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Two-dimensional chemo-elasticity under chemical equilibrium

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ABSTRACT

The coupling between solid state diffusion and mechanical stress arises in a number of important technological applications. The theory that describes such coupling is termed chemo-elasticity. In this paper, a solution approach is developed for two-dimensional chemo-elasticity problems. First, a coupled system of nonlinear partial differential equations is derived in terms of an Airy stress function and the solute concentration. Then, this coupled system of nonlinear equations is solved asymptotically using a perturbation technique. Finally, based on this approach, asymptotic solutions are obtained for three fundamental problems in two-dimensional chemo-elasticity, namely, a circular hole in an infinite plate under uniaxial tension, a straight edge dislocation and a disclination.

1. Introduction

In this paper, chemo-elasticity refers to the coupled theory of solid state diffusion and deformation in elastic solids. It deals with the thermodynamics of mechanically stressed solids that may change their composition through either solute redistribution within the solids, or mass exchange with the surrounding environment. Chemo-elasticity problems may arise in a number of technological areas including ionic solids in fuel cells (Swaminathan et al., 2007a,b), intercalation in batteries (Burch and Bazant, 2009; Bai et al., 2011; Cogswell and Bazant, 2012; Cui et al., 2012a,b, 2013a,b), and the growth of porous biogenic single crystals (Kienzler et al., 2006; Fratzl et al., 2010), just to name a few. In these applications, the solute is driven into or out of a host solid by various (electro-) chemical and mechanical deriving forces. A free-standing stress-free material element may expand (or shrink) to accommodate the solute insertion or extraction. However, such volumetric change may be restricted by either the surround materials or by the mechanical constraint imposed by the boundary conditions. Restriction to the composition-induced volumetric change will lead to mechanical stress in the solid. On the other hand, the stresses in the solid may affect solute diffusion in the solid. For instance, in thin film electrodes deposited on a substrate, the volumetric changes are restricted by the underlying current collector (Graetz et al., 2004). In the biomimetic growth of porous single crystals, cavities form and grow to accommodate significant volume reduction caused by crystallization of the amorphous precursor. However, formation of cavities gives rise to stress concentration and could increase the risk of failure (Fratzl et al., 2010). It is, therefore, of interest to investigate the interactive effects of the presence of the solute in the matrix on the mechanical stress fields.

Although chemo-elasticity problems have been investigated since the 1930s, e.g., (Fowler and Guggenheim, 1939), the development of a systematic framework is due to Larche and Cahn (1973). For a solid under chemical equilibrium, they showed that it is possible to introduce a set of modified material properties, namely open-system elastic constants, which account for the interplay between the non-uniform stress field and concentration within a linearized regime. This method hinges upon linearization of the chemical field in terms of stress components, and has been employed in the study of dislocations (Larche and Cahn, 1985; Sofronis, 1995), precipitates and inclusions (Johnson and Voorhees, 1985; King et al., 1991) and redistribution of solute in various interstitial sites in crystalline metals (Johnson and Huh, 2003; Voorhees and Johnson, 2004).

In this paper, we build upon Larche and Cahn's general framework (Larche and Cahn, 1973), and develop a solution approach to two-dimensional chemo-elasticity problems. By using the Airy stress function, we derive a coupled system of nonlinear partial differential equations for the Airy stress function and the solute concentration. Since an analytical solution does not seem to be feasible, we present a perturbation scheme that leads to an asymptotic solution for the coupled system of nonlinear equations. The small parameter $\hat{\eta}$ used in the perturbation scheme is a dimensionless parameter representing the coupling between the mechanical and chemical fields. Based on this approach, we obtain analytically the asymptotic solutions up to the second order of $\hat{\eta}$ for three

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fundamental problems in two-dimensional chemo-elasticity, namely, a circular hole in an infinite plate under uniaxial tension, a straight edge dislocation and a disclination. We also demonstrate that, for traction-prescribed problems, the leading order term in our asymptotic solution is equivalent to the solution obtained by Larche and Cahn (1973) using the open-system elastic constant approach.

The paper is arranged as follows. In Section 2, we derive the three-dimensional governing equations in chemo-elasticity. The corresponding two-dimensional equations are derived in Section 3 by introducing an Airy stress function. This system of two-dimensional equations are solved in Section 4 by an asymptotic approach whereby the field quantities are expanded in terms of the perturbation parameter $\hat{\eta}$. This asymptotic approach allows us to reduce the governing coupled nonlinear equations into a set of linear decoupled equations which can be solved recursively to obtain the higher order elastic and concentration fields. Using this asymptotic perturbation method, we investigate the disturbance of the concentration field as well as the elastic fields caused by the emergence of a hole, dislocation, and disclination under plane stress and/or plane strain conditions in an infinite medium. The connection between the asymptotic approach and the method of open-system material constants is also discussed. Finally, in Section 5, we conclude by summarizing the main findings of this work.

2. Governing equations for solid state diffusion

Without loss of generality, we consider an elastic solid A_xB that consists of species A and species B. It is assumed that the concentration of A in A_xB may vary from $x = 0$ to $x = x_{\max}$, where $x_{\max}$ is the solvability of A in B. One may also view species A as the solute and species B as the solvent. Furthermore, we assume that the solid in consideration can be represented by the network model of Larche and Cahn (1973), namely, the lattice sites of species B form a network within which species A can move (diffuse). This allows the definition of a displacement field and hence a strain field of the solid. To simplify the mathematics, we will only consider small strain deformation in the rest of this paper.

In the following, it is convenient to define molar concentration of the solute per unit volume of the solvent as $c = x/V_m$, where V_m is the molar volume of the pure solvent in its stress-free state. We assume that the solute-free solvent corresponds to a stress-free state, and the compositional change of the mixture causes a volumetric deformation according to

$$\varepsilon^c_{ij} = \eta x \delta_{ij} = \eta V_m c \delta_{ij}, \tag{1}$$

where δ_{ij} is the Kronecker delta, η is the coefficient of compositional expansion (CCE), which is a material property that characterizes the linear measure of the volumetric change due to unit change of the composition (Swaminathan et al., 2007a,b). For a given material, the CCE can be obtained either experimentally, or by conducting molecular dynamic simulations (Swaminathan and Qu, 2009; Cui et al., 2012a,b,c). The total strain caused by the compositional change and applied load can be written as

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) = \varepsilon^e_{ij} + \varepsilon^c_{ij}, \tag{2}$$

where u_i is the displacement and ε^e_{ij} is the elastic strain. The total strain needs to satisfy the compatibility condition,

$$\varepsilon_{pki}\varepsilon_{qlj}\varepsilon_{ij,kl} = 0, \tag{3}$$

where ε_{pki} is the permutation symbol.

We further assume that the solid is linear elastic so that its elastic state is uniquely determined by the elastic strain energy function

$$w = \frac{E}{2(1+\nu)}\left(\varepsilon^e_{ij}\varepsilon^e_{ij} + \frac{\nu \varepsilon^e_{kk}\varepsilon^e_{mm}}{1-2\nu}\right), \tag{4}$$

and the stress tensor is thus given by

$$\sigma_{ij} = \frac{\partial w}{\partial \varepsilon^e_{ij}} = \frac{E}{(1+\nu)}\left(\varepsilon^e_{ij} + \frac{\nu \varepsilon^e_{kk}}{1-2\nu}\delta_{ij}\right), \tag{5}$$

where E and ν are the Young's modulus and Poisson's ratio, respectively, of the solid, which are assumed to be independent of the solute concentration. This assumption is valid for most solids under dilute solute concentration. Eq. (5) can be inverted to give

$$\varepsilon^e_{ij} = \frac{1}{E}[(1+\nu)\sigma_{ij} - \nu\sigma_{kk}\delta_{ij}]. \tag{6}$$

In the absence of body forces, the stress needs to satisfy the static equilibrium equations,

$$\frac{\partial \sigma_{ji}}{\partial x_j} = 0. \tag{7}$$

In this stressed-solid, the chemical potential of species A will depend on the stress (Larche and Cahn, 1973). By assuming small strain and composition-independent isotropic elasticity, the stress-dependent chemical potential (more precisely, the diffusion potential of species A in species B) can be derived from the general expression of (Swaminathan et al., 2007a,b; Cui et al., 2012a,b,c),

$$\mu = \mu_0 + R_g T \log\frac{c}{c_{\max} - c} - V_m \eta \sigma_{kk}, \tag{8}$$

where μ_0 is a constant representing the chemical potential at a standard state, R_g is the standard gas constant, T is the absolute temperature, c is the molar concentration of the solute, and $c_{\max} = x_{\max}/V_m$ corresponds to the saturation state of the solution. The particular choice of the potential ensures that the stoichiometric state has the lowest energy (i.e., $\mu \to -\infty$ as $c \to 0$), and the state of saturation has the highest energy (i.e., $\mu \to \infty$ as $c \to c_{\max}$).

The governing equations presented above are valid within the elastic solid of interest. The stress and solute concentration within the solid depend also on what happens at the boundary of the solid. Therefore, boundary conditions are required in order to uniquely determine the stress and solute concentration fields.

Consider an elastic solid Ω with surface S with outward unit normal vector n_i. As usual, the mechanical boundary conditions can be prescribed as

$$\sigma_{ij}n_i\big|_{S_\sigma} = p_j, \quad u_i\big|_{S_u} = U_i, \tag{9}$$

where $S_u + S_\sigma = S$ and p_j and U_i are, respectively, the prescribed traction and displacement on the boundary. The chemical boundary conditions can be specified as

$$\mu\big|_{S_\mu} = \mu_s, \quad -\frac{cD}{R_g T}\nabla\tilde{\mu}\Big|_{S_J} = \mathbf{J}_s, \tag{10}$$

where $S_\mu + S_J = S$, and μ_s and $\mathbf{J}_s$ are, respectively, the prescribed chemical potential and the flux on the boundary.

3. Two-dimensional plane problems under electrochemical equilibrium

We assume that all field quantities are functions of x_1 and x_2 only, i.e.,

$$u_1 = u_1(x_1, x_2), \quad u_2 = u_2(x_1, x_2), \quad u_3 = u_3(x_1, x_2), \quad c = c(x_1, x_2). \tag{11}$$

Further, for plane strain, we assume

$$\varepsilon_{33} = \varepsilon_{23} = \varepsilon_{13} = 0. \tag{12}$$