Popis σ fáze VMi Modelem v soust Fe-Cr-Ni

$$P_f(Y) = \begin{pmatrix} {}^1y_{Fe} & \emptyset & {}^1y_{Ni} \\ \emptyset & {}^2y_{Cr} & \emptyset \\ {}^3y_{Fe} & {}^3y_{Cr} & {}^3y_{Ni} \end{pmatrix} = \text{např.} = \begin{pmatrix} 0.4 & \emptyset & 0.6 \\ \emptyset & 1.0 & \emptyset \\ 0.3 & 0.5 & 0.2 \end{pmatrix} \quad \begin{matrix} 8 \\ 4 \\ 18 \end{matrix}$$

celkem 6 členů

$$G_{ref} = G_{Fe:Cr:Fe} \cdot {}^1y_{Fe} \cdot {}^1y_{Cr} \cdot {}^3y_{Fe} + \boxed{G_{Fe:Cr:Cr}} \cdot {}^1y_{Fe} \cdot {}^2y_{Cr} \cdot {}^3y_{Cr} + \ldots$$
$$\underset{I}{}$$

G hyp. struktury
$Fe_8 Cr_4 Fe_{18}$

$${}^1y_{Fe} = \frac{{}^1h_{Fe}}{{}^1h_{Fe} + {}^1h_{Ni}}$$

$$G_I = f\left(G_{Cr}^{bcc}, G_{Fe}^{fcc}\right) \equiv g(T) \overset{\text{např.:}}{=} a + b \cdot T + c \cdot T^2 + d \cdot T^3 + e \cdot T \ln T +$$
$$+ f \cdot \frac{1}{T} + g \cdot \frac{1}{T^2} + h \cdot \frac{1}{T^3} + j \cdot T^7 + i \cdot T^{-9}$$

$$G^{id\,mix} = RT \cdot \left[\left({}^1y_{Fe} \cdot \ln {}^1y_{Fe} + {}^1y_{Ni} \cdot \ln {}^1y_{Ni}\right) \cdot 8 + \left({}^3y_{Fe} \ln {}^3y_{Fe} + {}^3y_{Cr} \cdot \ln {}^3y_{Cr} + \right. \right.$$
$$\left. \left. + {}^3y_{Ni} \cdot \ln {}^3y_{Ni}\right) \cdot 18 \right]$$

$$G^E = G^{E Bi} + G^{E Ter.} \qquad (\text{přísp. z binárních a tern. soust.})$$

G^{EBi}:

$L = a + b \cdot T + c \cdot T \ln T$

např.: $\ldots + L_{Fe:Cr:Fe,Cr} \cdot {}^1y_{Fe} \cdot {}^2y_{Cr} \cdot {}^3y_{Fe} \cdot {}^3y_{Cr} + \ldots$

$$= \left(L^0 + {}^1L \cdot \left({}^3y_{Fe} - {}^3y_{Cr}\right) + {}^2L \left({}^3y_{Fe} - {}^3y_{Cr}\right)^2 + \ldots\right)$$

$G^{E ter}$:

$\ldots L_{Fe,Ni:Cr:Fe} \cdot {}^1y_{Fe} \cdot {}^1y_{Ni} \cdot {}^2y_{Cr} \cdot {}^3y_{Fe}$

$$\Rightarrow G^{celk} = f\left(Y, G, L\right) \quad \text{interakční parametry (fit)}$$

složení

G.en. hypot. struktur (výpočet nebo fit)
resp. real. struktur.