High-Entropy Alloy Design Assisted by High-Performance Computing

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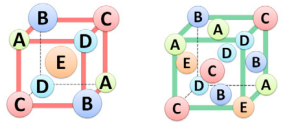
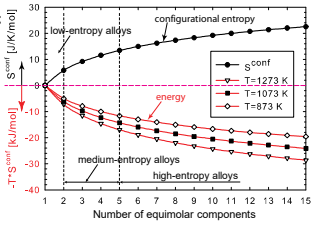
Basic Concept of High-Entropy Alloys (HEAs)

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



Solid solution alloys



$$\Delta G_{mix} = \Delta H_{mix} - T\Delta S_{mix} \qquad \Delta S_{mix} = \Delta S^{conf}_{mix} + \Delta S^{elec}_{mix} + \Delta S^{vib}_{mix} + \Delta S^{mag}_{mix}$$

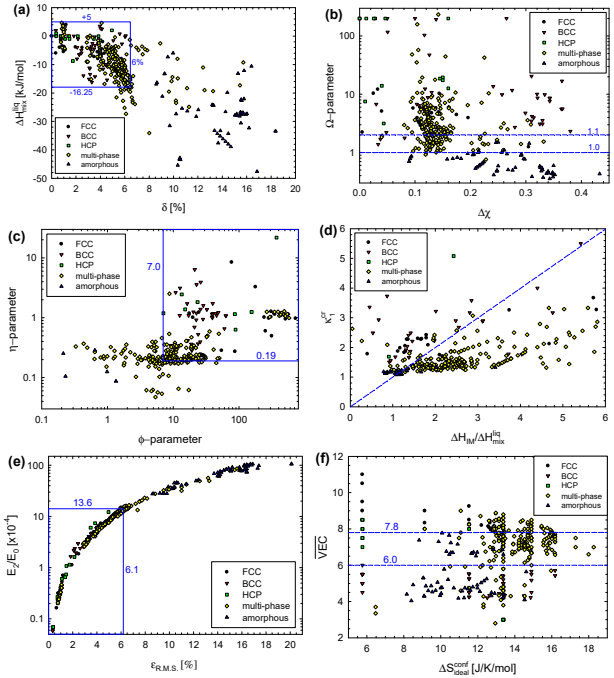
High Throughput Screening Single-Phase HEAs

$$\Delta H_{mix} = 4\sum_{i=1,i\neq j}^{N}\Delta H_{ij}^{mix}c_i c_j \quad \Omega = \frac{T_m\Delta S_{mix}}{|\Delta H_{mix}|} \quad \eta = \frac{T_{ann}\Delta S^{conf}_{ideal}}{|\Delta H^{IM}_{ij}|_{max}} \quad \phi = \frac{-R\sum_{i=1}^{N}c_i\ln c_i - |\sum_{i\neq j}4H_{ij}c_i c_j|/T_m}{|S_E|}$$

$$\kappa_1^{cr}(T) = 1 + \frac{T\Delta S_{mix}}{|\Delta H_{mix}|}(1-\kappa_2) > \Delta H_{IM}/\Delta H_{mix} \quad \Delta\chi = \sqrt{\sum_{i=1}^{N}c_i(\chi_i - \sum_{j=1}^{N}c_j\chi_j)} \quad VEC = \sum_{i=1}^{N}c_i VEC_i$$

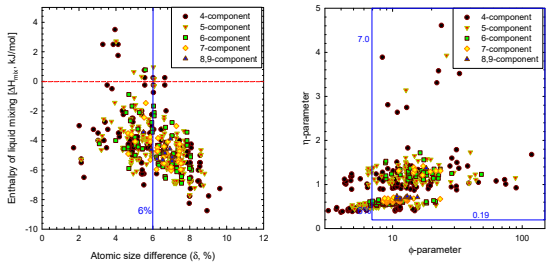
$$\delta = \sqrt{\sum_{i=1}^{N}c_i\left(1-c_i/\sum_{j=1}^{N}c_j r_j\right)^2} \quad <\varepsilon^2>^{1/2} \quad E_2/E_0 = \sum_{j\neq i}^{N}\frac{c_i c_j\left|r_i + r_j - 2\bar{r}\right|^2}{4(\bar{r})^2}$$

Experimental data evaluation

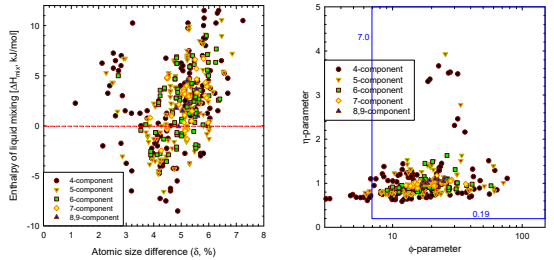


M.C. Gao, C. Zhang, P. Gao, F. Zhang, L.Z. Ouyang, M. Widom, and J.A. Hawk, "Thermodynamics of Composition Concentrated Alloys", *Current Opinion Solid State Mater. Sci.*, 2017, ***in press***.

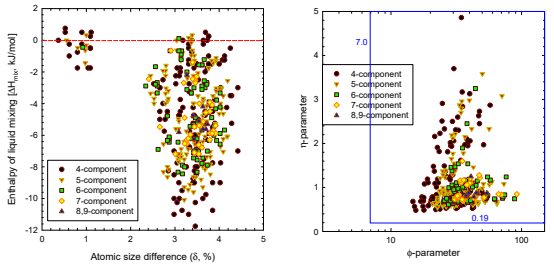
Cr-Hf-Mo-Nb-Ta-Ti-V-W-Zr system. BCC. Equimolar.



Ag-Au-Co-Cu-Ir-Ni-Pd-Pt-Rh system. FCC. Equimolar.

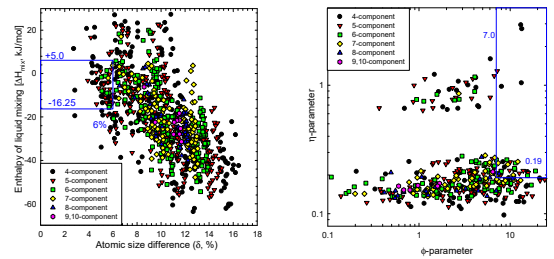


Co-Fe-Ir-Mn-Os-Re-Rh-Ru-Tc system. HCP. Equimolar.

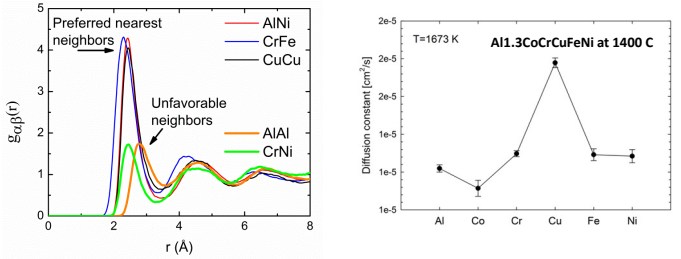


Out of 383 equimolar compositions (4, 5, 6, 7, 8 and 9-components) in each structure, there are 286 FCC compositions, 4 HCP compositions, and 174 BCC compositions that satisfy those constraints.

Al-Ga-Li-Mg-Sc-Si-Ti-V-Y-Zr system. Equimolar.

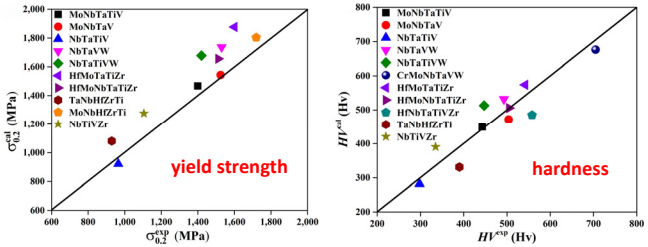


Ab Initio Molecular Dynamics Simulations



L.J. Santodonato, Y. Zhang, M. Feygenson, C. Parish, M.C. Gao, J.K.R. Weber, J.C. Neuefeind, Z. Tang, and P.K. Liaw, Nature Communication 6 (2015) 5964.

Solid Solution Strengthening Modeling



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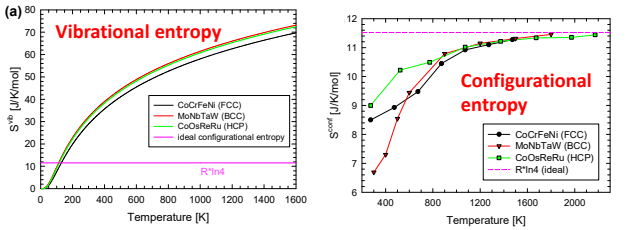
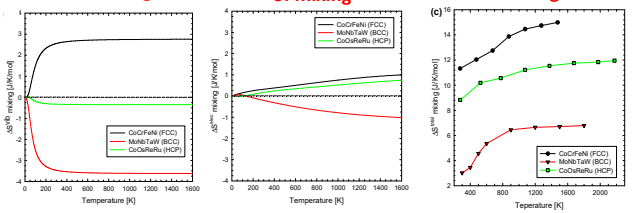
Entropy Sources Calculations



Vibrational entropy of mixing | Electronic entropy of mixing | Total entropy of mixing



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