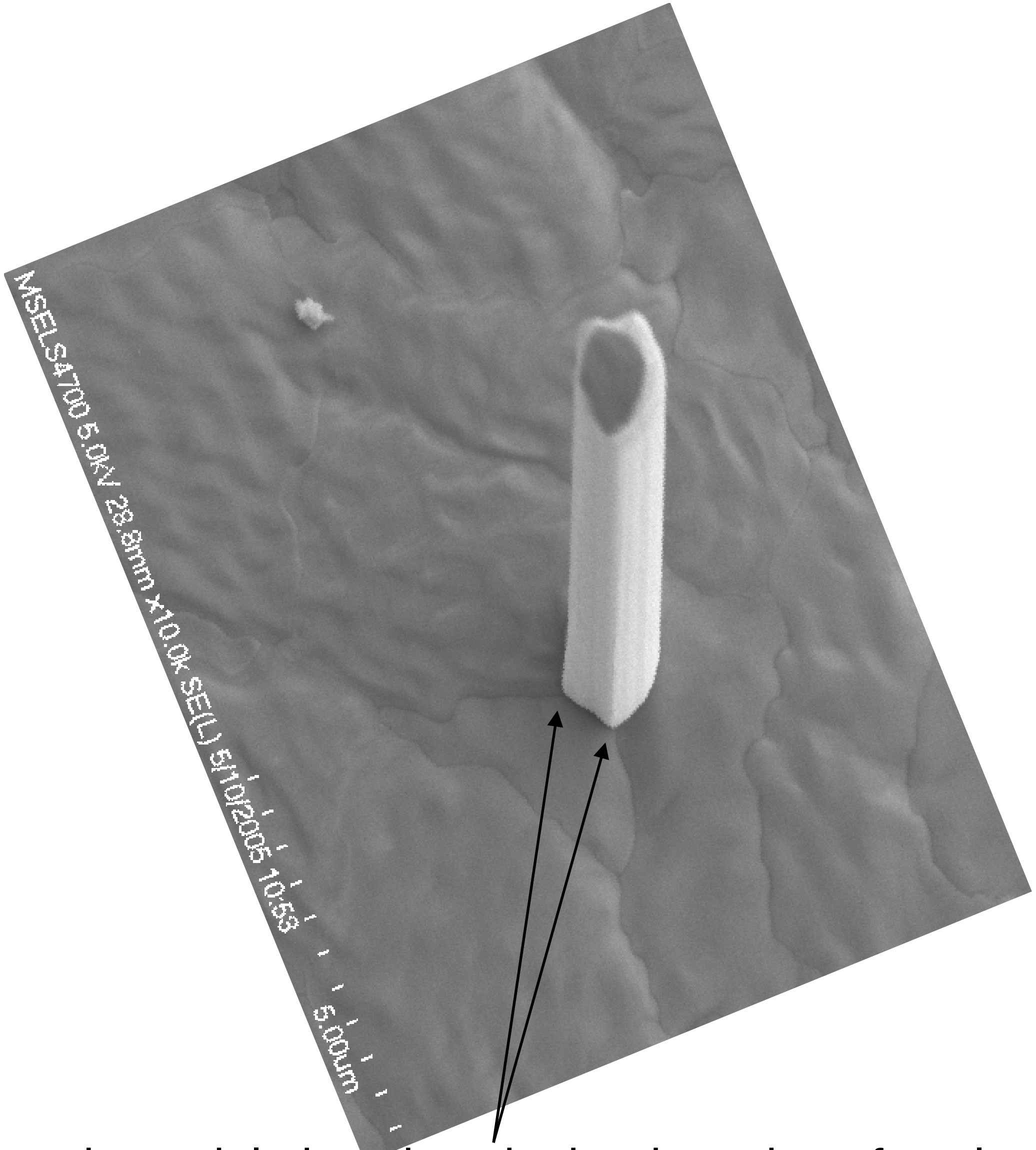
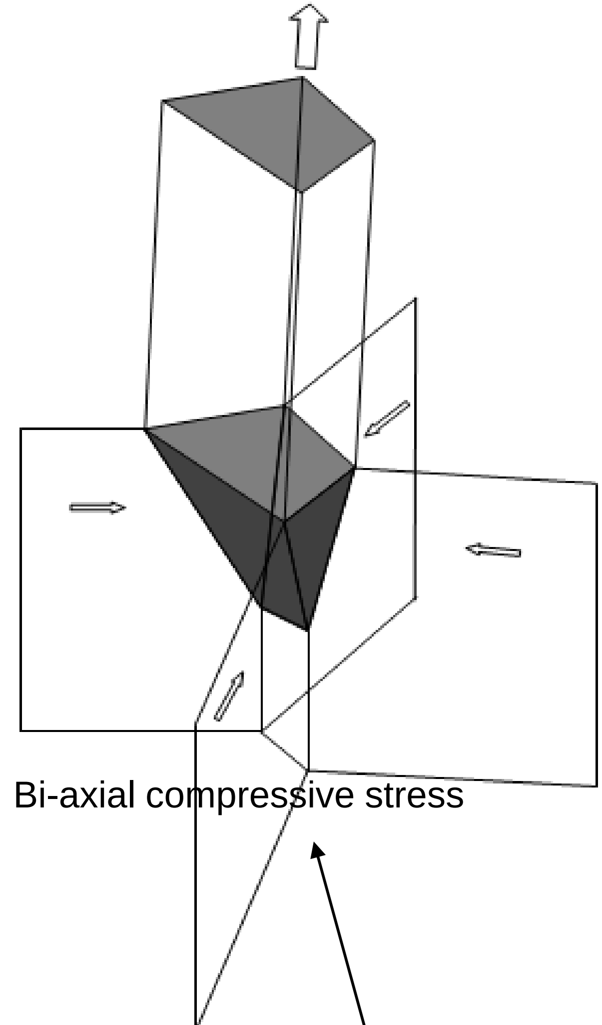


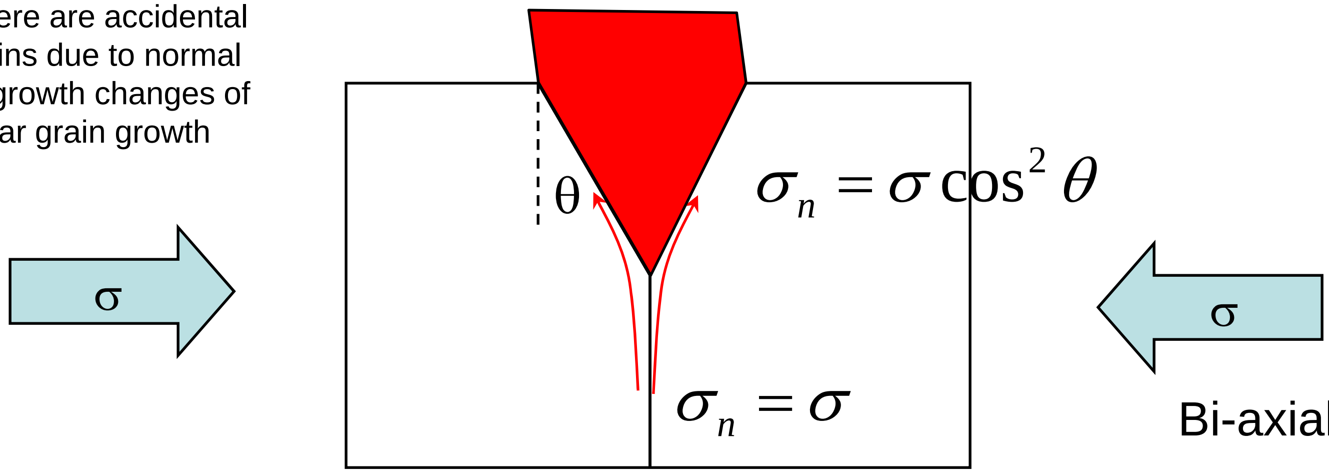


Can we model?

Note how triple junctions in the deposit surface leaves an edge on the whisker. This is evidence that the whisker grain penetrates into the deposit and was probably there at the beginning.

Diffusional Creep: Whisker/Hillock Growth Mechanism in Response to Bi-axial Compression

Presume there are accidental surface grains due to normal completive growth changes of a columnar grain growth



GB Chemical Potential depends on orientation of gb

$$\mu_{Sn-v}\big|_{gb} = -V_M \sigma_n(\theta)$$

Herring!

Flux of Sn (opposite of vacancy flux) is

$$J_{Sn} \approx \frac{D_{gb}\sigma}{RT}\left[1-\cos^2\theta\right]$$

- Atoms flow from GB's with small θ to GB's with large θ
- Accretion will occur on GB's with large θ
- Accretion will occur on the side of the GB that will not increase stress
- Grain grows at the bottom…pushes up grain above surface
- Whisker can grow at an angle to top surface if accretion on sides is unequal
- Flux along free surface need to be small for this mechanism to work!

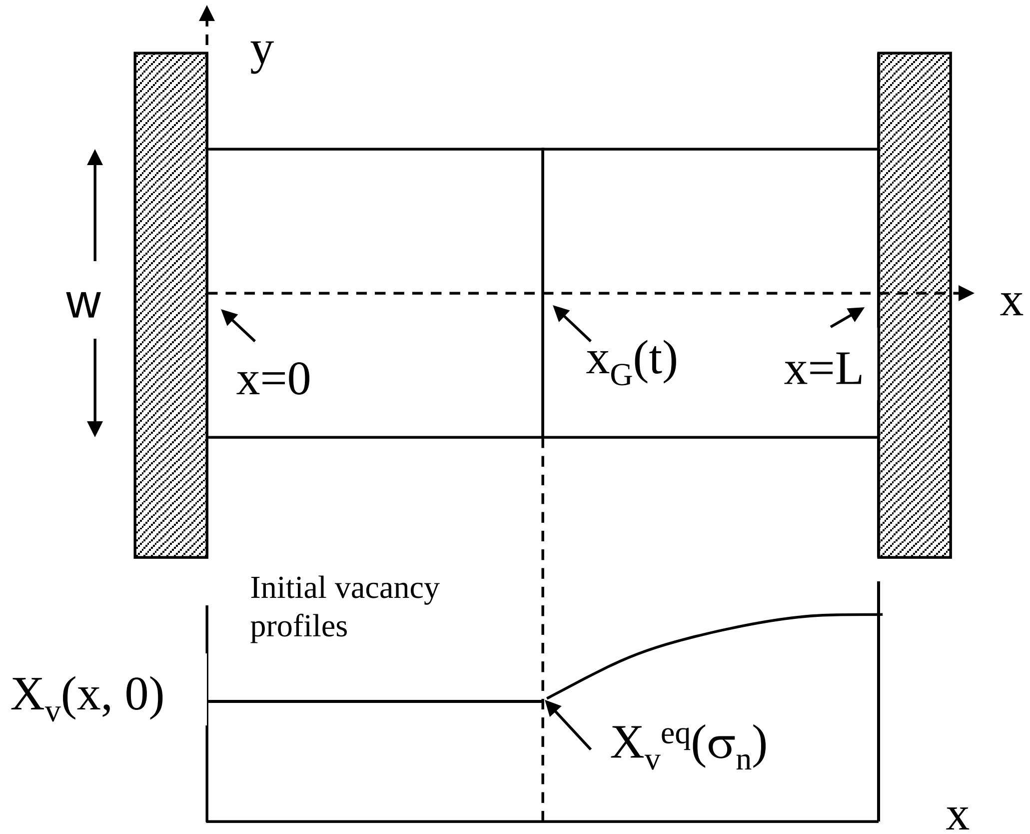
NIST

Creep of constrained bi-crystal

W. J Boettinger, G.B. McFadden

w/ J.E. Guyer,
J. A. Warren,
& R. F Sekerka

Problem



Compute how the grain boundary moves and what is the stress

Assume w is large

Model

In the grains (no source or sink of vacancies)

$$\frac{1}{V_m^{cell}}\left(\frac{\partial X_v}{\partial t}+\mathrm{v}_k\cdot X_{v,k}\right)=\left[\frac{D}{V_m^{cell}}X_{v,k}\right]_{,k}$$

$$\sigma_{ij,j}=0$$

$$\frac{1}{2}\left(\mathrm{v}_{i,j}+\mathrm{v}_{j,i}\right)=\frac{1+\nu}{E}\frac{\partial\sigma_{ij}}{\partial t}-\frac{\nu}{E}\delta_{ij}\frac{\partial\sigma_{kk}}{\partial t}$$

On the ends (no sinks, no x displacement)

$$X_{v,x}\left(0,t\right)=X_{v,x}\left(L,t\right)=0$$

$$\mathrm{v}_x\left(0,t\right)=\mathrm{v}_x\left(L,t\right)=0$$

tractions only in x-direction

On the grain boundary (from Herring or Larche-Cahn etc.)

$$X_v\big|_{left}=X_v\big|_{right}=X_v^{eq}\left[1+\frac{\sigma_{ij}n_in_jV_m^{cell}}{RT}\right]$$

Conservation of the A component gives

$$\mathrm{v}_x\left(x_G\left(t\right),t\right)\Big|_{left}-\mathrm{v}_x\left(x_G\left(t\right),t\right)\Big|_{right}=-\frac{D}{1-X_v}\left[X_{v,x}\big|_{left}-X_{v,x}\big|_{right}\right]$$

If we want the grain boundary to move only but the accreation/anhilation of vacancies, we demand that no flux of A atoms cross the grain boundary to an observer on the boundary. This gives individual equations on the left and right.

$$\begin{cases} \dot{x}_G(t) - \mathrm{v}_x\left(x_G(t),t\right)\Big|_{right} - \dfrac{D}{1-X_v} X_{v,x}\Big|_{right} = 0 \\ \dot{x}_G(t) - \mathrm{v}_x\left(x_G(t),t\right)\Big|_{left} - \dfrac{D}{1-X_v} X_{v,x}\Big|_{left} = 0 \end{cases}$$

Note that the difference of the bracketed equations gives the conservation equation above. In order to include other mechanisms for grain boundary motion, one changes the zeros on the RHS of each. For example for motion by mean curvature

$$\begin{cases} \dot{x}_G(t) - \mathrm{v}_x\left(x_G(t),t\right)\Big|_{right} - \dfrac{D}{1-X_v} X_{v,x}\Big|_{right} = -M\gamma_{gb}K_{gb} \\ \dot{x}_G(t) - \mathrm{v}_x\left(x_G(t),t\right)\Big|_{left} - \dfrac{D}{1-X_v} X_{v,x}\Big|_{left} = -M\gamma_{gb}K_{gb} \end{cases}$$

For the present problem we have K_{gb}=0

Solution

Seek 1-D solution (mostly),

Find

$$X_v\left(x,t\right)$$

$$\mathrm{v}_x\left(x,t\right)$$

$$\mathrm{v}_y\left(y,t\right)$$

$$\sigma_{xx}\left(t\right)$$

$$x_G\left(t\right)$$

$$V_m^{cell}\left(x,t\right)$$

With Initial Conditions

$$X_v\left(x,0\right)=specified$$

$$\mathrm{v}_{\mathrm{x}}\left(x,0\right)=0$$

$$\mathrm{v}_{\mathrm{y}}\left(y,0\right)=0$$

$$\sigma_{ij}\left(x,0\right)=0$$

$$V_m^{cell}\left(0\right)=V_m^0$$

$$x_G\left(0\right)=\frac{L}{2}$$

After some work we obtain

$$\mathrm{v}_x\left(x,t\right)=\begin{cases}\dfrac{1}{E}\dot{\sigma}_{xx}\left(t\right)x & 0\le x<x_G\left(t\right)\\ \dfrac{1}{E}\dot{\sigma}_{xx}\left(t\right)\left(x-L\right) & x_G\left(t\right)<x\le L\end{cases}$$

$$\mathrm{v}_y\left(y,t\right)=-\frac{\nu}{E}y\dot{\sigma}_{xx}\left(t\right)$$

$$\ln\left[\frac{V_m^{cell}}{V_{m0}^{cell}}\right]=\frac{1-2\nu}{E}\sigma_{xx}\left(t\right)$$

$$\begin{cases}\dfrac{\partial X_v}{\partial t}+\dfrac{1}{E}x\dot{\sigma}_{xx}X_{v,x}=DX_{v,xx} & 0\le x<x_G\left(t\right)\\ \dfrac{\partial X_v}{\partial t}-\dfrac{1}{E}\left(L-x\right)\dot{\sigma}_{xx}X_{v,x}=DX_{v,xx} & x_G\left(t\right)\le x<L\end{cases}$$

$$\begin{cases}\dfrac{-D}{1-X_v}X_{v,x}\Big|_{left}+\left[\dot{x}_G-\dfrac{1}{E}x_G\dot{\sigma}_{xx}\right]=0\\ \dfrac{-D}{1-X_v}X_{v,x}\Big|_{right}+\left[\dot{x}_G-\dfrac{1}{E}\left(x_G-L\right)\dot{\sigma}_{xx}\right]=0\end{cases}$$

$$X_v\left(x_G\left(t\right),t\right)=X_v^e\left(1+\frac{\sigma_{xx}\left(t\right)V_{m0}^{cell}}{RT}\right)$$

$$X_{v,x}\left(0,t\right)=X_{v,x}\left(L,t\right)=0$$

Numerical solution

Try approximate solution that satisfies BC and integrals of diffusion equations

$$\begin{cases} X_v(x,t) = a(t) + b(t)x^2 & 0 \le x < x_G(t) \\ X_v(x,t) = c(t) + d(t)(L-x)^2 & x_G(t) \le x < L \end{cases}$$

Normalizing x by L, t by $L^2/D, \sigma$ by E, X_v by X_v^e

Converts PDE's to ODE's

$$\begin{cases} \dot{a} + \dot{b}x_G^2 + 2bx_G\dot{x}_G - \dot{c} - \dot{d}(1-x_G)^2 + 2d(1-x_G)\dot{x}_G = 0 \\ \dot{a} + \dot{b}x_G^2 + 2bx_G\dot{x}_G - \dfrac{V_{m0}^{cell}E}{RT}\dot{\sigma}_{xx} = 0 \\ \dot{\sigma}_{xx} + 2X_v^e b x_G + 2X_v^e d(1-x_G) = 0 \\ \dot{x}_G - \dot{\sigma}_{xx}x_G - 2X_v^e b x_G = 0 \\ \dfrac{1}{3}\left[\dot{d} + 2\dot{\sigma}_{xx}d\right](1-x_G)^2 + \dot{c} - 2d = 0 \\ \dfrac{1}{3}\left[\dot{b} + 2\dot{\sigma}_{xx}b\right]x_G^2 + \dot{a} - 2b = 0 \end{cases}$$

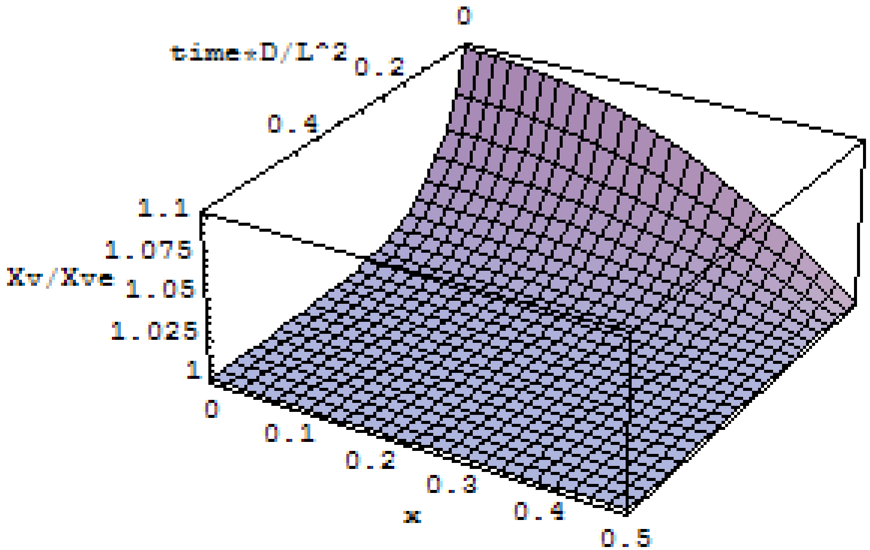
With initial data

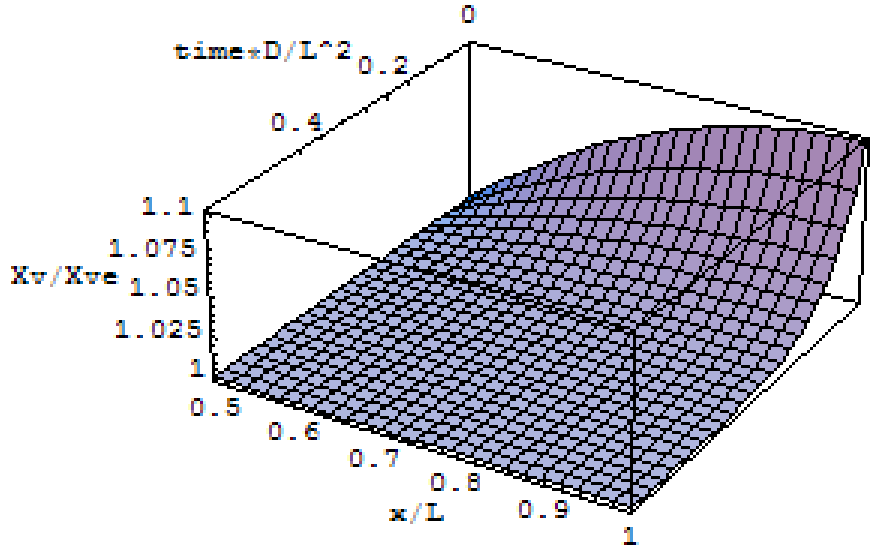
$$\begin{cases} a(0) = 1 + \alpha \\ b(0) = -4\alpha \\ c(0) = 1 + \beta \\ d(0) = -4\beta \\ \sigma(0) = 0 \\ x_G(0) = 1/2 \end{cases}$$

α and β control the initial profile shapes

Solution of ODE's by Mathematica

Case 1; Symmetric case, no grain boundary motion: $\alpha = 0.1$ $\beta = 0.1$ $\dfrac{V_{m0}^{cell} E}{RT} = 0.1$ $X_v^e = 0.01$





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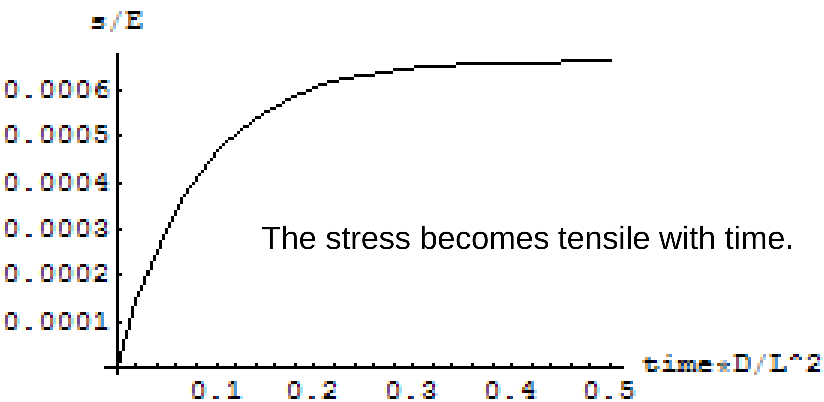
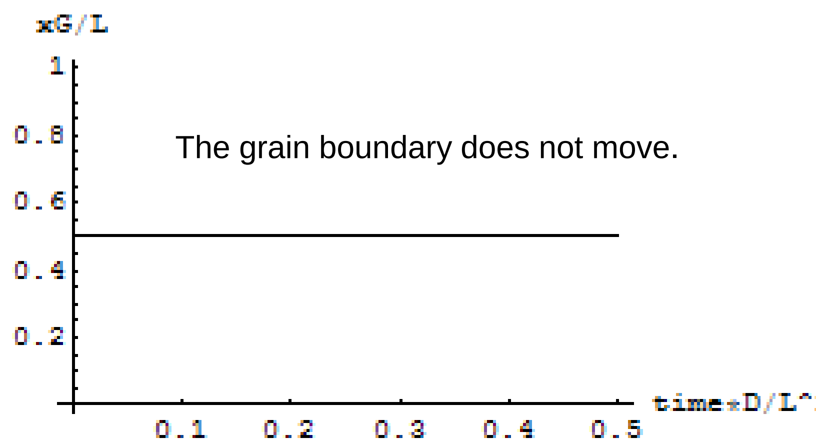
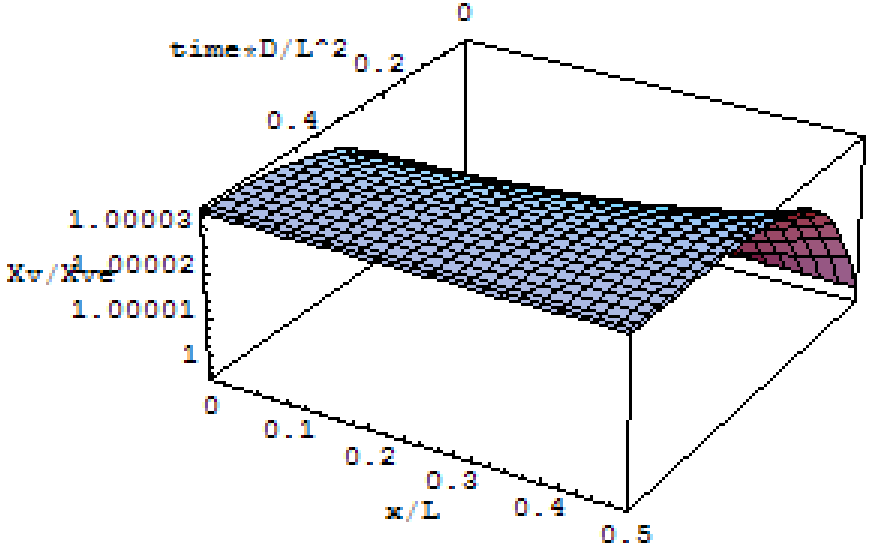




Case 2; Asymmetric case, profile on left is flat:

$$\alpha = 0.1 \qquad \beta = 0.1$$

$$\frac{V_{m0}^{cell} E}{RT} = 0.1 \qquad X_v^e = 0.01$$



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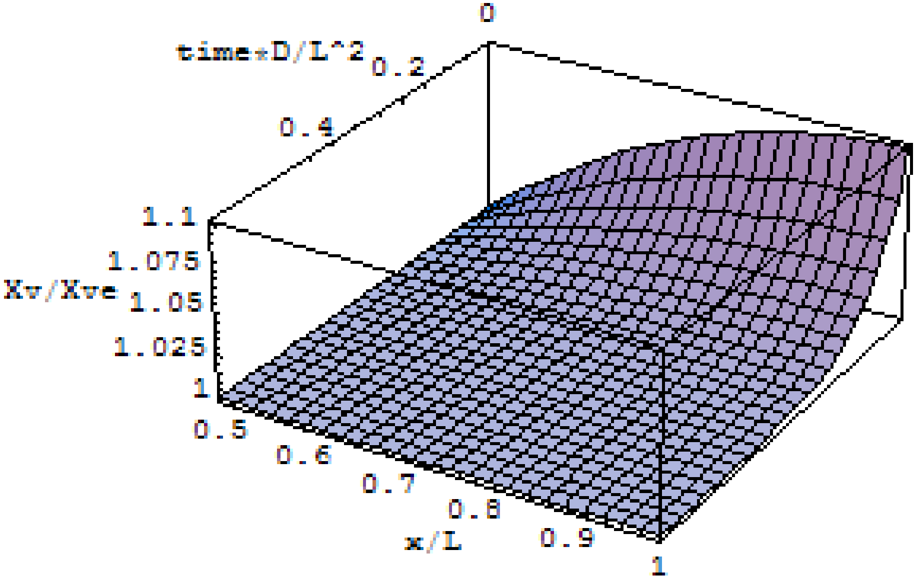
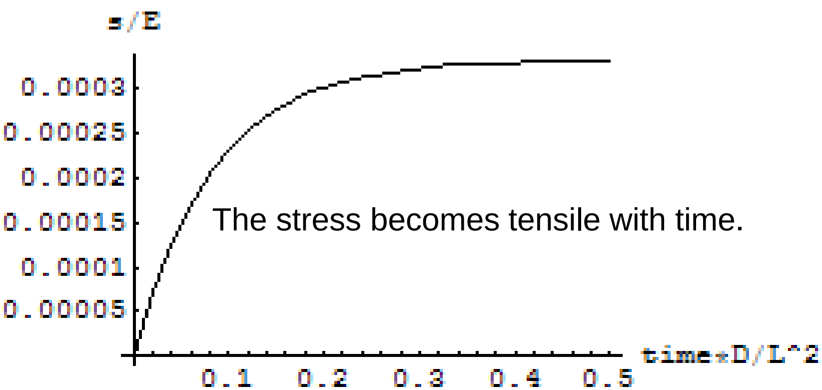
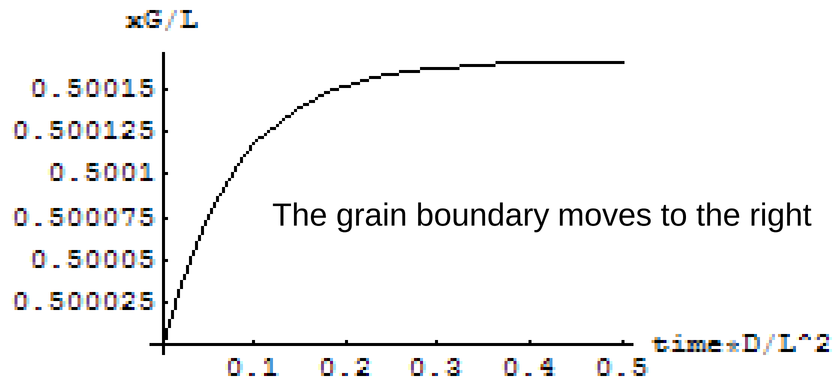




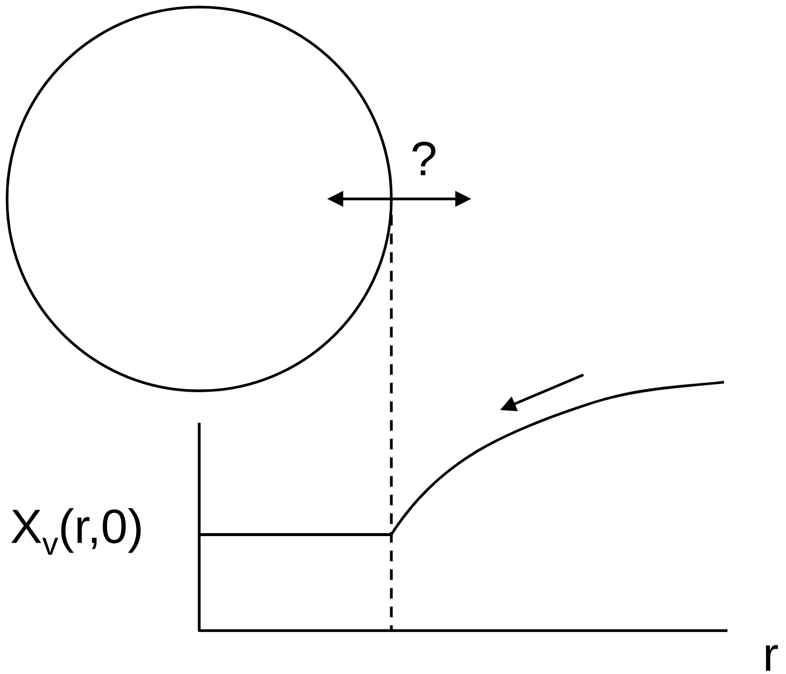
The stress becomes tensile with time.



The grain boundary moves to the right

Future Work

1. Spherical grain in a single crystal matrix



Can the flow of vacancies to the grain boundary overwhelm the usual interface energy motivated grain shrinkage?

2. Create a phase field model of this to treat more complex geometry …….
whisker!