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In the extended Miedema model and Gallego's method, the formation enthalpy of phases is written in the following form:

$$\Delta H = \Delta H^{\mathrm{chem}} + \Delta H^{\mathrm{elastic}} + \Delta H^{\mathrm{struct}}, \tag{1}$$

where ΔH^{chem}, $\Delta H^{\mathrm{elastic}}$ and $\Delta H^{\mathrm{struct}}$ stand for chemical, elastic and structural contributions to enthalpy. These three enthalpy terms are obtained in the following equations:

$$\Delta H^{\mathrm{chem}} = \sum_{\substack{i=1\\ i\neq j}}^{n} \Delta H_{ij}^{\mathrm{chem}}, \tag{2}$$

$$\Delta H^{\mathrm{elastic}} = \sum_{\substack{i=1\\ i\neq j}}^{n} \Delta H_{ij}^{\mathrm{elastic}}, \tag{3}$$

$$\Delta H^{\mathrm{struct}} = \sum_{\substack{i=1\\ i\neq j}}^{n} \Delta H_{ij}^{\mathrm{struct}}, \tag{4}$$

where n is the number of constituent elements. $\Delta H^{\mathrm{struct}}$ originates from the valence electrons and the crystal structure of the solvent and solute atoms, and are assumed to be negligible in comparison to ΔH^{chem} and $\Delta H^{\mathrm{elastic}}$. ΔH^{chem} and $\Delta H^{\mathrm{elastic}}$ stand for chemical and elastic contributions to the enthalpies of binary systems calculated by following equations:

$$\Delta H_{ij}^{\mathrm{chem}} = c_i c_j (c_j^s \Delta H^{\mathrm{inter}}(i \,\mathrm{in}\, j) + c_i^s \Delta H^{\mathrm{inter}}(j \,\mathrm{in}\, i)), \tag{5}$$

$$\Delta H_{ij}^{\mathrm{elastic}} = c_i c_j (c_i \Delta H^{\mathrm{elastic}}(i \,\mathrm{in}\, j) + c_j \Delta H^{\mathrm{elastic}}(j \,\mathrm{in}\, i)), \tag{6}$$

where

$$\Delta H^{\mathrm{inter}}(i \,\mathrm{in}\, j) = \frac{V_i^{2/3}}{\frac{1}{2}\left(\frac{1}{n_{wsi}^{1/3}} + \frac{1}{n_{wsj}^{1/3}}\right)} \left\{-P(\Delta\phi)^2 + Q(\Delta n_{ws}^{1/3})^2\right\}, \tag{7}$$

$$\Delta H^{\mathrm{elastic}}(i \,\mathrm{in}\, j) = \frac{2K_i G_j (W_{i\,\mathrm{in}\,j} - W_{j\,\mathrm{in}\,i})}{4G_j W_{i\,\mathrm{in}\,j} + 3K_i W_{j\,\mathrm{in}\,i}}, \tag{8}$$

$$c_i^s = \frac{c_i V_i^{2/3}}{c_i V_i^{2/3} + c_j V_j^{2/3}}, \quad c_j^s = 1 - c_i^s, \tag{9}$$

here, c_i and c_j are the compositions of the constituent elements, c_i^s and c_j^s are the surface fractions, V_i and V_j are the molar volumes, P and Q are empirical constants, $\Delta\phi$ stands for the difference of work function of the electrons (φ_i-φ_j), n_{ws} stands for the electron density at the boundary of the Wigner-Seitz cell, K is the compressibility, G is the shear modulus. $W_{i\,\mathrm{in}\,j}$ and $W_{j\,\mathrm{in}\,i}$ are the corrected molar volumes due to the electron transfer.

Considering the chemical short-range order of the alloy phases, the right-hand side of equation (5) should be multiplied by a factor

$$f = 1 + \gamma (c_i^s c_j^s)^2 . \tag{10}$$

The parameter γ in the factor is an empirical constant which is used to describe the short-range order of different alloys. For solid solution, amorphous phase and ordered compound, it usually takes 0, 5 and 8, respectively.

The formation enthalpy of an amorphous phase (ΔH^{AM}) is comprised of chemical ($\Delta H^{\mathrm{AM(chem)}}$) and topological enthalpy contributions (ΔH^{topo}), respectively. Thus, ΔH^{AM} can be written as:

$$\Delta H^{\mathrm{AM}} = \Delta H^{\mathrm{AM(chem)}} + \Delta H^{\mathrm{topo}}, \tag{11}$$

$$\Delta H^{\mathrm{topo}} = 3.5 \sum_{i=1}^{n} c_i T_m^i , \tag{12}$$

where T_m^i is the melting point temperature of constituent element.

For intermetallic compounds, the elastic and structural terms in the equation (1) are absent. Meanwhile, the formation enthalpy of solid solution (ΔH^{SS}) could be obtained by equation (1).

Generally, the Gibbs free energies of the possible competing phases are employed to determine whether amorphous phases could be formed or not. Thus, the Gibbs free energy of an alloy phase can be calculated by:

$$\Delta G = \Delta H - T \cdot \Delta S , \tag{13}$$

where ΔH and ΔS are the enthalpy and entropy terms, respectively. According to Miedema's model, the entropy term for the solid solutions and amorphous phases are both taken as ideal solution [11]. Thus, ΔS can be written as:

$$\Delta S = -R \sum_{i=1}^{n} c_i \ln c_i , \tag{14}$$

where R is the gas constant.

Furthermore, the parameter γ^* is employed to indicate the GFA of an alloy. According to Xia's and Wang's suggestion [13-15], the GFA is affected by two aspects: (1) the driving force for the formation of amorphous phases, i.e., $-\Delta H^{\mathrm{AM}}$, and (2) the resistance of the amorphous phases formation against crystallization, i.e., $\Delta H^{\mathrm{AM}} - \Delta H^{\mathrm{Inter}}$. Thus, γ^* is given by

$$\gamma^* = \mathrm{GFA} \propto \frac{-\Delta H^{\mathrm{AM}}}{\Delta H^{\mathrm{AM}} - \Delta H^{\mathrm{Inter}}} . \tag{15}$$

The larger the value of γ^*, the better the GFA of the alloy. The calculation of γ^* enables one to search for the alloy with superior GFA.