Interdiffusion in Binary Systems during Rapid Heating: Thermoelastic Stress Influence

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If vacancies of a binary metallic system A-B have the potential energy W_v depending on position, one can find the force, acting on a vacancy in such field

$$F_v = -\mathrm{grad}W_v \tag{1}$$

If the system is under stress σ, and if a vacancy in the solid is modelled as the centre of negative dilatation, the potential energy of a vacancy is given by

$$W_v = -(\Delta\omega\,\mathrm{tr}\sigma)/3 \quad \Delta\omega = \omega_v - \omega_{atom} \tag{2}$$

Consequently, one can determine vacancy flux due to potential energy gradient:

$$j_v^{\sigma} = C_V D_V\,F_v/(kT) + (D_B - D_A)\mathrm{grad}\delta C_B^{\sigma} \tag{3}$$

$$C_V D_V = C_A\,D_A^* + C_B\,D_B^*, \quad C_A + C_B = 1$$

This vacancy flux leads to appearance of atomic fluxes of atoms A and B in opposite direction (in the lattice reference system):

$$j_i = -C_i D_i J_v^{\sigma}/(C_V D_V) - D_A D_B/(C_A D_A + C_B D_B)\,\mathrm{grad}\delta C_i^{\sigma} \tag{4}$$

$$i = A,B$$

Besides, there are diffusion fluxes of atoms A and B (in the lattice reference system)

$$j_i = -D_i\,\mathrm{grad}\,C_i \qquad i = A,B \tag{5}$$

One can find resulting flux relatively to the Matano interface

$$J_B = -J_A = -(D\,\mathrm{grad}C_B + C_A C_B(D_B^* - D_A^*)\,F_v/(kT) + D\,\mathrm{grad}\delta C_B^{\sigma}) \tag{6}$$

$$D = C_A D_B + C_B D_A$$

Diffusion and Stresses

For describing of a phase growth with the range of homogeneity ΔC one can apply the constant flux approximation [1,2]

$$J_B \approx const = - (D\, \Delta C/\Delta X - D^*/(kT)(\Delta W_v/\Delta X) + D\Delta\delta C^\sigma/\Delta X), \quad C=C_B \qquad (7)$$

$$D = (1/\Delta C)\int_c^{c+\Delta c} D(C)dC ; \quad D^* = (1/\Delta C)\int_c^{c+\Delta c} C_A C_B(D_B^* - D_A^*)dC$$

Taking into account that concentrations at the interfaces practically are not changed under stress, one can neglect the last term:

$$J_B = - D\, \Delta C/\Delta X + D^*/(kT)(\Delta W_v/\Delta X) \approx const \qquad (8)$$

We have two situations (if, for example, $D_B^* > D_A^*$):

1. $\Delta W_V > 0$. The phase grows more slowly, if

$$\Delta W_v < D\, \Delta C\, kT/D^*.$$

And if $\Delta W_V/\Delta X = const = K$, one can find maximum width of phase

$$\Delta X_{max} = D\Delta C\, kT/(D^*K),$$

so stress gradient can stop the phase growth.

2. $\Delta W_V < 0$. The phase grows more rapidly.

If ΔW_V is small, the concentration profile tends to form a step ($\lceil$ -like shape).

If ΔW_V has a great value, it is possible for atoms to diffuse up to the concentration gradient, if mutual solubility of substances A and B is limited.

The analogical concentration profile is determined after interdiffusion during rapid heating of Fe-Ti samples ($\sim$ -like shape) [3].

The force, acting on a vacancy, is directed from Ti to Fe and $D_{Fe}^* > D_{Ti}^*$.

The stress gradient arises during rapid heating due to difference between thermal expansion coefficient of Fe and Ti ($\alpha_{Fe} \approx 2\, \alpha_{Ti}$).

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