Novel High-Entropy Alloys Designed to Overcome the Limitations of Conventional Materials

NETL-RUA Regional University Alliance

Motivation/Challenges

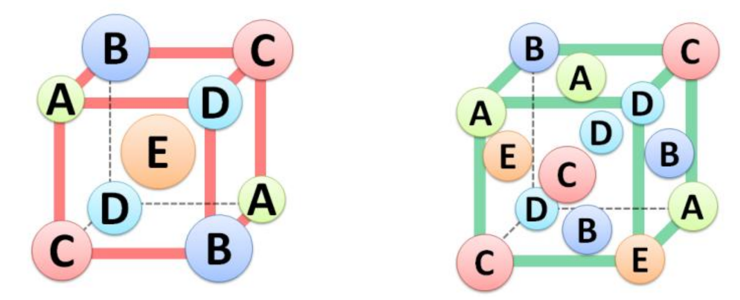
Existing alloys are vulnerable to environmental degradation at high temperatures, which causes rapid oxidation, loss of strength, undesirable phase transformations, rapid microstructure coarsening, accelerated creep, and thus much shortened lifetime. While expensive and mature Ni-based superalloys and stainless steels are the prime structural materials used for high-temperature applications in the market, they suffer from the limitations on temperature, pressure and environment. Consequently, there is urgent need in developing new materials with significantly improved properties (mechanical, thermal, and environmental) to be operated at higher temperature and higher pressure where environmental degradation is more severe for a wide array of industrial applications that demand high efficiency and long lifetime as well as lower cost.

Technology/Capability Overview

High-entropy alloys (HEAs) are loosely defined as solid solution alloys that often contain five principal elements in equal or near equal atomic percent. The basic principle of HEAs is the solution phase is stabilized by the significantly higher configurational entropy of mixing (≥1.61R) compared to conventional alloys. This stabilizing effect becomes even stronger as increasing temperature and the number of components in the system. A direct consequence of thermodynamic stabilization of the high-entropy phase is reducing the thermodynamic driving force towards oxidation and phase transformation. Another striking merit is the slow atomic diffusion due to highly saturated solid solution.

- Improve efficiency and reduce pollution by allowing HEAs to operate at higher temperature and pressure and lower cost
- Formation of simple FCC and BCC solid solution phases renders large freedom in microstructure manipulation and easy processing control
- Alloy chemistry can be tailored for specific property requirement, such as ductility, strength, oxidation, or balanced properties

Body-Centered Cubic (BCC) Face-Centered Cubic (FCC)

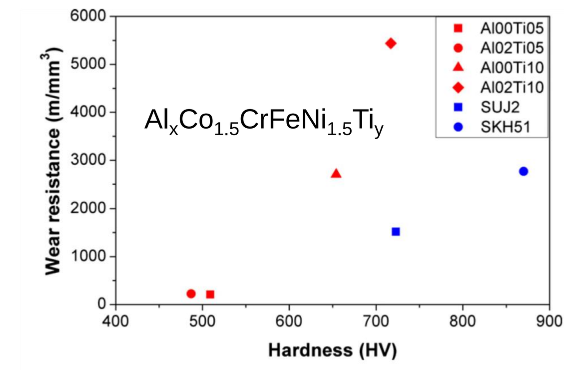


$$\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix}$$

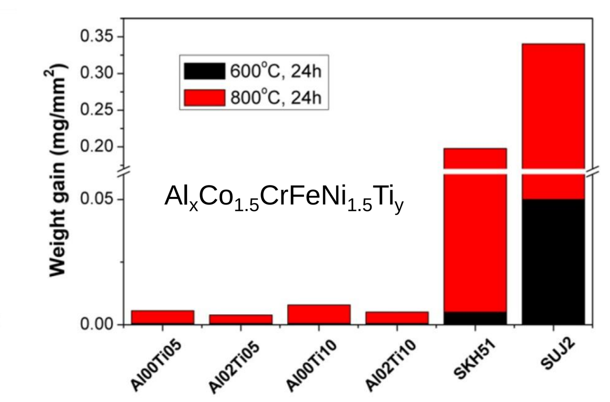
$$\Delta S_{mix} = -R\sum_{i=1}^{N} x_i \ln x_i$$

$$\Delta S_{mix}^{\max} = R \ln N$$

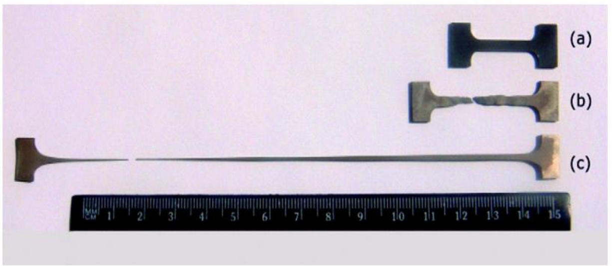
ΔG_{mix}: Gibbs energy of mixing
ΔH_{mix}: Enthalpy of mixing
ΔS_{mix} : Entropy of mixing
T: Absolute temperature. R: Gas constant. x_i: Molar composition



Pin-on-disk adhesive wear resistance

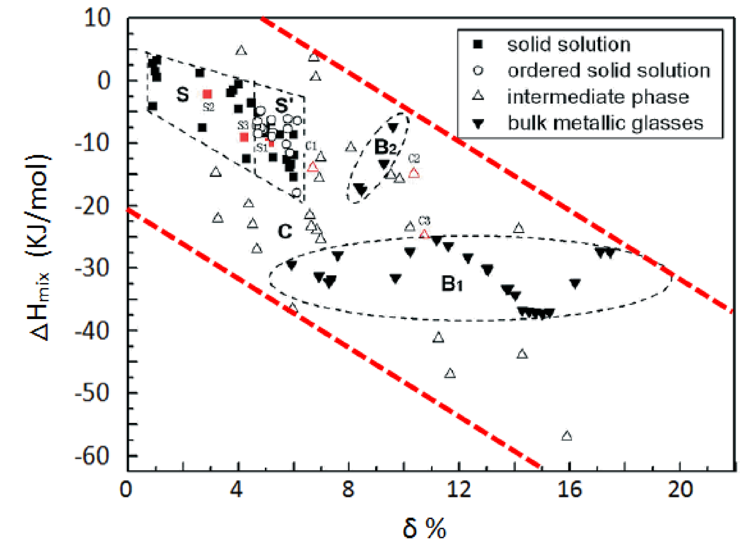


Acta mater **59** (2011) 6308

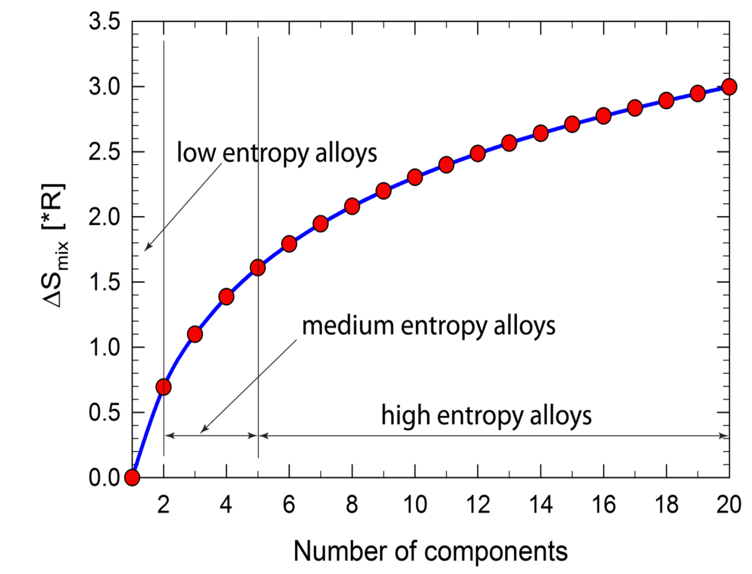


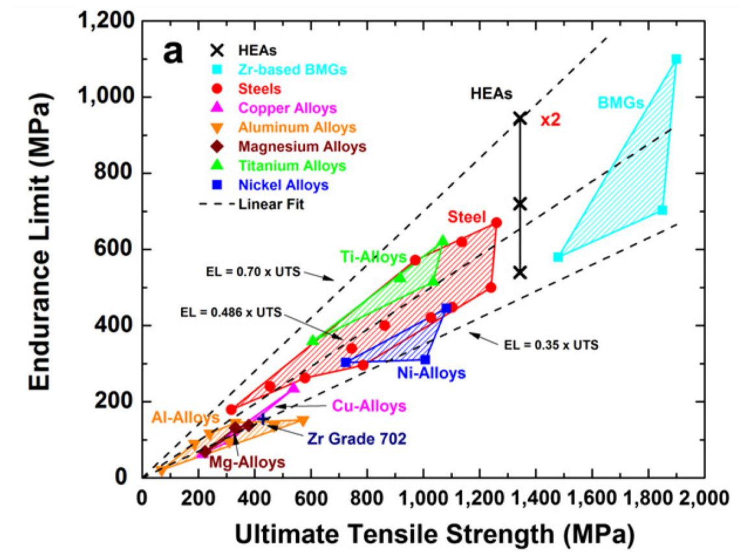
Photographs of tensile samples after deformation at 1,000 C: (a) a non-deformed sample; (b) as-cast sample (δ = 77%); and (c) forged sample (δ = 864%). Strain rate: 10^{-3}/s.

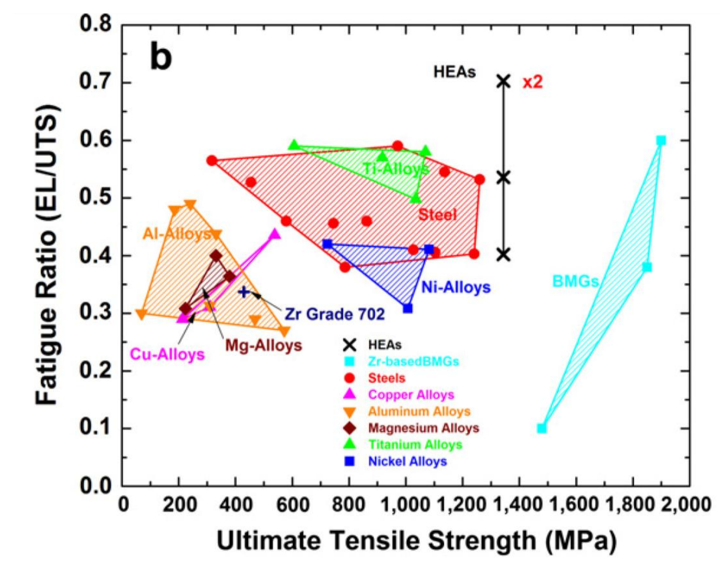
Mat . Sci. Eng. A, 2012. **533**: pp. 107-118. (AlCoCrCuFeNi)



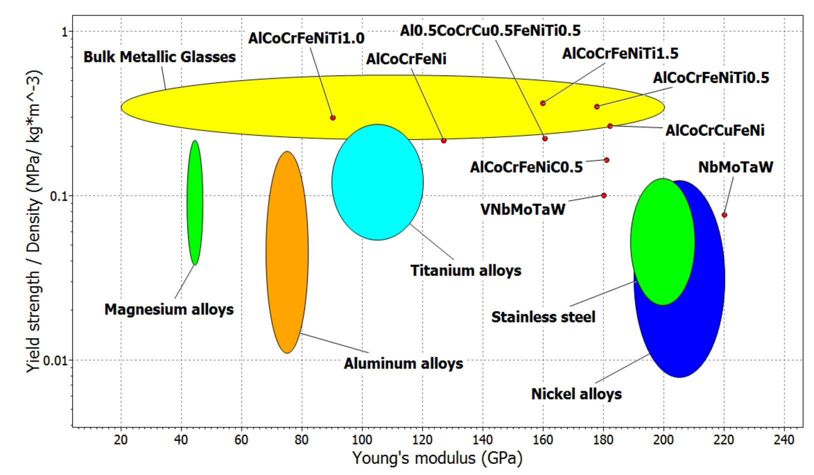
Adv. Eng. Mat. 2008;**10**:534



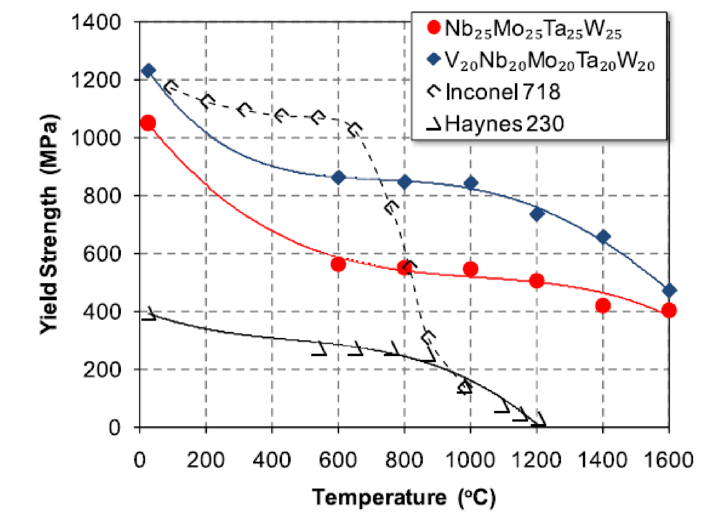




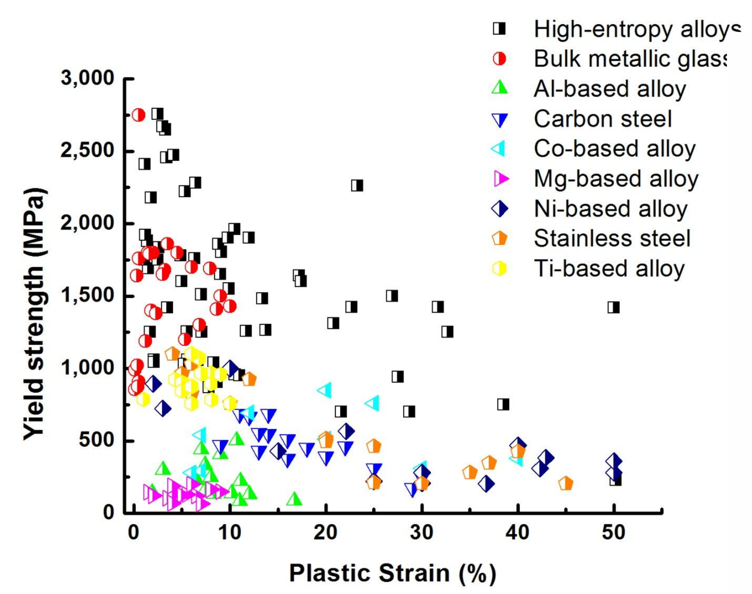
Acta Mater. 2012. **60**: 5723



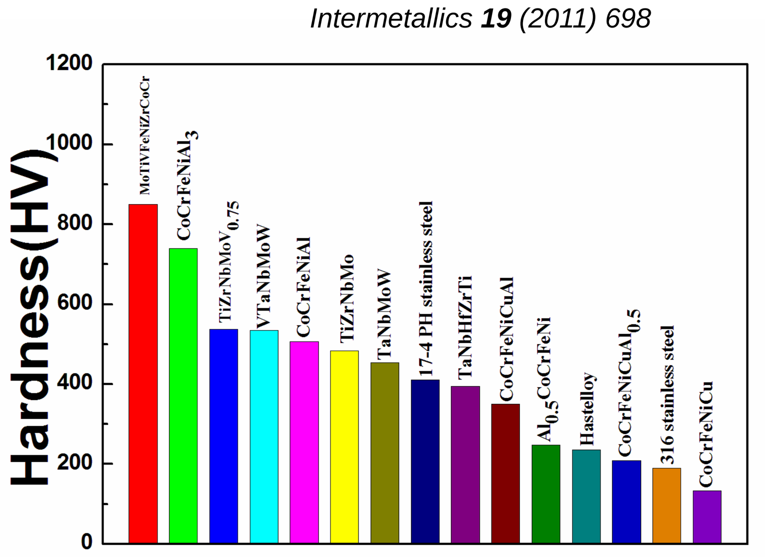
Zhang et al, unpublished, 2012



Intermetallics **19** (2011) 698



Courtesy of P.K. Liaw of University of Tennessee



Zhang et al, unpublished, 2012

Industry Significance

- Combination of ductility, strength, and oxidation resistance distinguishes HEAs as high-performance structural materials in extreme environment, superior to existing materials in the market.
- Slow diffusion and low thermal conductivity make HEAs suitable for diffusion barrier and thermal barrier applications
- Exceptional wear resistance allows HEAs ideal for forging industry, tool cutting, bioengineering, etc. where surface property plays a big role in materials lifetime

Benefits to Partner

Developing HEAs holds the key to applications in extreme environment where high temperature, high pressure and aggressive oxidation impose limitations to existing materials. Collaboration with NETL will create opportunities in sharing patents and publications and establishing joint-venture companies.

Opportunity

- Seek collaboration on high-temperature structural materials development: bulk, diffusion barrier, and thermal barrier coatings
- Seeking collaboration on developing hard coatings of outstanding wear and oxidation resistance

Development Status

- Combine multiscale computer modeling and critical experiments: *ab initio* density functional theory calculations, *ab initio* molecular dynamics and Monte Carlo simulations, and CALPHAD modeling
- Various HEAs: refractory metals, 3d transition metals, light-weight alloys, diffusion barriers, hydrogen separation membranes
- Benchmark HEAs are being processed and tested at NETL including corrosive environment at high temperatures

Contact

Michael Gao, NETL/URS, 1450 Queen Ave SW,
Albany, OR 97321. Email: michael.gao@contr.netl.doe.gov;
Tel: (541) 967-5869. Fax: (541) 918-4493.

NETL Carnegie Mellon PENNSTATE University of Pittsburgh VirginiaTech WestVirginiaUniversity URS