Designing high entropy alloys based on the tabulated physical properties of the constituent elements

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The tabulated physical properties data of the possible constituent elements for high entropy alloys will be revisited. The binary mixing enthalpy, $\Delta H_{\rm mix}$, the atomic radius, r, the valence, z, the electronegativity, χ, the elastic, E, and bulk modulus, B, will be reviewed from different sources and the most appropriate data will be selected and presented for calculating the characteristic quantities for alloy designing:

Mixing enthalpy $$\Delta H_{\rm mix} = \sum_{i=1,j>1}^{n} 4\Delta H_{AB}^{\rm mix} c_i c_j \,,$$

configuration entropy $$\Delta S_{\rm mix} = -R \sum_{i=1}^{n} c_i \ln c_i \,,$$

atomic size mismatch $$\delta r = \sqrt{\sum_{i=1}^{n} c_i 1 - r_i / \sum_{i=1}^{n} c_i r_i} \,,$$

and electro negativity $$\Delta \chi = \sqrt{\sum_{i=1}^{n} c_i (\chi_i - \sum_{i=1}^{n} c_j \chi_j)^2} \,.$$

Differences are used for calculating the alloy designing parameters such as:
$\Omega = T_m \Delta S_{\rm mix}/|\Delta H_{\rm mix}|$. New designing parameters will be proposed, such as:
$P = \overline{T}_m \Delta S_{\rm mix}/E\delta^2$ and $Q = \Delta H_{\rm mix}/E\delta^2$, where $E = \sum_{i=1}^{n} c_i V_i E_i / \sum_{i=1}^{n} c_i E_i$ and V_i is the molar volume.
Selection rules for solid solution phases in high entropy alloys can be established from diagrams representing Ω, P. and Q versus atomic size mismatch. Electron densities for high entropy alloys obtained by *ab initio* calculations will be compared to those obtained from tabulated data: $n = \sum_{i=1}^{n} c_i z_i / \sum_{i=1}^{n} c_i V_i^a$.
Some diagrams correlating the mechanical properties (hardness and elastic modulus) with electron densities will be presented for bulk amorphous and single-phase high entropy alloys.

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