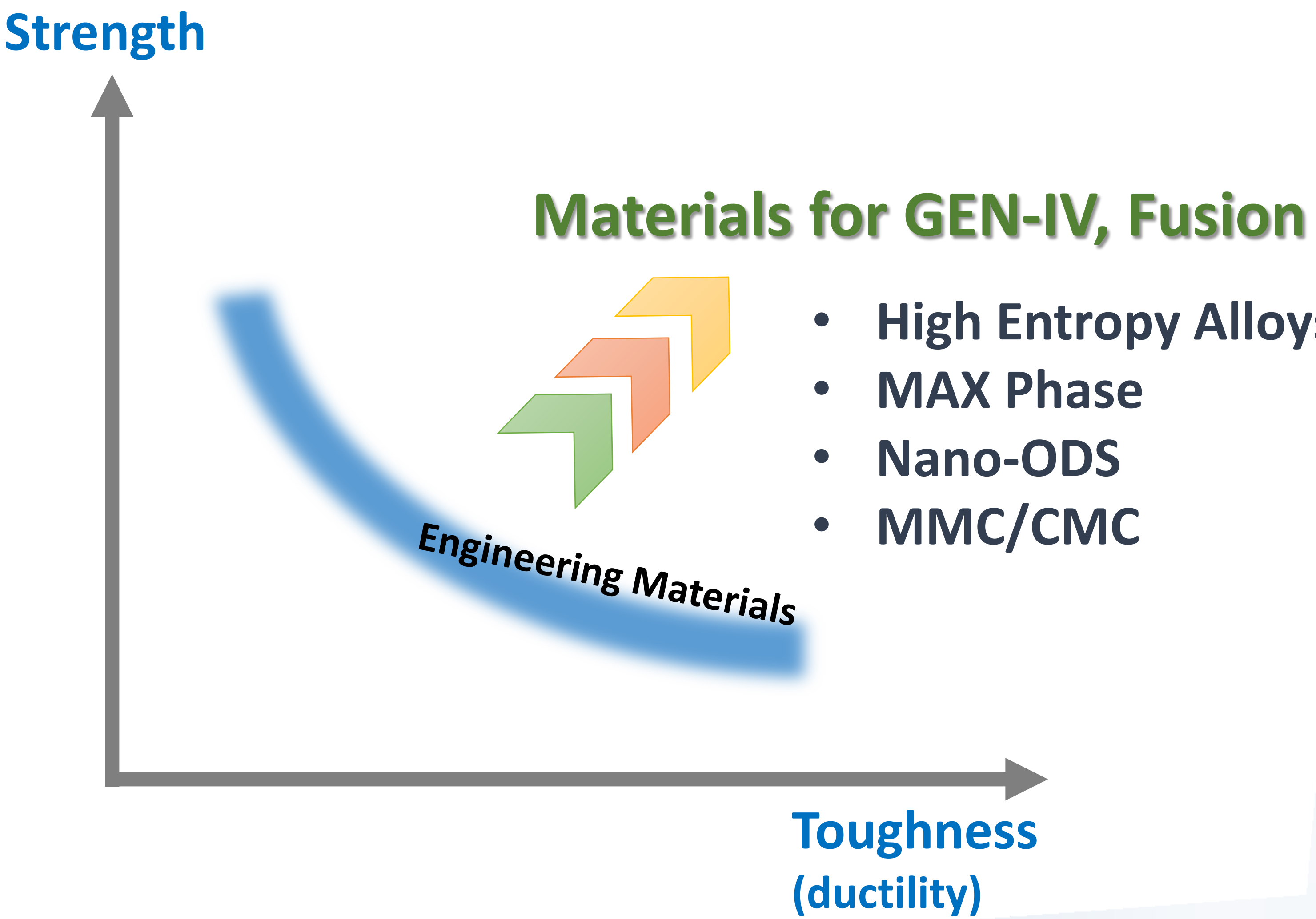


- Irradiation Resistance
- Creep Resistance



- Ablation Resistance
- Oxidation Resistance

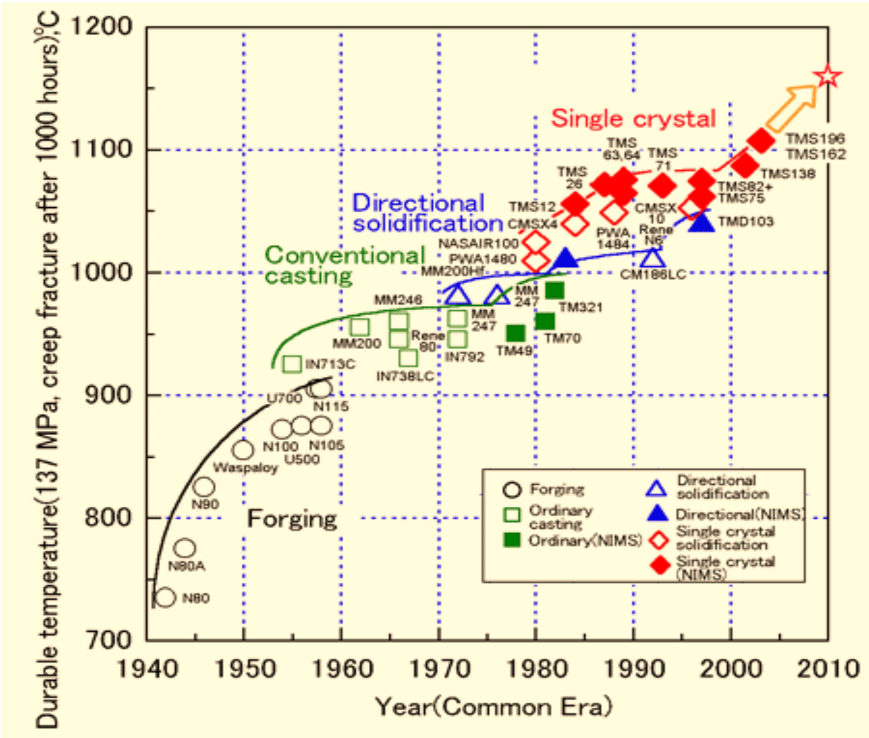
Materials breakthroughs required



- High Entropy Alloys
- MAX Phase
- Nano-ODS
- MMC/CMC

Incremental vs. Disruptive Approach

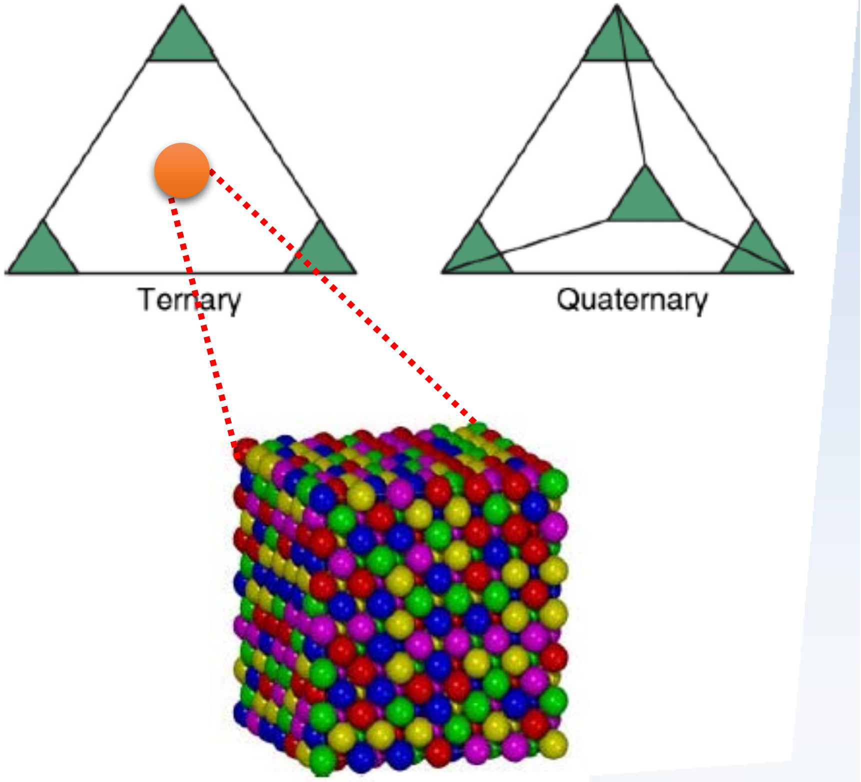
- Ni-base superalloy development



http://www.mst.or.jp/Portals/0/prize/english/winners/material/material2013_en.html

- High entropy alloys

2004

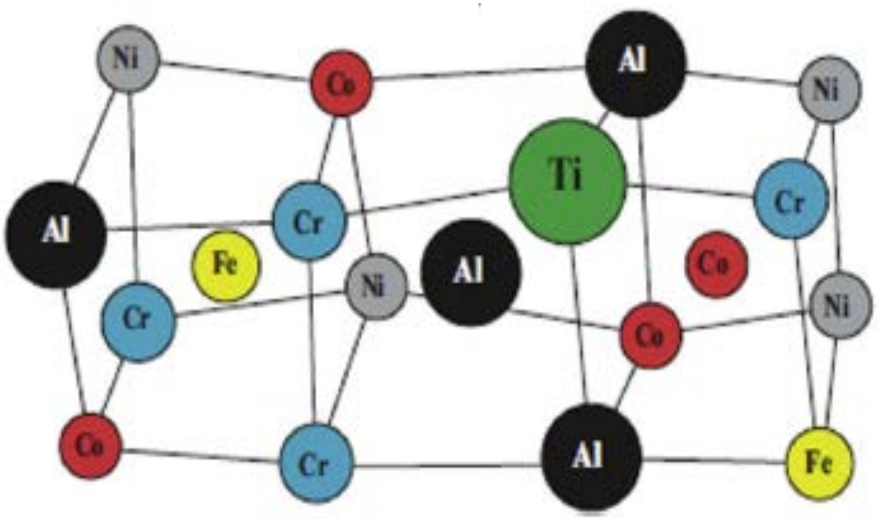


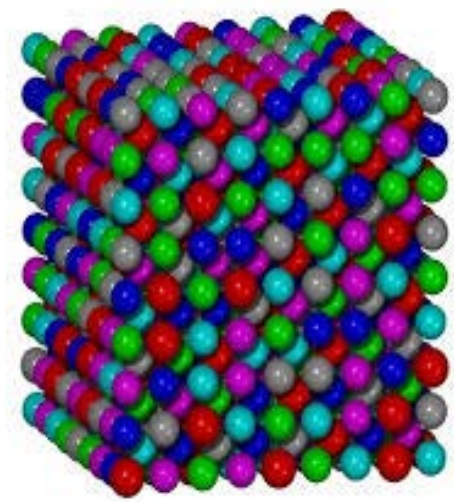
High-Entropy Alloys (HEA) are alloys that are formed by mixing equal or relatively large proportions of (usually) five or more elements.
Normally, in steel or other alloys, additional elements can be added to improve its properties, thereby creating, but typically in fairly low proportions.

«High entropy alloys" was coined because the entropy increase of mixing is substantially higher when there is a larger number of elements in the mix, their proportions are nearly equal.

These alloys are currently the focus of significant attention in materials science and engineering because they have potentially desirable properties (better strength-to-weight ratios, with a higher degree of fracture resistance, tensile strength, corrosion and oxidation resistance)

What is "High Entropy Alloy"?





Multicomponent alloys without solute and base atoms

- ➔ **Multi-principal element alloy**
- ➔ **Equiatomic alloys**
- ➔ **Compositionally complex alloy**
- ➔ **Concentrated solid solution alloys**

Four core effects have been proposed in HEAs:

(1) the entropic stabilisation of solid solutions,

(2) the severe distortion of their lattices,

(3) sluggish diffusion kinetics

(4) that properties are derived from a cocktail effect.

It is clear that HEAs represent a stimulating opportunity for the metallurgical research community

The idea is to choose a sufficient number of elements so that the configurational entropies of alloys would be high enough to overcome the enthalpies of formation of intermetallic phases, resulting in stable solid solution

For a solution comprising n components, each with mole fractions X_i, the configurational entropy is: $\Delta S_{\text{config}} = -\mathrm{R} \sum_{i=1}^{n} X_i \ln X_i$.

To maximise configurational entropy, these materials must have a configurational entropy of mixing

$$\Delta S_{\text{config}} > 1.5\mathrm{R}.$$

Therefore at least 5 components

Configurational Entropy vs. Enthalpy

$$\Delta S_{conf} = k \ln w = -R \sum_{i=1}^{n} X_i \ln X_i = -R \ln \frac{1}{n} = R \ln n$$

No of components	ΔS_{conf}
2	0.69 R
3	1.1 R
4	1.39 R
5	1.61 R

$$\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$$

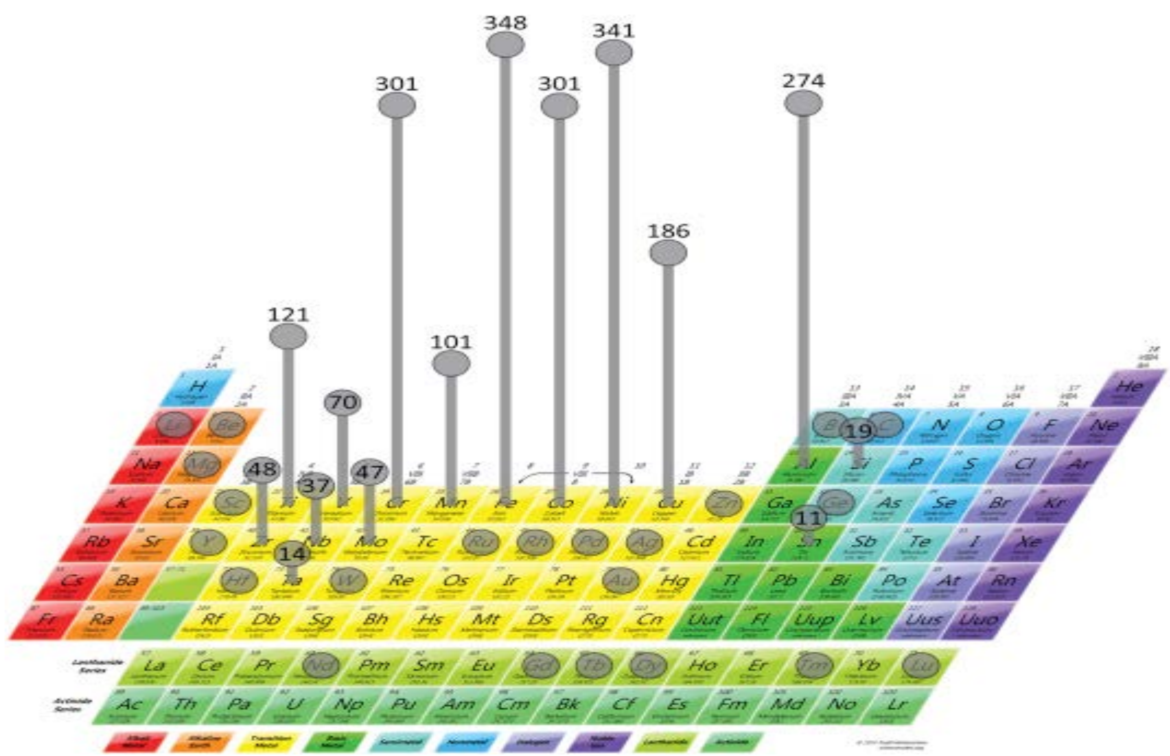
$\Delta H/T_m$ (NiAl) = 1.38 R

- The tendency of ordering would be lowered by the high mixing entropy
- **More easily form solid solution alloys**

design is based around the concept that their high configurational entropies of mixing should stabilise solid-solution phases relative to the formation of potentially-embrittling intermetallic phases.

Infinite Degrees of Freedom in Alloy Design

~40 elements, 1% → $(100/1)^{40-1} = 10^{78}$
(10^{66} atoms in the galaxy)



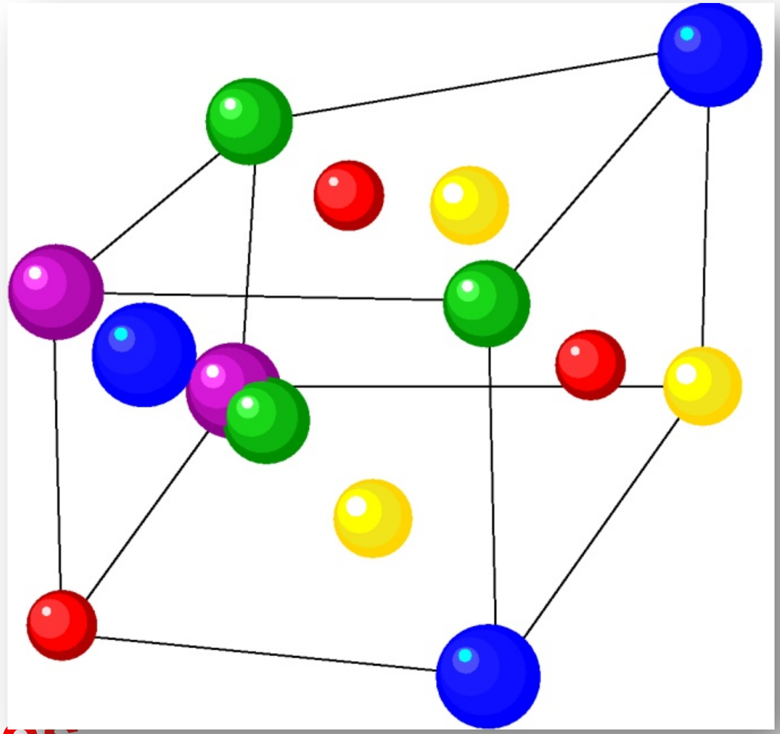
Miracle & Senkov, Acta mater 2017

AlHfNbTaTiZr
AlMoNbTaTiZr
AlNbTaTiV
AlNbTaTiVZr
AlNbTaTiZr
AlNbTiV
CrHfNbTiZr
CrMoNbTaTiZr
CrNbTiVZr
CrNbTiZr
HfMoNbTiZr
HfNbTaTiZr
HfNbTiVZr
HfNbTiZr
MoNbTaVW
MoNbTaW
NbTaTiV
NbTiVZr
NbTiVZr

High Entropy Alloys (HEAs)

Examples: Co Cr Fe Mn Ni & Al Hf Sc Ti Zr

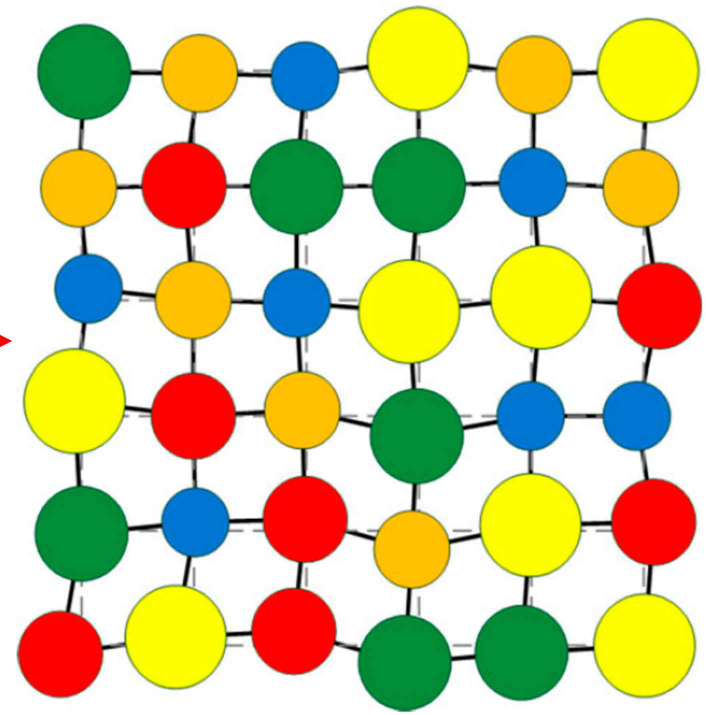
- **> 5 metallic components**
- **~ equal proportions**
- **disordered solid solutions**
- **single phase, no precipitates**



High Entropie Alloys (HEA)

Examples: Co Cr Fe Mn Ni & Al Hf Sc Ti Zr

- high entropy
- severe lattice distortion
- "cocktail" effect
- sluggish diffusion



5 Schematic representation of strained lattices in HEAs. Reprinted from[5] with permission from Springer

Sluggish diffusion

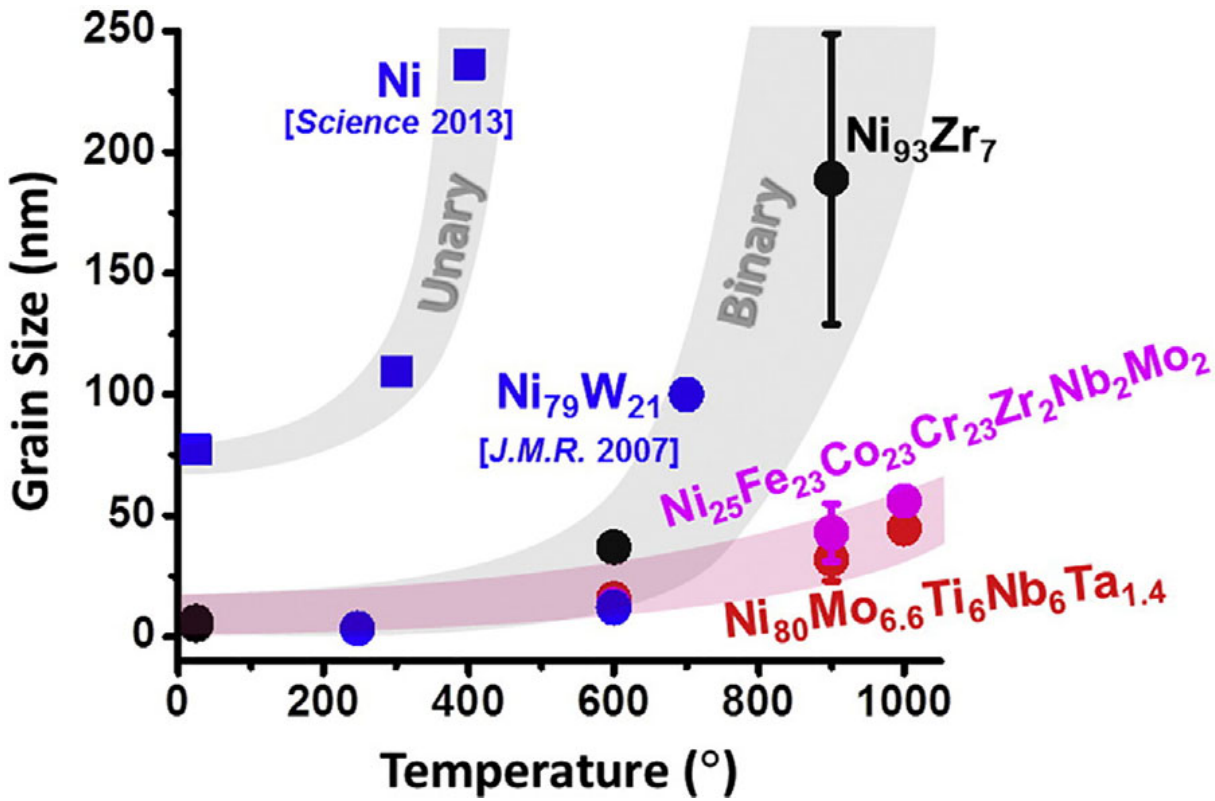
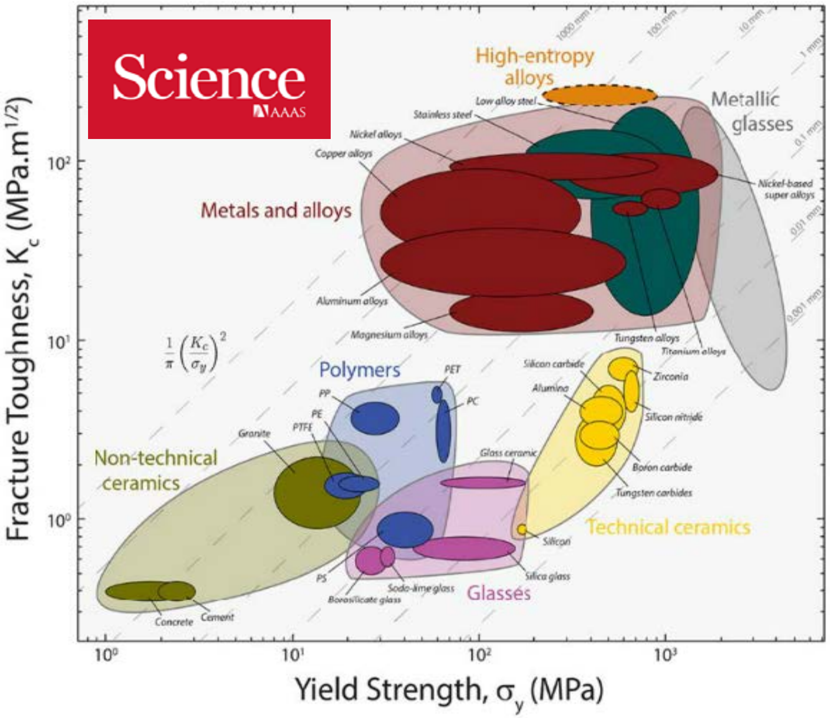


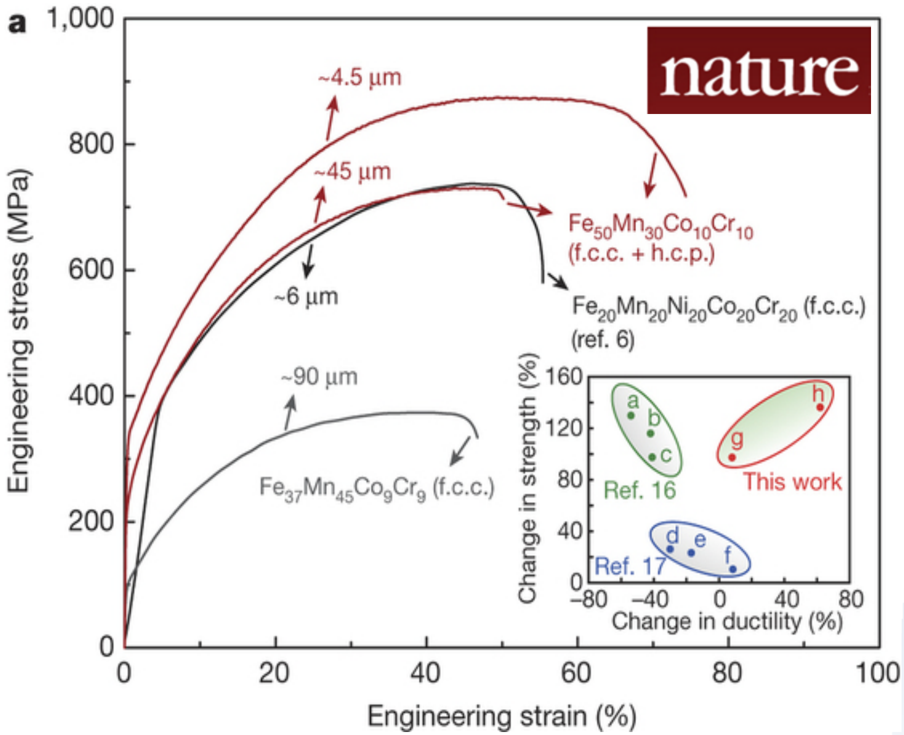
Figure 2. Exceptional resistance to grain growth in $Cr_{23}Fe_{23}Co_{23}Ni_{25}Zr_2Nb_2Mo_2$ HEA by utilizing the concept of grain boundary energy reduction.

Extraordinary Properties of High Entropy Alloys

CoCrFeMnNi



FeMnCoCr



Un altro sistema interessante: NbMoTaW

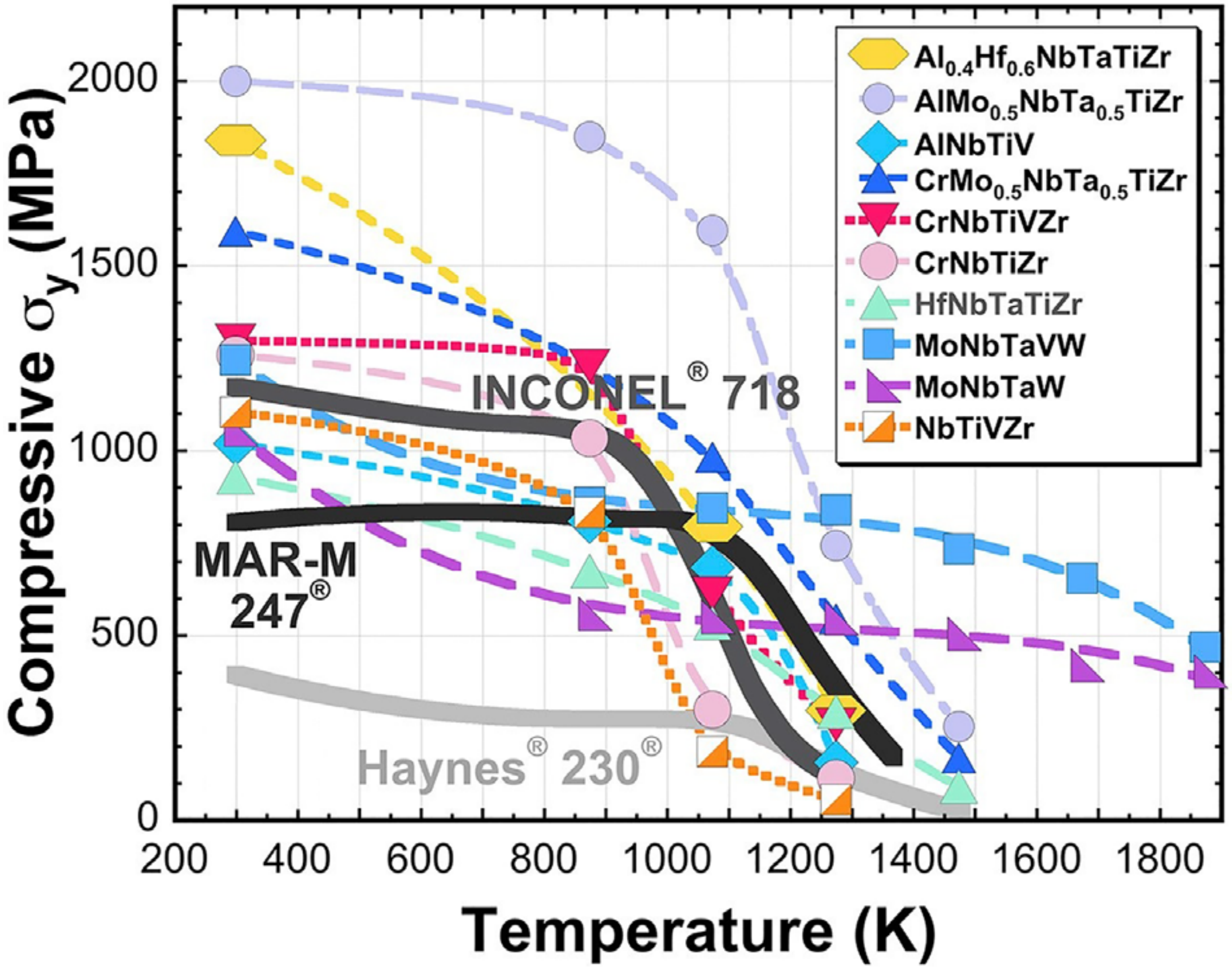
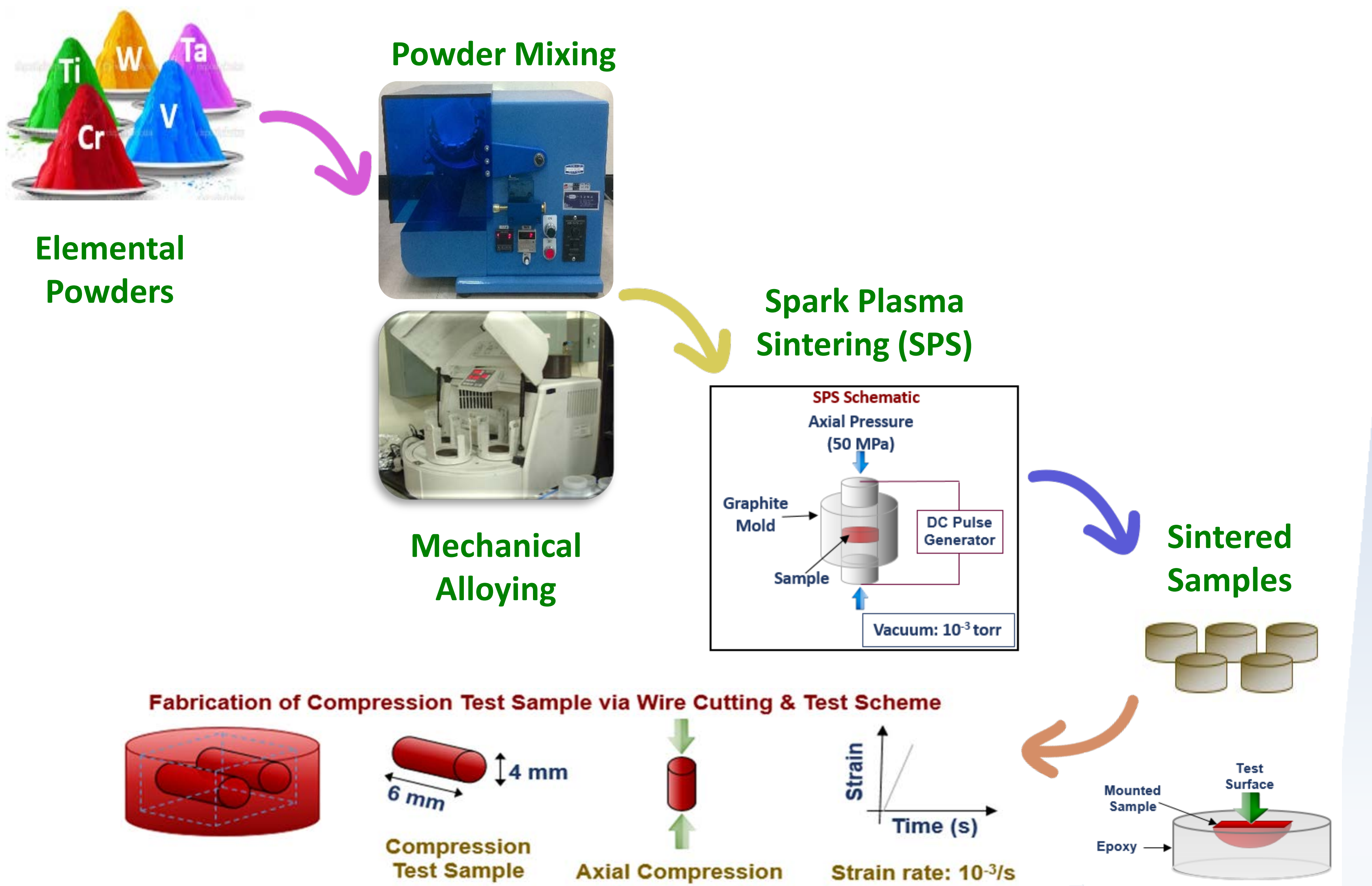
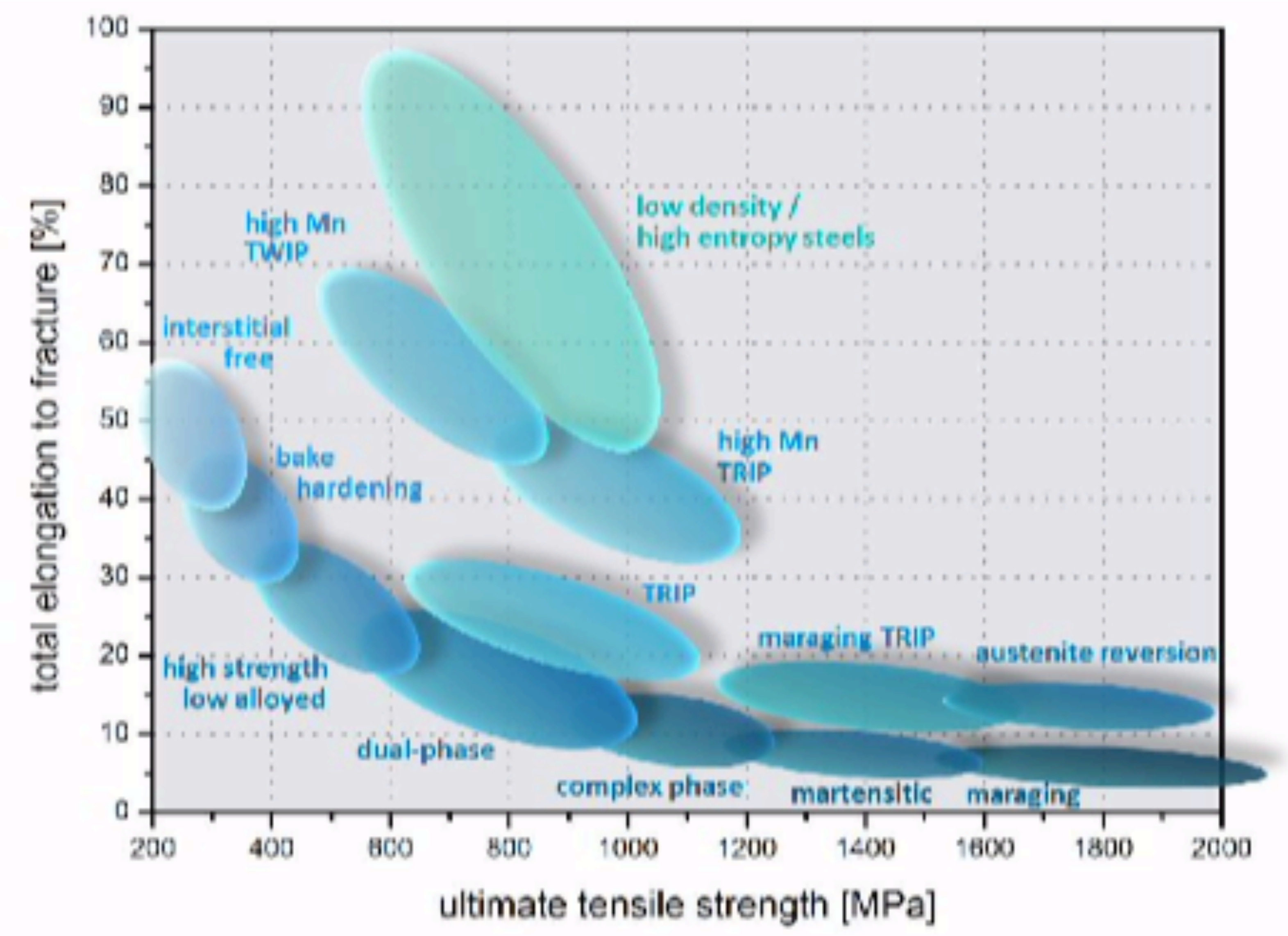


Figure 16. Yield strength variation of refractory HEAs illustrating superior strength retention at a higher temperature than superalloys.[6]

Powder Metallurgy Processing





total elongation to fracture [%]
ultimate tensile strength [MPa]
0
10
20
30
40
50
60
70
80
90
100
200
400
600
800
1000
1200
1400
1600
1800
2000
high Mn TWIP
low density / high entropy steels
interstitial free
bake hardening
high Mn TRIP
TRIP
maraging TRIP
austenite reversion
high strength low alloyed
dual-phase
complex phase
martensitic
maraging