

# Phase field evolution equation

## 1 Governing equation

The evolution equation for the phase field parameter  $d$  is given by Eqn.(41) in [1] as

$$\frac{g_c}{l} [d - l^2 \Delta d] = -g'(d) \Psi_0, \quad (1)$$

where  $g(d)$  is the strain energy degradation function,  $g_c$  and  $l$  are constants, and  $\Delta$  denotes the Laplacian operator. We rearrange Eqn.(1) and get

$$\Delta d - \frac{d}{l^2} = \frac{g'(d) \Psi_0}{g_c l}. \quad (2)$$

The “reference” strain energy density,  $\Psi_0$ , is defined in Eqn.(19) from [1] as

$$\Psi_0 = \frac{1}{2} \boldsymbol{\varepsilon} : \mathcal{C} : \boldsymbol{\varepsilon}, \quad (3)$$

where  $\boldsymbol{\varepsilon}$  is the total infinitesimal strain tensor and  $\mathcal{C}$  is the elastic stiffness tensor. Per Eqn.(23) in [1], the Cauchy stress  $\boldsymbol{\sigma} = g(d) \mathcal{C} : \boldsymbol{\varepsilon}$  but by definition  $\boldsymbol{\sigma} = \mathcal{C} : \boldsymbol{\varepsilon}_e$ , where  $\boldsymbol{\varepsilon}_e$  is the elastic strain. Therefore,

$$\boldsymbol{\varepsilon}_e = g(d) \boldsymbol{\varepsilon}.$$

Replacing  $\boldsymbol{\varepsilon}$  with  $\boldsymbol{\varepsilon}_e$  in Eqn.(3) we get

$$\Psi_0 = \frac{1}{2} \frac{1}{g(d)^2} \boldsymbol{\varepsilon}_e : \mathcal{C} : \boldsymbol{\varepsilon}_e. \quad (4)$$

Note that the strain energy density  $\Psi = g(d) \Psi_0$  is *not* the typical definition of the strain energy density and has an additional multiplicative factor of  $1/g(d)$  in Miehe’s formulation. If we define an elastic compliance tensor as  $\mathcal{S} = \mathcal{C}^{-1}$ , then  $\boldsymbol{\varepsilon}_e = \mathcal{S} : \boldsymbol{\sigma}$  and

$$\Psi_0 = \frac{1}{2} \frac{1}{g(d)^2} \boldsymbol{\sigma} : \mathcal{S} : \boldsymbol{\sigma}. \quad (5)$$

Substituting this into Eqn.(2), we get

$$\Delta d - \frac{d}{l^2} = \frac{1}{2g_c l} \frac{g'(d)}{g(d)^2} \boldsymbol{\sigma} : \mathcal{S} : \boldsymbol{\sigma} \quad (6)$$

## 2 Broadening phenomenon?

### 2.1 Displacement controlled

Consider a semi-infinite long strip in  $x$  direction that is subjected to an homogeneously applied total strain  $\boldsymbol{\varepsilon}_0$  in  $y$  direction, as shown in Fig. 1. Then the governing equation

$$\Delta d - \frac{d}{l^2} = \frac{g'(d)}{2g_c l} \boldsymbol{\varepsilon} : \mathcal{C} : \boldsymbol{\varepsilon}. \quad (7)$$

with  $g(d) = (1-d)^2$  becomes

$$d'' - \frac{d}{l^2} = -\frac{E \boldsymbol{\varepsilon}_0^2}{g_c l} (1-d) \quad (8)$$

From Eq. 8 we have

$$d'' - d/l^2 = \frac{-E\epsilon_0^2}{2cl} (c-d)$$

$$\tilde{d}(\xi) = d(\xi a), \quad \xi = \gamma/a; \quad \frac{d(\cdot)}{dx} = \frac{1}{a} \frac{d(\cdot)}{d\xi}; \quad \frac{d^2(\cdot)}{dx^2} = \frac{1}{a^2} \frac{d^2(\cdot)}{d\xi^2}$$

In terms of the new non-dimensional var:

$$\text{eq. 8} \Rightarrow \tilde{d}''(\xi) - \frac{\tilde{d}(\xi)}{(\gamma/a)^2} = \frac{-E\epsilon_0^2 a^2}{2cl} (1 - \tilde{d}(\xi))$$

$$\text{Let's set } \tilde{\lambda} = \gamma/a; \quad \tilde{\beta} = \frac{-E\epsilon_0^2 a^2}{2cl};$$

$$\tilde{d}'' - \left(\frac{1}{\tilde{\lambda}^2} + \tilde{\beta}\right)\tilde{d} + \tilde{\beta} = 0$$

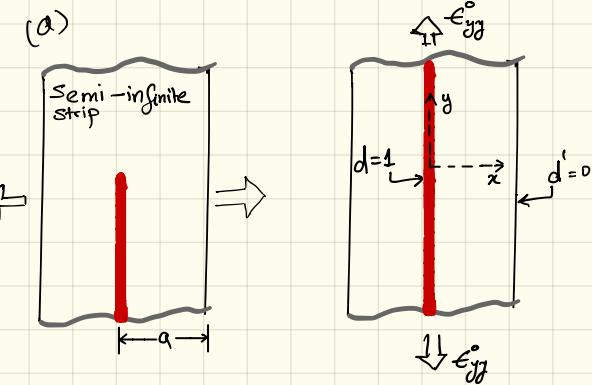
$$\tilde{d}'' - 2\tilde{\lambda}\tilde{d} + \tilde{\beta} = 0 \quad \dots \quad (8)$$

where,  $\tilde{\alpha} \hat{=} \frac{1}{\tilde{\lambda}^2} + \tilde{\beta}$ . The solution of eq. 8 is

$$\tilde{d}(\xi) = \frac{\beta}{\alpha} + C_1 e^{-\sqrt{\alpha}\xi} + C_2 e^{+\sqrt{\alpha}\xi}$$

Using the boundary conditions we get

$$C_1 = \frac{C_2 \alpha (\alpha - \beta)}{(1 + e^{\sqrt{\alpha}\xi})\alpha} \quad C_2 = \frac{(\alpha - \beta)}{(1 + e^{\sqrt{\alpha}\xi})\alpha}$$



$$\tilde{\beta} = \frac{-E\epsilon_0^2 a^2}{2cl};$$

So  $\beta$  can be increased by increasing  $\epsilon_0$ , i.e. by pulling harder, making the solid more stiff or by decreasing the cohesive strength of the solid. Now as you will note  $\alpha$  and  $\beta$  are coupled as you increase  $\beta$ , you also increase  $\alpha$ . I the correct way to think about this that the system will converge to the brittle crack solution as  $\tilde{\lambda} \rightarrow 0$ . However the problem might be that how small should  $\tilde{\lambda}$  be? Let's take a look the sol. once again.

Say  $\beta=0$ , then the equation is  $\tilde{d}''(\xi) - 2\tilde{\lambda}\tilde{d}=0$ , whose solution is  $\tilde{d}(\xi) = e^{-\sqrt{\alpha}\xi} = e^{-\sqrt{\lambda}\xi}$ . So when  $\tilde{\lambda}$  is small then the mi

the thickness of the crack is need much smaller than the dimensions of the solid. That is  $\tilde{\ell} \ll 1 \Rightarrow \frac{\ell}{a} \ll 1$ , i.e.,  $\ell \ll a$ . This matches the classical understanding make  $\ell$  much smaller than (dimensions of the solid to have the thickness of the crack much smaller than the dimensions of the solid however, if you recall this result was derived only for the special case,  $\tilde{\beta}=0$ . So, what happens when  $\tilde{\beta} \neq 0$ ?

Let's take a more careful look at  $\tilde{\beta} = \frac{Ea^2\tilde{\epsilon}_0^2}{\tilde{\ell}l}$  ← this quantity has units of length, so let,  $l_c = \frac{Ea^2\tilde{\epsilon}_0^2}{\tilde{\beta}c}$  be much small length.

Now  $\tilde{\ell}$  is always small since the analyst is always going to be running the case  $\ell \ll a$ . Now since  $\tilde{\beta} \ll 1$ , we have  $\tilde{\alpha} \gg 1$  anyways (on account of  $\tilde{\ell}$ ). Let's see now what this has on the solution. Let's begin by looking at  $C_1$  and  $C_2$ .

Put  $\tilde{\beta} \rightarrow 0$ , and  $\tilde{\alpha} \rightarrow \infty$  in the following expression. we get

$$C_1 = \frac{e^{2x}(\alpha-\beta)}{(1+e^{2x})\alpha} \underset{x \rightarrow \infty}{\sim} 1 - \frac{\beta}{\alpha}$$

We need  $\tilde{\beta}/\alpha \rightarrow 0$ , so  $\tilde{\alpha}/\beta \rightarrow \infty$

So  $\tilde{\ell}^2\tilde{\beta} \rightarrow 0 \Rightarrow$  Since,

$$\begin{aligned} C_1 &= \frac{\tilde{\ell}^2 c}{\alpha^2(1+e^{2x})} \cdot \frac{\tilde{\alpha}}{\tilde{\beta}} = \frac{1}{e^{2x}} + 1. \text{ Now } \tilde{\ell} \rightarrow 0 \text{ and } \tilde{\beta} \rightarrow 0. \frac{\tilde{\ell}^2}{\alpha^2} \times \frac{Ea^2\tilde{\epsilon}_0^2}{\tilde{\beta}l} = \frac{Ea^2\tilde{\epsilon}_0^2}{\alpha^2} = \frac{El\tilde{\epsilon}_0^2}{\alpha^2} \\ &\quad \cancel{\tilde{\ell}^2\tilde{\beta} \rightarrow 0} \\ C_1 &= \frac{1}{1+e^{2x}} \rightarrow 1 \text{ as } x \rightarrow \infty \end{aligned}$$

$$C_2 = \frac{l(\alpha-\beta)}{(1+e^{2x})\alpha} \underset{x \rightarrow \infty}{\sim} \frac{e^{2x}-\beta}{e^{2x}} = 1 - \frac{\beta}{e^{2x}}$$

$$\begin{aligned} &\frac{Ea^2\tilde{\epsilon}_0^2}{\tilde{\beta}l} = \frac{El\tilde{\epsilon}_0^2}{\alpha^2} = \frac{El\tilde{\epsilon}_0^2}{\alpha^2} \\ &\quad \cancel{\tilde{\ell}\tilde{\beta} \rightarrow 0} \\ &= \frac{l\tilde{\epsilon}_0^2}{\alpha^2 E} \rightarrow 0 \end{aligned}$$

case (i)  $\beta/\alpha = 0$ , or  $\beta/\alpha \rightarrow 0$  we get the correct solution,  $C_1 = \text{some number}$ , doesn't really matter, the case (ii)  $\beta/\alpha$  remains bounded  $\frac{l\tilde{\epsilon}_0^2}{\alpha^2 E} \sim 1$   $C_2 \rightarrow 0$  term decays fast over a distance the solution quickly converges to  $\frac{l\tilde{\epsilon}_0^2}{\alpha^2}$

$$= \frac{l \sigma_0^2}{g_c E} \longrightarrow 0$$

Example theoretical strength calculation.

$$\sigma_{th} = 0.7 \left( \frac{10^{9} \text{ N/m}^2}{10^{-9} \text{ m}} \right)^{1/2} = 0.7 \times 10^9 \text{ N/m}^2 = \underline{\underline{0.7 \text{ GPa}}}$$

which implies that

$$l \ll \left( \frac{g_c E}{\sigma_0^2} \right)$$

$$\ll \left( \frac{E g_c^2}{\sigma_0} \right); \quad E = 20 \times 10^9 \text{ N/m}^2 \sim 10 \text{ GPa} \quad \text{The strain calculation.}$$

$G_c = 0.1$  (GPa).  $\sim 1 \text{ J/m}^2$  (is a bit confusing)  
 $\sim 1 \text{ J/m}^2$  (Silicon).  
(Copper)

$$E g_c = 10 \times 10^9 \text{ N/m}^3 = \frac{10^9 \text{ N/m}^2}{(10^{-12} - 10^{-18} \text{ N/m}^4)} = 10^{-3} - 10^{-9} \text{ m}$$

An alternate way to calculate this is to set  $\sigma_{th} = c \left( \frac{E g_c}{x_0} \right)^{1/2}$ , where  $x_0$  is the length scale of the fracture mechanism.

$$\frac{E g_c}{c^2 \left( \frac{E g_c}{x_0} \right)} = 4$$

$$l_0 \ll 4x_0$$

$$\tilde{\beta} = \frac{Ea\epsilon_0^2}{\tilde{g}_c \tilde{l}} = \frac{1}{\tilde{l} c \tilde{l}} ; \quad \frac{v}{\tilde{\beta}} = \frac{1}{\tilde{l}^2} \times 1$$

$$= \frac{1}{\tilde{l}^2} \times \tilde{l} c \tilde{l} + 1 = \frac{1}{\tilde{l}^2} \tilde{\beta} + 1$$

$$\frac{\tilde{a}}{\tilde{\beta}} = \left( \frac{\tilde{l}_c}{\tilde{l}} \right) + 1 \rightarrow \infty$$

when  $\frac{\tilde{l}_c}{\tilde{l}} \rightarrow \infty$ , i.e.,

$\tilde{l}_c$  is much larger than

$\tilde{l}$ . That is  $\tilde{l}$  is much smaller than  $\tilde{l}_c$

$$\tilde{l} \ll \tilde{l}_c$$

$$\begin{aligned} l_c &= \frac{Ea\epsilon_0^2}{\tilde{g}_c} \\ \tilde{l}_c &= \frac{Ea^2\epsilon_0^2}{\tilde{g}_c a} = \frac{EA\epsilon_0^2}{\tilde{g}_c} \\ &= \frac{\sigma_0^2 a}{\tilde{g}_c E} \end{aligned}$$

$$\frac{l}{a} \ll \frac{\sigma_0^2 a}{\tilde{g}_c E}$$

$$l \ll \frac{\sigma_0^2 a^2}{\tilde{g}_c E}$$

Prepare a to do for  
Kaushik. This should be  
about the plasticity sec:

Rough Calculation

$$\frac{Ea\epsilon_0^2}{\tilde{g}_c} \times a^2 \times \frac{m^2 L}{m^2 \times 8 \pi^2 / 3} \times \frac{m^2 L}{m^2 \times 8 \pi^2 / 3}$$



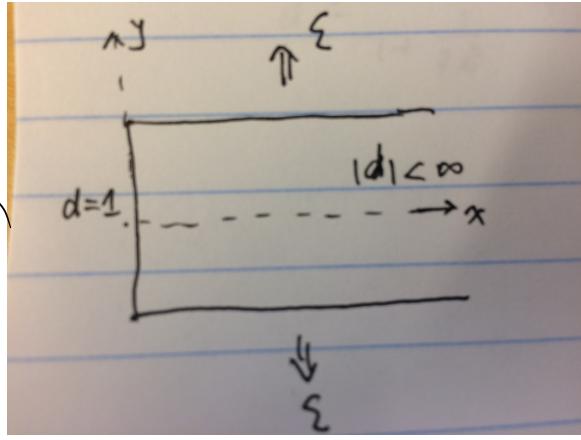


Figure 1: A semi-infinite long strip subjected to an applied total strain.

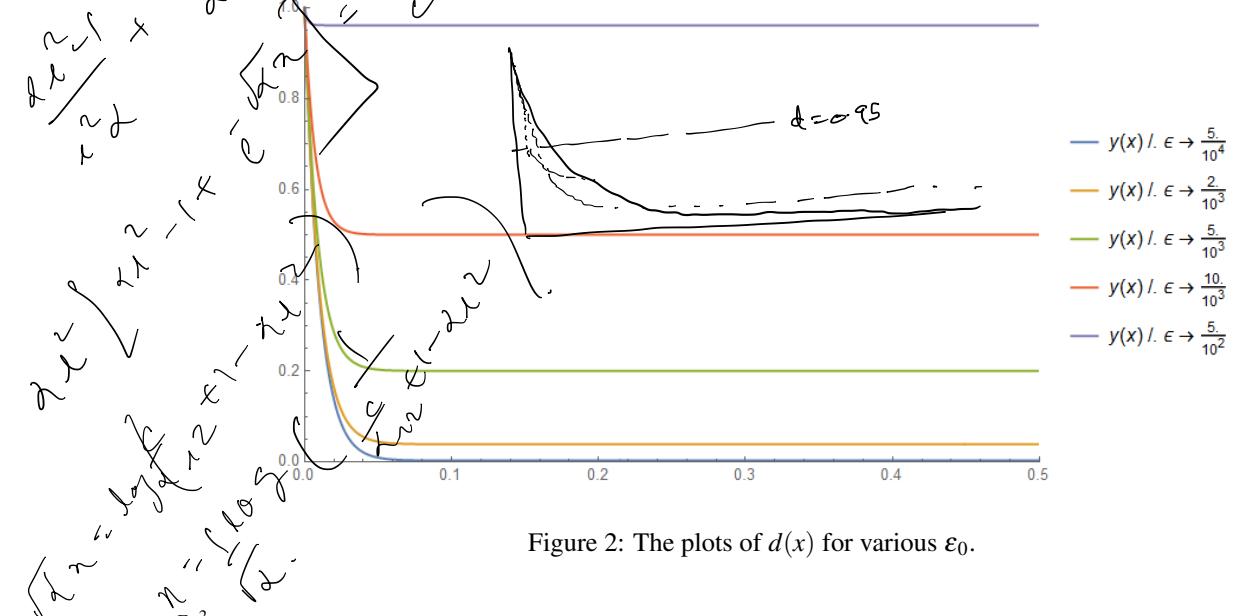


Figure 2: The plots of  $d(x)$  for various  $\epsilon_0$ .

Let  $\beta = \frac{E\epsilon_0^2}{g_c l}$ ,  $\alpha = \beta + \frac{1}{l^2}$ . The general solution of

$$d'' - \alpha d + \beta = 0 \quad (9)$$

is

$$d(x) = \frac{\beta}{\alpha} + C_1 e^{-\sqrt{\alpha}x} + C_2 e^{\sqrt{\alpha}x} \quad (10)$$

According to the boundary conditions

$$d(0) = 1 \quad \text{and} \quad |d(x)| < \infty \quad \text{for } x \in [0, \infty], \quad (11)$$

we determine the constants to be  $C_1 = \frac{1}{1+\beta l^2}$  and  $C_2 = 0$ . Thus

$$d(x) = \frac{\beta}{\alpha} + \frac{1}{1+\beta l^2} e^{-\sqrt{\alpha}x}. \quad (12)$$

As an example, let  $E = 5.0 \times 10^{-5}$ ,  $g_c = 0.5$ ,  $l = 1.0 \times 10^{-2}$ . The plots of  $d(x)$  at different strain levels are shown in Fig. 2. We still need to check the equilibrium of stress to be satisfied. We note that

$$\sigma = g(d)\mathcal{C} : \epsilon \quad (13)$$

with components  $\sigma_{xx} = 0$ ,  $\sigma_{xy} = 0$ , and  $\sigma_{yy} = (1 - d(x))^2 E \epsilon_0$ . Then the equilibrium follows by substituting the stress into the equation  $\nabla \cdot \sigma = 0$ .

## 2.2 Load controlled

Instead of applying displacement, we prescribe traction  $\sigma_0$  at the top and bottom boundary. According to equilibrium equation, the only non-zero stress is  $\sigma_{yy} = \sigma_0$ . Then the governing equation of  $d(x)$  is

$$d'' - \frac{d}{l^2} = -\frac{\sigma^2}{g_c l} \frac{g'(d)}{g(d)^2} = -\frac{\sigma^2}{g_c l E} \frac{1}{(1-d)^3}, \quad (14)$$

or written as

$$d'' - \alpha d + \beta (1-d)^{-3} = 0 \quad (15)$$

with  $\alpha = \frac{1}{l^2}$  and  $\beta = \frac{\sigma^2}{g_c l E}$ . The boundary conditions are Eq. 11.

## References

- [1] Christian Miehe, Martina Hofacker, and Fabian Welschinger. A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits. *Computer Methods in Applied Mechanics and Engineering*, 199(45):2765–2778, 2010.