Atomistic interpretation of the interface transfer coefficients for interdiffusion in AB binary phase separating system

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During intermixing in A/B diffusion couple the actual compositions (c'_α and c'_β) on the left as well as on the right hand side of the α/β interface gradually will decrease (from unity) as well as increase (from 0) until the equilibrium c_α and c_β will be reached (α and β refer to the A- and B-rich phases, separated by the interface). The diffusion flux of A atoms across this interface, J_I, is determined from the expression of atomic fluxes given in the modified Martin model [1,2]. Assuming that J_I, is proportional to the deviations, $\Delta_\alpha = c'_\alpha - c_\alpha$ and $\Delta_\beta = c_\beta - c'_\beta$, from the equilibrium

$$J_I = (1/\Omega)[K_{I\alpha\beta}\Delta_\alpha + K_{I\beta\alpha}\Delta_\beta),$$

where $\Omega = \Omega_A = \Omega_B$ is the atomic volume. It is shown that the $K_{I\alpha\beta}$ and $K_{I\beta\alpha}$ interface transfer coefficients are positive and equal to each other for symmetric miscibility gap and can be given as

$$K_{I\beta\alpha} = K_{I\alpha\beta} = K = z_v a \Gamma_{I\alpha\beta} c_\alpha \xi.$$

Here $\Gamma_{I\alpha\beta}$ is the jump frequency from α to β phase across the interface, a is the lattice parameter z_v is the vertical coordination number, $\xi = [1 + exp(ZV\{c_\alpha - c_\beta\}/kT)]$, V is the well-known solid solution parameter, kT has its usual meaning. The above expression justifies the conjecture, frequently used in the literature (see e.g. [3]), that *only one interface transfer coefficient is enough for the description of mass transfer across an interface*. For short diffusion times the finite value of $\Gamma_{I\alpha\beta}$ will restrict the flux, leading to linear kinetics. It will also be shown that for the estimation of the critical interface shift (giving the transition from the interface to diffusion control, i.e. from linear to parabolic kinetics) the

$$x_c \cong a\,exp[-ZM(1-2c_\beta)/kT]$$

relation can be used, where a is the lattice spacing and the exponential factor is the ratio of factors describing the composition dependence of the jump frequencies in the β phase and across the interface, respectively. Thus x_c is independent of the value of V and only the composition dependence of the jump frequencies is important. For composition independent jump frequencies $x_c \cong a$, (i.e. it can not be detected), while for the case when the diffusivity changes by seven orders of magnitude from pure A to B [2,4], x_c is about 150nm.

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