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Nanovoid dynamics based on temperature dependent Young modulus and void formation energy in Nickel: a phase field study

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ABSTRACT: In the present work, a phase field method is used to study the growth/annihilation of nanovoids under thermal and mechanical loadings. To do so, the coupled system of the Cahn-Hilliard and elasticity equations is solved using the nonlinear finite element method in 2 dimensional. This coupling is due to the presence of elastic energy in the Cahn-Hilliard free energy and the dependence of total strain on the void misfit strain. The novel point in the present physical model is including the temperature dependence of elastic properties and void formation energy. Then, examples of nanovoid structure evolution are presented consisting of planar gas-solid interface formation and evolution, growth/annihilation of circular nanovoids at different temperatures, growth/annihilation of nanovoids under biaxial compression and at different temperatures and nanovoid structure evolution with initially, randomly distributed void pattern. The obtained results show a faster growth with larger amounts of void concentration at lower temperatures. Also, the stress field significantly varies during nanovoids growth/annihilation especially inside the solid-gas interface and its value depends on the nanovoid size and the concentration.

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1. Introduction

Voids appear in materials by natural activities, and aging in working environments. When voids are behave as defects, they are regarded as having a bad result on material properties. In the most highly engineered dense materials, defects such as voids will make trouble for the design of real structures. Nanovoid were discovered in nickel in 1970 [1]. Several models were built based on the rate theory to simulate void evolution [2,3]. While rate theory is an important method for forecast the average behavior of the material, cannot prepare information on the micro/nanostructure property evolution. The computational cost of rate theory high, and therefore is primarily done in 1 Dimensional (1D) for sizes up to 100 nm.

Phase Field Approach (PFA) has been extensively used to simulate evolution of nano/microstructure [4,5]. The essential advantage of the PFA is to obtain the microstructure without need to track interfaces. The PFA, as an intermediate between continuum thermodynamic and the atomistic approaches, resolves issue at the nanoscale and also allows one to consider case and time much larger than in atomistic modeling. It also consist of much more information than traditional thermodynamic approaches since the Phase Field (PF) potential is determined for all intermediate states between phases and at interfaces.

In this paper PFA is used to study the evolution of nanovoids under thermal and mechanical loadings. To do so, the coupled system of the Cahn-Hilliard and elasticity equations is solved using the nonlinear finite element method in 2D. This coupling is due to the presence of elastic energy in the Cahn-Hilliard free energy and the dependence of total strain on the void misfit strain. The novel point in the present physical model including the temperature dependence of elastic properties and void formation energy, the obtained results show a faster growth with larger amounts of void concentration at lower temperatures. Also, the stress field significantly varies during nanovoids evolution especially inside the solid-gas interface and its value depends on the nanovoid size and the concentration.

2. Coupled Mechanic and Phase Field Equation

The total free energy of the system is:

$$\psi(c,\nabla c,T,\boldsymbol{\varepsilon}) = \int_V [\psi^e + \tilde{\psi} + \hat{\psi} + \psi^{\nabla}]dV \qquad (1)$$

ψ^e is the elastic energy and $\tilde{\psi}$ is the chemical free energy employed to describe the equilibrium between the matrix and nanovoids, $\hat{\psi}$ is the free energy of mixing and ψ^{∇} shows the solid-gas gradient energy as [6,7]:

$$\begin{aligned} \tilde{\psi} &= g_v c + g_a(1-c) \\ \hat{\psi} &= E_v^f c(1-c) + k_B T\left[c\ln c + (1-c)\ln(1-c)\right] \\ \psi^{\nabla} &= \kappa(\nabla c)^2 \end{aligned} \qquad (2)$$

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where κ is the constant of gradient energy for the void matrix interface, *gv* is the chemical energy of vacancy and ga the chemical energy of matrix atom per unit volume. *kB* is the Boltzmann's constant, *T* is the absolute temperature and E_v^f is vacancy formation energy.
The Cahn-Hilliard equation can be written as:

$$\frac{\partial c}{\partial t}=\nabla.\left[M\nabla(\frac{\partial(\psi^e+\tilde{\psi}+\hat{\psi})}{\partial c}-2\kappa\nabla^2 c)\right] \quad (3)$$

The elastic energy can be expressed as

$$\psi^e=\frac{1}{2}\boldsymbol{\sigma}_e(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^0) \quad (4)$$

$$\boldsymbol{\varepsilon}=\frac{1}{2}\left[\nabla\boldsymbol{u}+(\nabla\boldsymbol{u})^T\right] \quad (5)$$

where $\boldsymbol{\varepsilon}$ is total strain, *u* is the displacement vector and $\boldsymbol{\varepsilon}^0$ describes the misfit strain between nanovoid surface and matrix with form of $\varepsilon_{ij}^0=2\varepsilon_0\delta_{ij}(1-c)c$. A positive $\boldsymbol{\varepsilon}_0$ describes pressure operating on a bubble surface and a negative describes a force toward the center of a nanovoid. Thus, the elastic stress from Eq. (4) can be written as:

$$\boldsymbol{\sigma}_e=\boldsymbol{C}^0(1-c)(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^0) \quad (6)$$

where $\boldsymbol{C}^0$ is the elastic tensor of solid.

3. Result

The finite element method and the COMSOL code are used to solve the coupled mechanics and Cahn-Hilliard equations. An adoptive remeshing is used to prevent mesh divergence. The mesh size is chosen fine enough and equal to 0.1 so that the solution is mesh-independent. The following material property have been used (Table 1) for nanovoid dynamics modeling in Nickel [8];

Table 1. Nano nickel property

$E(T)$	E_v^f	κ	M
$-0.004T+8.4$	$-6.6\times10^{-8}T^2-3.3\times10^{-5}T+14$	0.25	0.3

In order to validate, concentration profile of present work in stationary situation compared with the analytical solution [9] in Fig. 1 which show good agreement.

A square sample with the size of 10×10 nm^2 and periodic boundary conditions is considered. For the initial conditions, a circular void with the radius of 1 nm and the value of $c=0.4$ is located at the center of the square and the rest of the sample is $c=0.15$. The misfit strain for the void is $\varepsilon_0=-0.1\%$. The evolution of void in three different temperature are represented in Fig. 2. Fig. 2 represent amount effect of temperature and

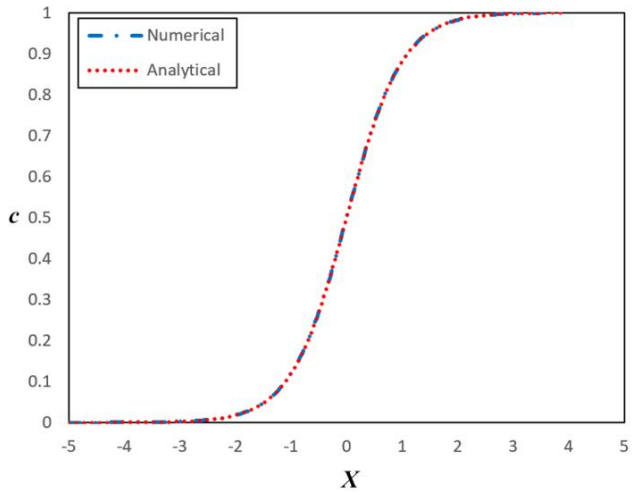

Fig. 1. Comparison of concentration of void between Numerical and analytical solution.

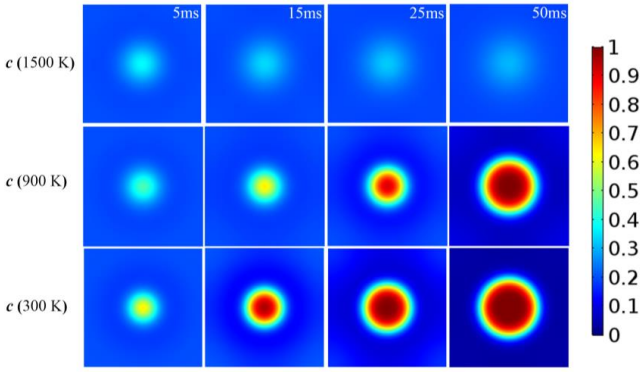

Fig. 2. Effect of temperature on void evolution.

consequently change in elastic modulus and energy barrier in growth/annihilation of void in different time. As can be seen, void shrinkage in 1500 K but grow at 900 K and 300 K with different velocity.

4. Conclusions

In the present work, a phase field method is used to research the evolution of void under thermal and mechanical loadings. For this goal, the coupled system of the Cahn-Hilliard and elasticity equations is solved using the finite element method. This coupling is due to the presence of elastic energy in the Cahn-Hilliard free energy and the dependence of total strain on the void misfit strain. Results show a faster growth with larger amounts of void concentration at lower temperatures. Also, the stress field significantly varies during void evolution inside the solid-gas interface and its value depends on the void size and the concentration.

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