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Intermediate phase cone growth kinetics along dislocation pipes inside polycrystal grains

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Dislocation-pipe diffusion (DPD) becomes a major contribution to device failure in microelectronic components at working temperatures. Usually, the simple random walk law for diffusion (Type C kinetics $t^{1/2}$) is employed to calculate of DPD coefficients. The article presents an analytically solvable model of describing the diffusion phase cone growth along dislocation pipes inside polycrystal grains involving outflow from dislocation lines (Type B kinetics). Correlative analytical method to solve differential diffusion equations for such model is suggested. Competition between phase cone growth along dislocation lines involving outflow and phase wedge growth along grain boundaries (GBs) involving outflow is analyzed. It is shown that while phase wedge growth law along GBs is the Fisher regime $t^{1/4}$, phase cone growth law along dislocation lines is another diffusion regime $t^{1/6}$. Real experimental data are analyzed using such diffusion regime. It is shown that it is possible to calculate DPD coefficients not only for the phase cone formation, but for migration of atoms along dislocations and self-diffusion along dislocation pipes too.
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INTRODUCTION

Model of intermediate phase growth with a narrow concentration range of homogeneity, ΔC_1, between low-soluble components during diffusion along grain boundaries involving outflow was suggested[1] and criteria for a transition from the Fisher regime $t^{1/4}$ to a parabolic one ($t^{1/2}$) was analyzed. It was analytically proved[2] that perpendicular grain boundaries do not influence phase growth kinetics in B-regime. This result enables using the well-known model of a polycrystal as a 3-D array of grain boundaries to be perpendicular to the interface for describing the phase growth. A model to describe analytically the diffusion spherical phase growth from point source inside polycrystal grains was presented.[3] It was shown that spherical phase growth law from point source is $t^{1/3}$.

MODEL

Physical model of dislocation-pipe diffusion involving outflow is as follows (Fig.1). Diffusion flux, j_d, flows along dislocation pipe with diffusion coefficient D_d and, simultaneously, outflows into volume from each point, dy, with bulk diffusion coefficient $D<<D_d$[4] in 2-D space to be perpendicular to the dislocation pipe (Eq.1).

$$\pi R_d^2 C_1 \frac{dy}{dt} = \pi R_d^2 j_d - 2\pi R_d \int_0^{y(t)} j_1 dy \tag{1}$$

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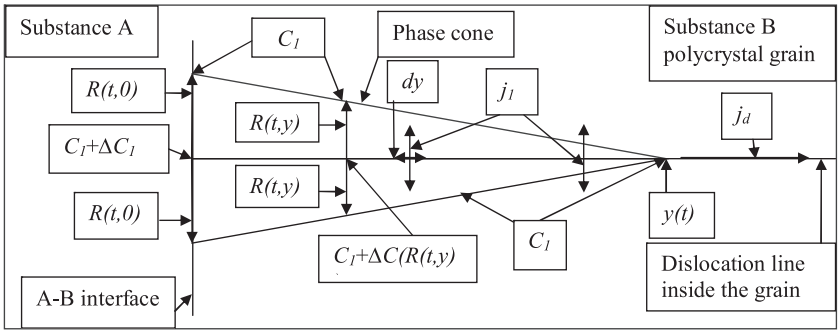

FIG. 1. Model of the intermediate phase cone formation during A-atoms diffusion along dislocation line involving outflow from the dislocation pipe.

where R_d is the radius of dislocation pipe.

$$\text{Here} \quad j_d(t) = \frac{D_d \Delta C_1}{y(t)} \quad \text{and} \quad j_1(t) = D\frac{\partial C}{\partial R} = \frac{D\Delta C_1}{R(t,0)} = \frac{D\Delta C(R(t,y))}{R(t,y)}. \tag{2}$$

Concentration profiles are approximately linear[1] along dislocation line and along the phase cone radii.

Correlative differential diffusion equation is as follows:

$$\frac{dy}{dt} = \frac{D_d \Delta C_1}{C_1 y(t)} - \frac{2D\Delta C_1 y(t)}{C_1 R(t,0) R_d}. \tag{3}$$

Phase grows law for *R(t,0)* is unknown, so we can slightly modify the model (Fig.2). A model is based on the following assumptions.

1. Diffusion flux flows along dislocation line only up to the first dislocation step, then it flows in spherical symmetry and along dislocation line, simultaneously, up to the second dislocation step and so on. The dislocation steps are regarded as the point sources having a diameter of $\delta \approx 1nm \approx 2R_d$.
2. Ratio $\frac{D_{GB}}{D_d} \approx 10^1 \rightarrow 10^2$ depends on temperature[5] (D_{GB} is the grain boundary diffusion coefficient).
3. Formed spherical phases *1* broadens in 3-D space from the dislocation steps due to diffusion with a diffusion coefficient $D_1 \approx D$. It is important for the analysis.
4. Phase grows law for *R(t,0)* is[3]

$$R(t,0) = \sqrt[3]{\frac{3D_1 \Delta C_1 \delta}{2C_1}} \sqrt[3]{t}. \tag{4}$$

Here *R(t,0)* is the radius of spherical phase formed from the first dislocation step, *R(t,y)* are the radii of spherical phases formed from the next dislocation steps.

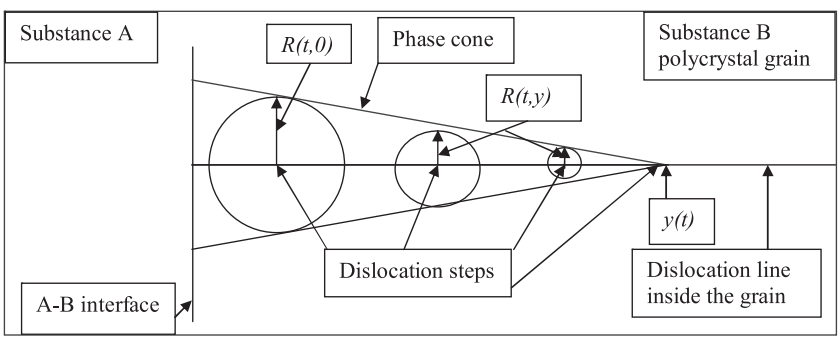

FIG. 2. Model of the intermediate phase cone formation during A-atoms diffusion along dislocation line involving outflow from the dislocation steps.

METHOD

One can get from eq.3 differential equation for intermetallic compound cone cusp, *y(t)*, growing inside polycrystal grains along dislocation lines involving outflow from the dislocations steps:

$$\frac{dy(t)}{dt} = \frac{A}{y(t)} - B_d \frac{y(t)}{\sqrt[3]{t}} \tag{5}$$

where $A = \frac{D_d \Delta C_1}{C_1}$, $B_d = \sqrt[3]{\frac{2^7 D_1^2 (\Delta C_1)^2}{3 C_1^2 \delta^4}}$.

In the Appendix we prove that the phase growth law during Type B kinetics is

$$y(t) = \sqrt{\frac{A}{B_d}\sqrt[3]{t}}$$

or

$$y(t) = \sqrt{\frac{A}{B_d}}\sqrt[6]{t} = \left(\frac{D_d}{D_1}\right)^{1/3} D_d^{1/6} \left(\frac{\Delta C_1}{C_1}\right)^{1/6} \frac{3^{1/6}\delta^{2/3}}{2^{7/6}} t^{1/6}. \tag{6}$$

The physical dimensionalities method shows that $[y(t)] = \left[\frac{m^2}{s}\right]^{1/6}[m]^{2/3}[s]^{1/6} = [m]$ so the solution (6) is reasonable.

ANALYSIS

The equation for $y_{GB}(t)$ of the growing phase wedge nose along GB involving outflow has such form:[1,2]

$$\frac{dy_{GB}(t)}{dt} = \frac{A_{GB}}{y_{GB}(t)} - B_{GB}\frac{y_{GB}(t)}{\sqrt{t}}, \tag{7}$$

where

$$A_{GB} = \frac{D_{GB}\Delta C_1}{C_1},\ B_{GB} = \sqrt{\frac{2D\Delta C_1}{C_1\delta^2}}, \tag{8}$$

and

$$y_{GB}(t) = \sqrt{\frac{A_{GB}}{B_{GB}}\sqrt{t} - \frac{A_{GB}}{4B_{GB}^2}(1 - e^{-4B_{GB}\sqrt{t}})}. \tag{9}$$

Equation (9) show the Fisher diffusion regime

$$y_{GB}(t) = \sqrt{\frac{A_{GB}}{B_{GB}}}\sqrt[4]{t} \tag{10}$$

for $t_{GB\to wedge} > \frac{C_1\delta^2}{2D\Delta C_1}$ and $y_{GB}(t_{GB\to wedge}) > \sqrt{\frac{D_{GB}}{2D}}\delta$.

Ratio $\frac{D_{GB}}{D} \approx 10^3 \to 10^5$ depends on temperature[1] so $y_{GB}(t_{GB\to wedge}) > 30nm \to 300nm$ dependently on temperature. Equation (6) shows diffusion regime $t^{1/6}$ for $t_{d\to cone} > \frac{\sqrt{3}C_1\delta^2}{2^5 D_1 \Delta C_1}$ and $y(t_{d\to cone}) > \sqrt{\frac{D_d}{D_1}}\frac{\sqrt[4]{3}}{4}\delta$. Ratio $\frac{D_d}{D_1} = \frac{D}{D_1}\frac{D_{GB}}{D}\frac{D_d}{D_{GB}} \approx \frac{D}{D_1}10^2 \to \frac{D}{D_1}10^3$ so $y(t_{d\to cone}) > 3nm \to 10nm$ dependently on temperature. We can analyze competition between phase cone growth along dislocation pipes involving outflow and phase wedge growth along grain boundaries involving outflow (Fig.3). Here *x(t,0)* is the phase layer thickness formed in A-B planar specimen due to volume diffusion, *x(t,y)* is the phase wedge thickness formed in A-B planar specimen (B is bicrystal) due to grain boundary diffusion with simultaneous outflow in volume,[1,2] *y(t)* is the growing phase cone cusp along dislocation line, $y_{GB}(t)$ is the growing phase wedge nose along GB.

Ratio $\frac{y_{GB}(t_{d\to cone})}{y(t_{d\to cone})} = \frac{\sqrt{2}}{3^{1/8}}\sqrt{\frac{D_{GB}}{D_d}}\sqrt[4]{\frac{D_1}{D}} \approx 4 \to 12$ dependently on temperature. Ratio $\frac{D_{GB}}{D_d}$ is more important than ratio $\frac{D_1}{D}$.

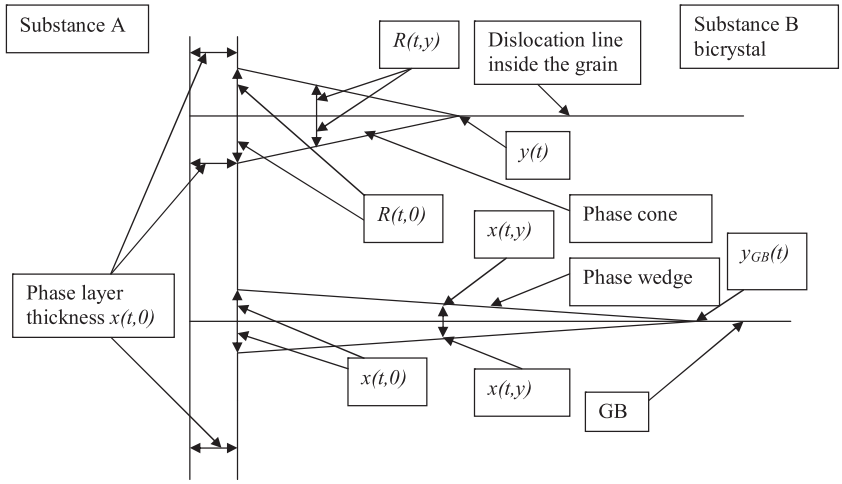

FIG. 3. Growing phase wedge along GB involving outflow and growing phase cone along dislocation line involving outflow competition.

Ratio $\frac{R(t_{GB\to wedge},0)}{x(t_{GB\to wedge},0)} = \frac{2D_1 D_{GB}^{1/6}}{DD_d^{1/6}} \approx 2\frac{D_1}{D} \approx 2$. Ratio $\frac{D_1}{D}$ is more important than ratio $\frac{D_{GB}}{D_d}$.

It seems that Fig.3 is like Figure 3.[5] The diffusion length penetration of Hf into a HfN/ScN superlattice sample was directly measured and an average value was calculated[5] (*y(24h)=4.5nm at* 950^0C). The shape of the Hf diffusion front is like as shown in Fig.3 (diffusion cone *R(t,y)*). One can estimate,[1] $\left(\frac{\Delta C_1}{C_1}\right) \approx 10^{-1}$, and $y^6(t) = \left(\frac{D_d}{D_1}\right)^2 D_d \left(\frac{\Delta C_1}{C_1}\right) \frac{3\delta^4}{2^7} t \approx \left(\frac{D_d}{D_1}\right)^2 D_d \frac{\delta^4 t}{400}$, and $D_d^{Hf} \approx \left(\frac{D_d}{D_1}\right)^{-2} \frac{400}{t} \left(\frac{y}{\delta}\right)^4 y^2 \approx 4\left(\frac{D_d}{D_1}\right)^{-2} * 10^{-17} \frac{m^2}{s} \approx 3.8 * 10^{-21} \frac{m^2}{s}$ if $\frac{D_d}{D_1} \approx 10^2$ at such temperature. Figure 3[5] shows that *y(48h)* ≈*5nm at* 950^0C and $D_d^{Hf} \approx 3.6 * 10^{-21} \frac{m^2}{s}$. The authors[5] obtained $D_d^{Hf} \approx 2.34 * 10^{-22} \frac{m^2}{s}$.

SUMMARY

The growth law of the phase cone during the intermetallic compound formation with a narrow concentration range of homogeneity inside polycrystal grains is parabolic for diffusion time $t_{d\to cone} < \frac{\sqrt{3}C_1\delta^2}{2^5 D_1 \Delta C_1}$ and $y(t_{d\to cone}) < 3nm \to 10nm$ dependently on temperature. Phase growth law $t^{1/2}$ transit into phase growth law $t^{1/6}$ when $t_{d\to cone} > \frac{\sqrt{3}C_1\delta^2}{2^5 D_1 \Delta C_1}$ and $y(t_{d\to cone}) > 3nm \to 10nm$ dependently on temperature. Phase growth law $t^{1/6}$ is valid during Type B kinetics of dislocation-pipe diffusion. It is possible to calculate DPD coefficients not only for the phase cone formation, but for migration of atoms along dislocations and self-diffusion along dislocation pipes too.

APPENDIX

One can simplify equation (4) by the following way

$$\frac{dz(t)}{dt} = 2A - \frac{2B_d}{\sqrt[3]{t}} z(t), \tag{A1}$$

where $z(t) = u(t)v(t) = y^2(t)$.

One can transform equation (A1) into

$$\frac{du(t)}{dt} v(t) + u(t)\left(\frac{dv(t)}{dt} + \frac{2B_d}{\sqrt{t}} v(t)\right) = 2A. \tag{A2}$$

$$\text{Assumption} \quad \frac{dv(t)}{dt} + \frac{2B_d}{\sqrt[3]{t}} v(t) = 0 \quad \text{leads to} \quad v(t) = e^{-3B_d \sqrt[3]{t^2}} = e^{-m^2}, \tag{A3}$$

where

$$m^2 = 3B_d t^{2/3} \quad \text{or} \quad m = \sqrt{3B_d} t^{1/3}. \tag{A4}$$

Next step gives:

$$u(t) = 2A \int_0^t e^{3B_d t^{2/3}} dt = \frac{2A}{\sqrt{3B_d^3}} \int_0^m e^{m^2} m^2 dm = \frac{A}{\sqrt{3B_d^3}} \left(m e^{m^2} - \int_0^m e^{m^2} dm \right) \tag{A5}$$

and

$$z(t) = \frac{A}{\sqrt{3B_d^3}} \left(m - e^{-m^2} \int_0^m e^{m^2} dm \right) = \frac{A}{B} t^{1/3} - \frac{A e^{-m^2}}{\sqrt{3B_d^3}} \int_0^m e^{m^2} dm \tag{A6}$$

or

$$y(t) = \sqrt{\frac{A}{B_d} \sqrt[3]{t} - \frac{A e^{-m^2}}{\sqrt{3B_d^3}} \int_0^m e^{m^2} dm}. \tag{A7}$$

It is well known that $\int e^{-m^2} dm = \frac{\sqrt{\pi}}{2} erf(m)$ and $\int e^{m^2} dm = \frac{\sqrt{\pi}}{2i} erf(mi)$, where $i = \sqrt{-1}$.

It was shown[6] that exact solution $erf(m) = \frac{2}{\sqrt{\pi}} \int_0^m e^{-n^2} dn$ can be approximated by the following expression: $erf(m) \approx th(\frac{2}{\sqrt{\pi}} m) = \frac{1 - e^{-\frac{4}{\sqrt{\pi}} m}}{1 + e^{-\frac{4}{\sqrt{\pi}} m}}$ because of $\left. \frac{d(erf(m))}{dm} \right|_{m=o} = \left. \frac{d\left(th\left(\frac{2}{\sqrt{\pi}} m \right) \right)}{dm} \right|_{m=0} = \frac{2}{\sqrt{\pi}}$. It has a deviation from the exact solution of less than 1.9%. It is a precise solution for the main part of the diffusion zone (the deviation is less than 0.1% if $m = \frac{x(t,y)}{x(t,0)} < \frac{1}{4}$). Here *x(t,0)* is the phase layer thickness formed in A-B planar specimen due to volume diffusion, *x(t,y)* is the phase wedge thickness formed in A-B planar specimen (B is bicrystal) due to grain boundary diffusion with simultaneous outflow in volume.[1] It is possible to analyze the experimental results presented[7] using the methods described[6,8] but it is not the problem being considered in this article. We can get finally:

$$y(t) = \sqrt{\frac{A}{B_d} \sqrt[3]{t} - \frac{A e^{-m^2}}{\sqrt{3B_d^3}} \frac{\sqrt{\pi}}{2i} \frac{1 - e^{-\frac{4}{\sqrt{\pi}} mi}}{1 + e^{-\frac{4}{\sqrt{\pi}} mi}}}. \tag{A8}$$

So the phase growth law during Type B kinetics is $y(t) = \sqrt{\frac{A}{B_d} \sqrt[3]{t}}$.

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