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NUMERICAL MODELING OF THE INFLUENCE OF CRACKS ON THE FORMATION OF HYDRIDES IN METALLIC MATERIALS

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Summary. The formation of hydrides at a crack tip is studied by using a numerical model based on the Ginzburg-Landau phase field formulation.

1 INTRODUCTION

For metallic structures and components exposed to hydrogen-rich environments there is an impending risk of hydrides forming, which can have a detrimental effect on the performance of the material and it may lead to a premature failure of the structure at hand. This threat is particularly real for fuel cladding materials in nuclear power reactors and components in rocket engines, where not only the exposure to hydrogen is imminent, but also the severe thermo-mechanical loading can reduce the life-time significantly. Moreover, experimental observations have indicated that the presence of high stress concentrators, such as cracks and dislocations, may promote the formation of hydrides. Hence, the aim of this work is to model nucleation and eventual growth of precipitates in the presence of a crack.

2 DESCRIPTION OF THE MODEL

The phase field formulation of Ginzburg-Landau [1,2] is adopted to describe the precipitation of a second phase in a linear elastic crystalline solid in the presence of crack. The non-conservative time-dependent Ginzburg-Landau (TDGL) equation for a single component structural order parameter $\eta(\boldsymbol{\rho}, t)$ is used to study the spatio-temporal evolution of a low-order phase ($\eta \neq 0$) in the vicinity of a crack tip in a high-order matrix material ($\eta = 0$). Neither the influence of concentration gradients, nor thermal fluctuations are included in the present model. The formulation is based on the free energy $\mathcal{F}$ that includes structural energy, elastic strain energy and structure-strain interaction energy [3]:

$$\mathcal{F} = \int \left[g_a \left(\nabla \eta \right)^2 + \frac{r_1}{2}\eta^2 + \frac{u_1}{4}\eta^4 + \frac{v_0}{6}\eta^6 \right] d\boldsymbol{\rho}, \tag{1}$$

where g_a is a constant that accounts for the existence of interface in a inhomogeneous system. The coefficient r_1 is a temperature and load dependent variable, u_1 a constitutive parameter

including elastic constants, and v_0 a constant. The TDGL equation can then be express as

$$\frac{\partial \eta}{\partial t} = g_a \nabla^2 \eta - (r_1 \eta + u_1 \eta^3 + v_0 \eta^5). \tag{2}$$

Phase transitions limits in space is governed by the parameter r_1, which is related to temperature as follows:

$$r_1 = a\left[T - T_c\left(\rho, \theta\right)\right], \tag{3}$$

where a is a material parameter and T_c the space dependent critical temperature for phase transition for the system containing a mode I crack (with its tip at $\rho = 0$, and $\theta = 0$ in the crack plane). Equation (3) is here expressed as

$$r_1 = |r_0| \left(sgn\left(r_0\right) - \sqrt{\frac{\rho_0}{\rho}} \cos\frac{\theta}{2} \right), \tag{4}$$

where $r_0 = r_1$ for a defect free system. A characteristic length ρ_0 accounts for the strength of the crack induced stress singularity and some material properties. For further details of the model, see e.g. Bjerkén and Massih[4].

3 NUMERICAL METHOD

We use the FiPy module[5], based on the finite volume method, together with in-house shell scripts, to simulate the phase transition process in a two dimensional space, $(x, y) = \rho_0(\cos\theta, \sin\theta)$. A linear system of partial differential equations is solved using the preconditioned conjugate gradient method (PCG) with symmetric successive over-relaxation (SSOR) preconditioning by default. We use a square mesh consisting of 200×200 equally-sized square elements with the element size $dx = 0.05\rho_0$, and the time increment $\Delta t \approx \min(t_{ss}) \cdot 10^{-3}$ (t_{ss} is time to reach steady state for the different cases studied). At the outer boundaries $\bar{n} \cdot \nabla\eta = 0$, where $\bar{n}$ is a unit vector perpendicular to a boundary. Initially, random values of η of the order of 10^{-4} of the maximum η value are distributed in the mesh. Regarding convergence, we have shown in a previous, unpublished study that the chosen numerical parameters give solutions that are precise enough to validate the results.

4 RESULTS AND DISCUSSION

To investigate the nucleation and growth of hydrides in the vicinity of a semi-infinite crack, a wide range of combinations of load, temperature and material are explored by varying g_a, r_0, ρ_0, u_1 and v_0. Here, results for two different values of the coefficient u_1 are presented, with r_0 set equal to unity, $g_a = 3 \cdot 10^{-3}$, and $\rho_0 = v_0 = 1$. A positive r_0 represents the situation where no precipitation should occur in a defect-free crystal.

Figure 1a) shows the distribution of η at the crack tip when steady state is reached for the case $u_1 = -1$. The largest values is found in the very vicinity of the tip, further away η decreases relatively slowly until the interface area between phases is reached and η declines rapidly. To more clearly illustrate the spatial distribution, a contour plot is given in Fig. 1b). Precipitation is found to occur in front of the crack as well as along the crack flanks, however to a much smaller extension.

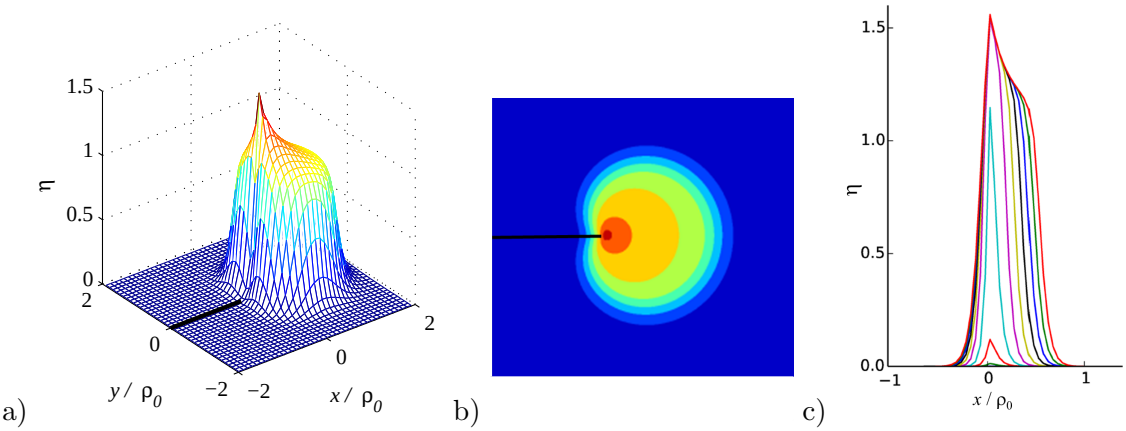

Figure 1: a) Surface plot of η in the crack tip vicinity for the case $r_0 = 1$ and $u_1 = -1$ at a steady state, b) contour plot of the same situation as in a), and c) η-profiles in the crack plane ($y = 0$) for different times during the evolution of a hydride. (The crack is given as a black line and the tip is located at (x,y)=(0,0))

The temporal evolution of a hydride is illustrated by showing η-profiles along the crack plane ($y = 0$) for different times until a steady state is reached. Figure 1c) shows the nucleation and growth of η for the case $u_1 = -1$. It is found that nucleation starts in an limited area near the crack tip where η increases until a peak value is reached, thereafter continuous growth of the hydride takes place. For positive r_0 this evolution pattern is found for all $u_1 < 0$, but with $u_1 > 0$ no broadening will occur. In the case of $r_0 < 0$, the whole material will eventually transform into the second phase. However, the transition is completed first in the same area as for $r_0 > 0$. It can be concluded that the stress singularity will in all cases effectively trigger the formation of a nucleus. In the cases shown here, the formed nuclei are stable, but the stability is strongly influenced by the interface interaction between phases, i.e. larger values of g_a may result in dissolution of the second phase before a steady state is obtained.

To validate the numerical calculations, a comparison with an analytic solution is made. At a

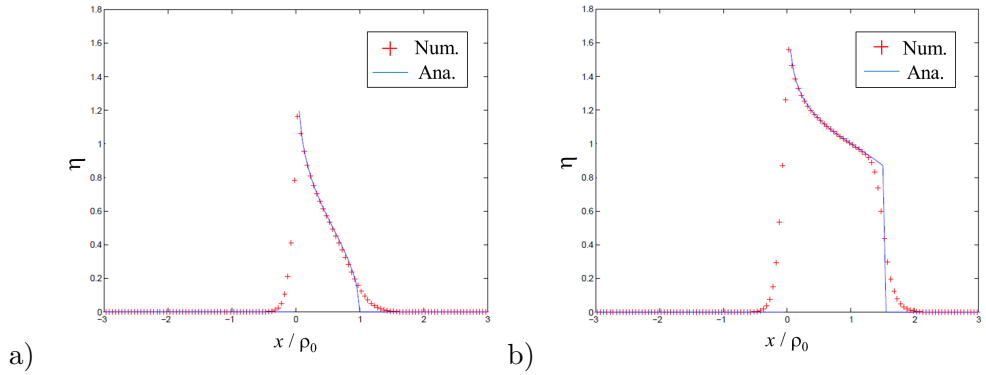

Figure 2: Comparision between numerical results (+) at steady state and an analytical solution of Eq. (2) (-) for a) $u_1 = 1$ and b) $u_1 = -1$, respectively.

steady state $\partial\eta/\partial t = 0$ and by setting $g_a = 0$, an analytical solution to Eq. 2 is found. Figure 2 shows the numerical results when steady state is reached together with this analytical solution for the two cases $u_1 = 1$ and $u_1 = -1$. A good resemblance is found, and the difference may be explained by that the numerical solution includes the influence of interfaces. Instead of having sharp boundaries between hydrides ($\eta \neq 0$) and solid solution ($\eta = 0$) as in the analytical results, smooth transitions are visible in the numerical results due a non-zero g_a. Hence, this proximity may justify our method to study the phenomenon of phase transformations in presence of cracks.

The results shown here are part of a larger project exploring nucleation of hydrides at defects. At this stage of the project, there is a lack of material data connected to hydride formation. In a work on dislocation induced nucleation of a second phase by Bjerkén and Massih [4], data for ferro-magnetism was used to validate the approach used also in the present project. To include anisotropy to explore microstructural features, such as preferable crystal planes for precipitation, will be the next step in this research. The long-term ambition of the project is to aid the development of advanced engineering alloys with improved resistance to hydrogen, to supplant experimental testing and to improve life-time predictions for metallic materials in hydrogen-rich environments.

5 CONCLUSION

The use of a numerical method based on a Ginzburg-Landau formulation to study the nucleation and growth of a second phase is highlighted. The spatio-temporal evolution can be simulated in detail, e.g. giving characteristics of the development of shape of the hydrides in an isotropic material is, and showing that a crack will in all cases induce of a hydride embryo.

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