A MODEL OF GROWTH OF AN INTERMEDIATE PHASE IN BI- AND POLYCRYSTALS

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An analytically solvable model of the growth of an intermediate phase between low-soluble components on diffusion at grain boundaries involving outflow is suggested. Criteria for a transition from the Fisher regime $t^{1/4}$ to a parabolic one are established. The formalism suggested is extended to the case of the growth of a solid-state solution with an exponential concentration dependence of the diffusion coefficient.

Although the Fisher solution for the impurity diffusion in a bicrystal and its modification for polycrystals have long been known [1-4], an analogous problem for the growth of intermediate phases in systems with limited solubility has been analyzed, as far as we known, only in [5] for the case where the diffusion coefficients for a solid-state solution are well in excess of those for a phase. In [5], solutions analogous to a conventional Fisher solution have been obtained on the assumption that the diffusion process is quasistationary:

$$\frac{\partial C_b(t, y)}{\partial t} = 0,$$

where $C_b$ is the grain boundary concentration of component B in the phase, and the Y axis runs along a grain boundary (GB). In the form of Eq. (1) this assumption is not fulfilled; it is inexact since at a fixed $y$ the quantity $C_b(y)$ changes from $C_1$ to $C_1 + \Delta C_1$ (within the limits of the homogeneity interval) and incorrectly predicts the form of the phase wedge. The assumption

$$\frac{\partial C_b(\xi)}{\partial t} = 0,$$

is more exactly fulfilled, where $\xi = y/y_0(t)$, $y_0(t)$ is the maximum length of the phase wedge. For instance, in the middle of the phase wedge $C_b$ is virtually unchanged throughout the period of phase growth (the homogeneity interval is from $C_1$ to $C_1 + \Delta C_1$). Use of assumption (2), as shown below, leads to correct prediction of the form of the phase wedge.

Our developed model is rather simple, and it may be generalized to the case of growth of several phases and allows prediction of the phase composition and sufficiently easy calculation of diffusion coefficients.

The model is based on the following assumptions:

1. An intermediate phase forms at first on the basis of the GB; the latter, transforming from the boundary A-A to the boundary I-I, remains, due to easy influx with a diffusion coefficient $D_b$ and having a thickness of $\delta \approx 1$ nm (i.e., the GB is not overgrown with a new phase and does not bifurcate).

2. Formed phase I broadens normal to the GB due to volume diffusion with a diffusion coefficient $D$.

3. At all thee points of the formed I-A phase boundary between the broadening phase I and the matrix A the concentration of the component B is $C_1$ on the side of phase I and is zero on the side of phase A (solubility of B in A is ignored).

4. Consideration is given to the following variants:

a) following [5], we assume that outflow from the GB is the same at all GB points:

\[
\frac{\partial C}{\partial x} = \frac{\Delta C'}{x(t, y)} = \frac{\Delta C_1}{x_0} \quad ; \quad x_0 = x(t, 0);
\]  

\(\text{(3)}\)

b) following [5], in which a linear approximation for \(C_0(y)\) is shown to be a permissible one for a rigorous solution, we also assume here that \(C_0(y)\) changes approximately linearly with \(y\).

Conditions 4a) and 4b) will be considered independently and then the results obtained will be compared.

5. A flow in the volume of a phase wedge normal to the GB is constant along \(x\) (a corresponding property is proved in [6]) in a reference system associated with the moving nose of the wedge.

At first, we employ assumption 4a).

The balance equation of the flows at the nose of the growing phase wedge is as follows

\[
C_1 \frac{dy_0}{dt} = \frac{D_0 \Delta C_1}{y_0} - \frac{2}{\delta} \int_0^{y(t)} D \frac{\partial C(t, x/y)}{\partial x} \ dy,
\]  

\(\text{(4)}\)

where the second term on the r.h.s. accounts for the decrease of the flow, reaching the nose, due to lateral outflow into the volume of the phase.

Taking into consideration assumption (3) on the outflow being the same, we obtain from (4)

\[
C_1 \frac{dy_0}{dt} = \frac{D_0 \Delta C_1}{y_0} - \frac{2y_0(t)}{\delta} \frac{D \Delta C_1}{x_0(t)}.
\]  

\(\text{(5)}\)

The dependence \(x_0(t)\) is determined from the usual equation for transverse motion of the phase boundary

\[
C_1 \frac{dx_0}{dt} = \frac{D \Delta C_1}{x_0},
\]

so that \(x_0(t)\) grows according to the parabolic law

\[
x_0(t) = \left( \frac{2D \Delta C_1}{C_1} t \right)^{1/2}.
\]

Thus, the equation for \(y_0(t)\) has the simple form

\[
\frac{dy_0}{dt} = \frac{A}{y_0} - B \frac{y_0}{t^{1/2}}; \quad A = \frac{D_0 \Delta C_1}{C_1}, \quad B = \frac{1}{\delta} \left( \frac{2D \Delta C_1}{C_1} \right)^{1/2}.
\]  

\(\text{(6)}\)

Its general solution is as follows:

\[
y_0^2 = \frac{A}{B} t^{1/2} - \frac{A}{4B^2} (1 - e^{-4B t^{1/2}}).
\]

In the case of frozen outflow ((\(D \Delta C_1 t)^{1/2} \ll \delta\), i.e., \(B t^{1/2} \ll 1\)), this gives the parabolic law (regime A)

\[
y_0^2 = 2At.
\]

On passing to large times of annealing, \(t >> 1/B^2\), we arrive at the Fisher regime of diffusion (regime B):

\[
y_0^2 = \frac{A}{B} t^{1/2} \left( 1 - \frac{1}{B t^{1/2}} \right) \approx \frac{A}{B} t^{1/2},
\]

i.e., \(y_0 \approx t^{1/4}\). The characteristic time of the transition from A to B is

\[
t_{A-B} \approx C_1 \delta^2 / 2D \Delta C_1,
\]

which agrees with an analogous estimate for tracer diffusion [4]. Here the corresponding length of the phase wedge is

\[
y_{A-B} \approx \delta (D_0 / 2D)^{1/2}.
\]  

\(\text{(7)}\)

877