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Computation of Electropulse-driven Regeneration of Magnetic Heterogeneous Materials

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Abstract— When a material with heterogeneous microstructure degraded in a service environment, both the local and overall magnetic and electric properties inside the materials changed drastically. This is particularly significant for the magnetic properties. The diffusion of solute elements from one to another zones causes drastic alteration of magnetic permeability. When an electric field is applied to the materials, the electromagnetic responses of the degraded materials to the applied electromagnetic field are different from that of the state before degradation. In some special cases, the applied electric field can drive the degraded materials to recover to the original state. This article reports our detailed theoretical and numerical calculation of the electropulse-driven regeneration project. The changes of electrical and magnetic properties during the materials degradation were analysed and investigated. The microstructures during the degradation and regeneration were reconstructed using a phase field method. The chemical free energy was obtained from commercial thermodynamic database. The electromagnetic thermodynamics was calculated according to the change of microstructure and electromagnetic properties in the materials. The proposed computational electromagnetic method can be implemented to the investigation of regeneration of many engineering materials.

1. INTRODUCTION

Many engineering alloys are in non-equilibrium states. This is due to the advanced mechanical properties that a non-equilibrium alloy can possess than that of its counterpart equilibrium state. The dual phase stainless steel implemented in the nuclear power plants is an example in this case. It contains two phases called ferrite and austenite, which is a non-equilibrium structure obtained by quench of the material from a thousand degrees Celsius to ambient environments. Its equilibrium states would contain more phases including the decomposed ferrite into iron-rich and chromium-rich zones and other precipitates [1]. Ferrite phase is ferromagnetic and austenite is paramagnetic phases. The materials has a heterogeneous structure in terms of magnetic property, electrical property and crystallography. Solute diffusion takes place in the material during the engineering service. The magnetic property of the material changes drastically during the usage of the material [2], together with the change of many other changes such as electrical properties [3] and charpy impact toughness [4]. This property degradation is called aging. Aged materials need to be replaced when the degradation has achieved to a certain content to prevent the failure.

In our previous study, electric current was applied to the aged materials. The degraded materials were found to be regenerated according to experimental measurement [5]. However, the theoretical consideration and numerical calculation in the project has not been reported in details. The present work aimed to address this. The method for generation of magnetic heterogeneous microstructure is described in Section 2. The calculation of electric current processing and results are presented in Section 3. The conclusion remarks are outlined in Section 4.

2. CONSTRUCTION OF HETEROGENEOUS MICROSTRUCTURES

According to the predictions made by the calculation of phase diagram and the observations made by experiments, the microstructure of a dual phase stainless steel is formed by the growth of austenite grains with dendrite morphology in the matrix of δ -ferrite during the cooling of the materials. Both austenite and ferrite phases are in cubic crystal structures with the former in face-centered-cubic and the later in body-centered-cubic symmetry. The volume fraction of austenite is found to be 30%. A phase-field model is implemented in the present work to calculate the microstructure of this material. The details of phase-field theory were described in several review papers [6, 7]. The anisotropic interface energy between the face-centered-cubic austenite and the body-centered-cubic ferrite is not available. In the present simulation, the anisotropic surface energy of pure iron

has been implemented to represent the ferrite-austenite interface as an approximation [8]. The governing equations for the phase-field simulation are in the followings.

$$\frac{\partial \phi}{\partial t} = M_\phi \left\{ \sum_{\alpha=x,y,z} \frac{\partial}{\partial \alpha} \left[|\nabla \phi|^2 \epsilon(\hat{n}) \frac{\partial \epsilon(\hat{n})}{\partial \phi_\alpha} \right] + \nabla [\epsilon(\hat{n})^2 \nabla \phi] + \frac{1}{2\omega} \phi(1-\phi)(1-2\phi) - \frac{\partial g_b}{\partial \phi} \right\} \quad (1)$$

where ϕ is the phase-field order parameter with $\phi = 0$ represents ferrite, $\phi = 1$ austenite and $0 < \phi < 1$ the interface. $\epsilon(\hat{n})$ is the anisotropic interface gradient energy coefficient and is dependent on the anisotropic interface energy. $\hat{n}$ is the unit vector at the normal direction of the interface. The expression for cubic anisotropic interface energy and the coefficients were implemented in the calculations [8]. g_b is the free energy density of bulk phase. The value of g_b for the material is available from the commercial thermodynamic database such as MTDATA. The solute diffusion in the computation of microstructure was calculated using

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(M_c \nabla \frac{\partial \mu_b}{\partial c} \right) \quad (2)$$

where c is the solute concentration, M_c is the mobility and μ_b is the chemical potential. μ_b can be obtained directly from the thermodynamic database. The mobility is related to the diffusivity. Solute fluctuation were introduced in the simulation to include the statistical effect in mesoscopic system. The austenite grains were supposed to grow from some random sites to represent the nucleation. The growth of austenite grains was suspended when the total fraction of austenite has achieved 30%.

The numerical calculations were performed using finite difference method. The initial solute compositions were taken from the average values in the real alloys. The time step and space distance between lattice were selected according to the recommendations in literature [8]. The microstructure of austenite grains when its volume fraction achieved 30% is plotted using MatVisual software and is illustrated in Figure 1. The different colours represent different crystallographic orientations. The ferrite phase is matrix, which is not plotted in the figure.

Figure 1: The morphology of austenite grains. The different colours represent the different crystallographic orientations.

From this point, the spinodal decomposition in ferrite phase starts to take place. The phase-field model for spinodal decomposition has been reported in several papers [9]. The solute distributions of Cr in ferrite phase before and after the spinodal decompositions are presented in Figures 2(a) and (b), respectively. The microstructure is similar to that observed by experimental observations using atom probe tomography.

3. EFFECT OF THE PASSING ELECTRIC CURRENT

When an electric field is applied to the two ends of the alloy, electric current forms due to the conductivity of material. The local electric current density is obtainable via Ohm's law of $\vec{j}(r) = \sigma(r) \cdot \vec{E}(r)$, where r is a spatial position in material, $\vec{j}(r)$ is the electric current density at space r .

Figure 2: The distribution of Cr composition in ferrite (a) before and (b) after spinodal decompositions.

$\sigma(r)$ is the local electrical conductivity which is dependent on the phase and solute composition at the spatial position. $\vec{E}(r)$ is the electric field. The electric field is determined by the gradient of the electric potential via $\vec{E}(r) = -\nabla\phi(r)$, where $\phi(r)$ is the local electrical potential. For a metallic matrix, the electrical potential inside the materials satisfies $\nabla^2\phi(r) = 0$. This Poisson equation can be solved using a relaxation method. The distribution of electric current density can then be obtained. According to the thermodynamic theory on the electric-current-carrying system [10], the electric current free energy can be obtained by the following equation.

$$G_j - G_{ref} = \frac{1}{8\pi} \iint_V \frac{\mu(r)\vec{j}(r) \cdot \vec{j}(r')}{|r - r'|} dr dr' \quad (3)$$

where $G_j - G_{ref}$ is the electric current free energy difference from its reference state. The integration of position r goes throughout the whole volume of material V . $\mu(r)$ is the local magnetic permeability which is dependent on the phases as well as the solute composition. The numerical method to obtain the electric-current free energy according to Equation 3 has been described in literature [10].

The electrical conductivity of ferrite and austenite phases before the spinodal decomposition is 8.48×10^5 S/m and 9.27×10^5 S/m, respectively. After the spinodal decomposition, the electrical conductivity of ferrite in iron-rich and chromium-rich zones is changed slightly into 9.29×10^5 S/m and 9.17×10^5 S/m, while that of the austenite phase remains unchanged. The spinodal decomposition causes drastic change of magnetic permeability in the ferrite phase, from $2087\mu_0$ before spinodal decomposition changes into $162\mu_0$ and $49\mu_0$ respectively in iron-rich and chromium rich zones after the spinodal decomposition [3]. Those values were substituted into the electromagnetic

equations to calculate the electric current density distribution followed by the calculation of the electric current free energy for the microstructures presented in Figures 1 and 2. The electric current density distribution before and after the spinodal decomposition is presented in Figures 3(a) and 3(b) respectively. The electric current free energy is found 891 J/mol higher for the microstructure formed by spinodal decomposition than that before decomposition. This means that electric current prefers to the microstructure before decomposition. In another word, electric current intends to drive the decomposition to reverse back. This is the fundamental mechanism for the experimentally observed microstructure and property regeneration for dual phase stainless steel.

Figure 3: The distribution of electric current density in the materials (a) before and (b) after the spinodal decompositions.

4. CONCLUSION

From the computation of effect of electric current on the microstructure change in magnetic heterogeneous materials, it has been found that the electric current possesses an effect to interfere the microstructure transformation. In the particular case of ferromagnetic ferrite and paramagnetic austenite magnetic heterogeneous structure, electric current can be used to regenerate the microstructure of the material. The property will hence be regenerated. The method can be implemented to treat the engineering alloys.

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