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Nonlinear effects on impurity segregation in edge dislocation strain fields

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Elastic field coupling to solute concentration is known to produce dislocation-driven impurity segregation. Recent reports detailing the distribution of boron around edge dislocations in B2-ordered FeAl indicate that nonlinear coupling of species concentration and elastic strain to the chemical potential must be considered to assess the magnitude of boron segregation around edge dislocations. One type of nonlinear coupling spatially shifts the solute distribution relative to the dislocation strain field, while another maintains the centers of the respective distributions.
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The coupled phenomena of species diffusion and elastic deformation in materials give rise to a range of interesting effects [1–6]. One of great importance is the stress-induced redistribution of mobile/solute species in the presence of dislocation structures in materials, resulting in the formation of Cottrell atmospheres around these partially stable defects. The formation of regions enriched by solute species around dislocations, especially those of the edge type, directly affects dislocation mobility and impacts mechanical deformation characteristics. Consequently, the study of the distribution of solute species around dislocations has been an area of active research extending back to the work of Cottrell and Bilby [7]. However, recent advances in microscopy have provided unprecedented ability to quantitatively map the three-dimensional distribution of various species on the atomic scale around defect structures including edge dislocations. With these advances, information has been gathered that allows for refinement and reinterpretation of models describing the coupling of solute concentration to elastic deformation in materials.

Among the techniques that have been adapted to solute distribution mapping and imaging is atom-probe field ion microscopy, which has been used to quantitatively analyze atomic species distributions around edge dislocations [8–12]. Focusing primarily on the FeAl intermetallic system, Blavette et al. examined the preferential segregation of boron to edge dislocations and were able to successfully quantify the average radial distribution of aluminum, iron and boron around the dislocation line [8]. While attempts have been made to model the measured distribution of boron in this system [12,13], quantitative agreement has not been established. Wilde et al. mapped the carbon Cottrell atmosphere around a dislocation in iron but did not provide statistical measures of the distribution [14]. Beyond these studies, solute and vacancy diffusion in the presence of dislocations has been studied in an attempt to understand age-hardening and annealing kinetics in alloy systems [15–18]. Unfortunately, much early work has been hindered by an incomplete understanding of solute distribution around dislocation structures. In this paper, the nonlinear couplings of strain and concentration that affect chemical potential are explored to provide insight into species diffusion around edge dislocations.

Note that both the species concentration and the strain have components that are stationary with respect to the changes that are of interest in this treatment. However, these background values can depend on additional factors (such as temperature) and can influence the response of the material. Specifically,

$$\varepsilon_{ij} = \varepsilon^0_{ij} + \varepsilon'_{ij} \quad \text{and} \quad c = c^0 + c', \tag{1}$$

where ε_{ij} is the linear strain tensor, c is the concentration of the species of interest, the zero superscript indicates the average/background value and the prime indicates

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the varying portion. The initial, or reference, state is represented by a spatially uniform solute concentration field at finite temperature such that the relevant thermodynamic potential function can be expanded about this state, yielding the following constitutive relations for stress, σ_{ij}, and chemical potential, μ, [1,19]:

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl} - \beta_{ij}c - \frac{1}{6}g_{ij}c^2 + \frac{1}{2}c_{ijklmn}\varepsilon_{kl}\varepsilon_{mn} + \frac{1}{3}h_{ijkl}\varepsilon_{kl}c \tag{2}$$

and

$$\mu = mc - \beta_{ij}\varepsilon_{ij} - \frac{1}{3}g_{ij}\varepsilon_{ij}c + \frac{1}{6}h_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + \frac{1}{2}pc^2, \tag{3}$$

where indicial notation and the Einstein summation convention have been used. These nonlinear forms for the constitutive relations use strain and concentration as independent variables and include the following material constants: c_{ijkl}, the second-order elastic stiffness tensor; c_{ijklmn}, the third-order elastic stiffness tensor; β_{ij}, the linear stress–concentration coupling tensor; g_{ij} and h_{ijkl}, the nonlinear stress–concentration coupling tensors; m and p, the linear and nonlinear chemical potential coefficients.

For the development here, the chemical potential is of primary interest, however, a more general treatment would require consideration of diffusion potentials [3]. Generally, for small excursions from equilibrium, only linear coupling of strain to the chemical potential is considered. However, if concentrations are small, even modest strain levels can cause higher-order terms in Eq. (3) to become important. Under these conditions, only the nonlinear term in Eq. (3) that contains both the strain and the concentration should be retained. With this approximation in place, Eqs. (1) and (3) yield the following:

$$\mu' = mc' - \beta_{ij}\varepsilon'_{ij} - \frac{1}{3}g_{ij}(\varepsilon^0_{ij}c' + \varepsilon'_{ij}c^0 + \varepsilon'_{ij}c'), \tag{4}$$

where μ' specifically represents variations to the chemical potential related to species concentration and stress and the unperturbed, or initial state, requires $\mu^0 = mc^0 - \beta_{ij}\varepsilon^0_{ij}$. For static systems, it is assumed that variations in the strain and concentration fields are related so the chemical potential is uniform across the system. Consequently, Eq. (4) can be simplified to yield:

$$c'\left(m - \frac{1}{3}g_{ij}\varepsilon^0_{ij}\right) = \left(\beta_{ij} + \frac{1}{3}g_{ij}(c^0 + c')\right)\varepsilon'_{ij}. \tag{5}$$

Regrouping terms and using the background-modified material constants

$$m^* = \left(m - \frac{1}{3}g_{ij}\varepsilon^0_{ij}\right) \text{ and } \beta^*_{ij} = \left(\beta_{ij} + \frac{1}{3}g_{ij}c^0\right)$$

yields the result

$$c' = \beta^*_{ij}\varepsilon'_{ij}\left(m^* - \frac{1}{3}g_{ij}\varepsilon'_{ij}\right)^{-1}. \tag{6}$$

Note that the variation in concentration must obey the constraint $c' \geqslant -c^0$ since simple application of a strain field cannot cause concentration to be negative. This limits the values assumed by nonlinear constants under various conditions.

The Cottrell atmosphere around a dislocation in crystalline solids can be investigated in non-time-varying systems using the appropriate strain field in Eq. (6). The linear strain field tensor for an infinitely long, edge dislocation in an isotropic material with Burgers vector in the positive x_1 direction, b_1, has the following trace:

$$\varepsilon_{11} + \varepsilon_{22} = -\frac{b_1}{2\pi}\frac{2}{(\lambda + 2\mu)}\frac{\sin\theta}{r}, \tag{7}$$

where the angle θ is measured from the positive x_1 axis, λ and μ are the Lamé constants and r is the radial distance from the dislocation line. The strain tensor trace is associated with the dilatation of the material surrounding the dislocation providing the thermodynamic driving force for species diffusion. Using the linear term in Eq. (6) to determine the concentration in the edge dislocation strain field shows that there is a singularity at the origin where the dilatation is not defined. Including the nonlinear term yields two spatial locations where the concentration is singular—one at the origin and a second corresponding to the condition $m^* = \frac{1}{3}g_{ij}\varepsilon'_{ij}$ which occurs for certain strains away from the origin. The existence of this additional singularity serves to shift the concentration distribution away from the origin. If the only nonlinear terms retained in the description depended entirely on strain, then the concentration expression would only have a singularity at the origin.

Eqs. (6) and (7) can now be used to construct the average concentration variation as a function of the radial distance from the dislocation core. This is given by the following:

$$\overline{c'} = \frac{1}{\pi}\int_{\frac{-\pi}{2}}^{\frac{\pi}{2}} c'\mathrm{d}\theta \approx \frac{1}{\pi}\left(\frac{-3\beta}{g}\right)a\int_{\frac{-\pi}{2}}^{\frac{\pi}{2}} \sin\theta(1 + a\sin\theta)^{-1}\mathrm{d}\theta, \tag{8}$$

where

$$a = \frac{g}{3m^*}\frac{b_1}{2\pi}\left(\frac{2\mu}{\lambda + 2\mu}\right)\frac{1}{r}. \tag{9}$$

The integral is quite simple and yields the result:

$$\overline{c'} \approx \left(\frac{3\beta^*}{g}\right)(1 - (1 - a^2)^{-1/2}). \tag{10}$$

Here it has been assumed that the system of interest behaves isotropically such that $\beta^*_{ij} = \beta^*\delta_{ij}$ and $g_{ij} = g\delta_{ij}$. Note that the nonlinear coupling constant, g, appears both as a factor in the functional form and as an amplitude scaling coefficient for the average radial concentration. The former limits the maximum value for g since, at some minimum radius, a singularity in the domain of integration occurs, making the derived form invalid. Conveniently, for the values of g required, we can take this minimum radius to be in or near the dislocation core where other assumptions of the current derivation also break down.

Using materials-related parameters appropriate for the B2-ordered intermetallic FeAl with boron alloying [13,20,21] yields the results in Figure 1, showing the average radial boron concentration around an edge dislocation located at the origin. Both the measured results

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