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CRACKING BEHAVIOR OF CORED STRUCTURES

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ABSTRACT

The effects of compositional gradients, are considered based on a thermodynamic analysis, referred to as the Cahn-Hillard analysis, which describes the degree to which a local surface energy is modified by the presence of a composition gradient. The analysis predicts that both ductile and brittle fracture mechanisms are enhanced by the presence of a composition gradient. Data on stress corrosion cracking and fatigue crack growth in selected FCC alloys are used to illustrate the significance of microsegregation on mechanical properties.

INTRODUCTION

The presence of microsegregation and other compositionally non uniform conditions have been found to directly affect the mechanical properties of a wide variety of systems. For example, Johnson and Grimsley (1) improved the stress corrosion cracking resistance of 17-7 PH stainless steel by homogenization, a heat treatment which eliminates compositional gradients. In weldments, both Savage et al (2) and Berry et al (3) reported that stress corrosion cracks in as-solidified microstructures follow the location in the microstructure where the concentration gradient is the steepest. To illustrate this point, Figure 1 shows the chromium microprofile in solidified stainless steel, along with the observed location (at the steepest point in the gradient) of a stress corrosion crack (3).

Other forms of cracking are also dependent on the magnitudes of microcompositional gradients. For example, Choi et al (4) showed that post-weld heat treatments decreased the susceptibility of Monel Alloy 400 weld metal to high temperature creep cracking. The decrease in cracking susceptibility correlated directly to changes in the microcompositional gradients due to the post-weld homogenization heat treatments.

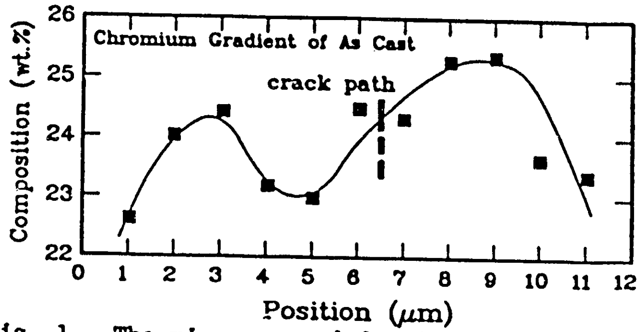

Fig. 1 - The microcompositional profile for chromium content across a stress corrosion crack of as-cast CK-20. Data were obtained on an unetched surface. Dashed line represents stress corrosion crack location (3).

These observations lead to fundamental questions about the role of microsegregation or compositional gradients on the local mechanical behavior and on the initiation and propagation of cracks. In this paper fundamental aspects of cracking in compositionally modulated structures are introduced. First-principle analyses are presented to illustrate the approach to the evaluation of both brittle and ductile cracking behavior in selected systems with controlled composition gradients.

BRITTLE FRACTURE

The magnitude of the brittle fracture stress of a material is strongly dependent on the specific surface free energy as suggested by the Griffith Crack theory (5) and described quantitatively by:

$$K_c = \alpha\sigma_F (\pi C)^{1/2} = \alpha (2\gamma E)^{1/2} \quad (1)$$

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where σ_F is the critical fracture stress, α is the geometric factor, γ is the specific surface free energy, K_c is the critical stress intensity factor, c is the crack length, and E is the modulus of elasticity. The specific surface free energy can be defined as the amount of the energy to create new surface. To correlate the specific surface free energy with fracture, it is necessary for the crack to form in a brittle manner, that is without energy being dissipated for deformation.

The specific surface free energy requires a reference energy state. For most materials this reference energy state is for a uniform (homogeneous) material. This concept is illustrated in Figure 2a where the energy difference between a reference energy state and the new surface is the specific surface free energy value to be used in the Griffith Crack Theory.

When considering the genesis of a crack through a compositionally non-uniform material a change in the reference energy state is required as shown in Figure 2b. Cahn and Hilliard (6) introduced an approach to calculate the energy change of a material if it has developed a non uniform compositional state. Cahn and Hilliard (6) considered the local free energy associated with a non uniform system. They defined the local free energy quantitatively such that this specific energy, conceptually a specific interfacial energy, can be written as:

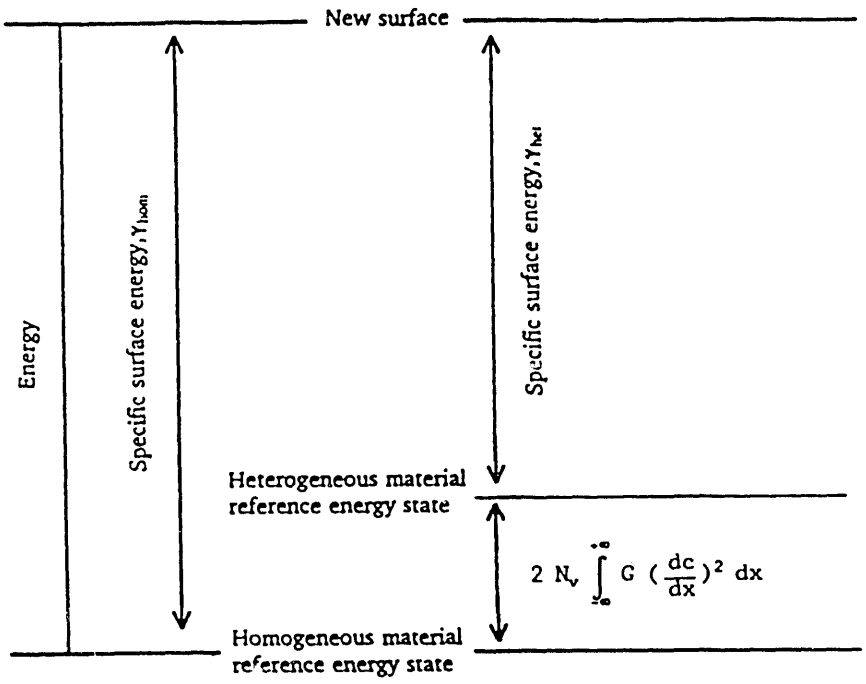
$$\gamma_i = N_v \int_{-\infty}^{+\infty} G \left(\frac{dc}{dx}\right)^2 dx \qquad (2)$$

In Equation 2, N is the number of atoms per unit volume, dc/dx is the composition gradient, γ_i is the local specific interfacial free energy, and G is an energy coefficient which can be calculated from a specific solution model with knowledge of the necessary chemical thermodynamic and physical data for the alloy system.

With the analytical approach summarized in Equation 2, the local specific free energy for this compositionally non uniform state can be calculated and used to correct the reference energy state. This procedure is illustrated in Figure 2b. From Figure 2b it can be seen that the specific surface free energy for a non uniform (heterogeneous) material can be given by the following mathematical expression:

$$\gamma_{het} = \gamma_{hom} - 2 N_v \int_{-\infty}^{+\infty} G \left(\frac{dc}{dx}\right)^2 dx \qquad (3)$$

where γ_{hom} is the specific surface free energy for the homogeneous system and the second term



(a) (b)

Fig. 2 - (a) Energy to create surface in a material in a compositionally uniform condition. (b) Energy to create surface in a material in a compositionally non-uniform condition.

is the Cahn-Hilliard expression which corrects the reference energy state for a non uniform condition. Equation 3 suggests that the local specific surface free energy is concentration gradient dependent. The steeper the concentration gradient the lower the localized specific surface free energy.

The specific surface free energy for the homogeneous system, γ_{hom}, which is a necessary quantity for Equation 3, can be calculated as a function of alloy content by using the expression derived by Guggenheim (7):

$$\exp\left[-\frac{(\gamma A)}{kT}\right] = N_1 \exp\left[-\frac{\gamma_1 A)}{kT}\right] + N_2 \exp\left[-\frac{(\gamma_2 A)}{kT}\right] \qquad (4)$$

In Equation 4, A is the molar surface area ($A = 1.612\ N^{1/3}\ V^{1/3}$), γ_1 and γ_2 are the specific free energies of the individual elemental components of the system, and kT has its usual significance. The application of this analysis is discussed in the following section with the copper-nickel system used as an example material.

THEORETICAL THERMODYNAMIC ANALYSIS OF SCC IN THE COPPER-NICKEL SYSTEM - Copper-nickel alloys will fracture in a brittle manner when subjected to a stress corrosion cracking environment (8). The following analysis is limited to a consideration of stress corrosion cracking. The copper-nickel system was chosen for this analysis as it is an isomorphous system that exhibits significant coring on solidification and there is sufficient thermodynamic and physical data (9) to allow property calculations. Calculated values of the specific free energy for a homogeneous materials as a function of alloy content are obtained from Equation 4 for specific free energies for copper and nickel of 1.665 and 2.236 J/m^2 (10). The calculation was performed by assuming that the microprofile in a compositionally non uniform system is described by the sinusoidal compositional profile given below.

$$C(x) = C_o \operatorname{Sin}\left(\frac{2\pi x}{\lambda} + \frac{\pi}{2}\right) \qquad (5)$$

In Equation 5, C_o is the compositional amplitude, λ is the dendritic spacing, and x is the location of interest in the interdendritic region. The locus of the steepest concentration gradient is at $x = \lambda/4$. To implement the Cahn-Hilliard concept, the interdendritic spacing, λ, needs to be determined, from which the energy coefficient, G, is calculated. The assumed sinusoidal profile has been found to be acceptable for systems that have a small interdendritic spacing and are partially homogenized, a condition which can occur on cooling for some alloys.

The calculated values of the specific surface free energy as a function of alloy composition are shown in Figure 3 and the calculations which include the heterogeneous correction term are shown in Figure 4. Figure 4 shows that the higher the compositional

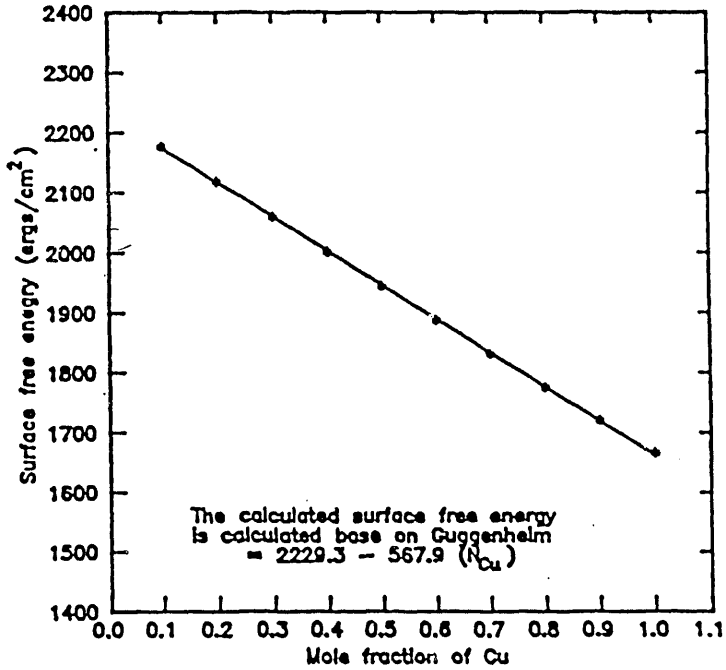


Fig. 3 - Calculated surface free energy of homogeneous copper nickel alloys as functions of compositional calculated based on Equation 4.

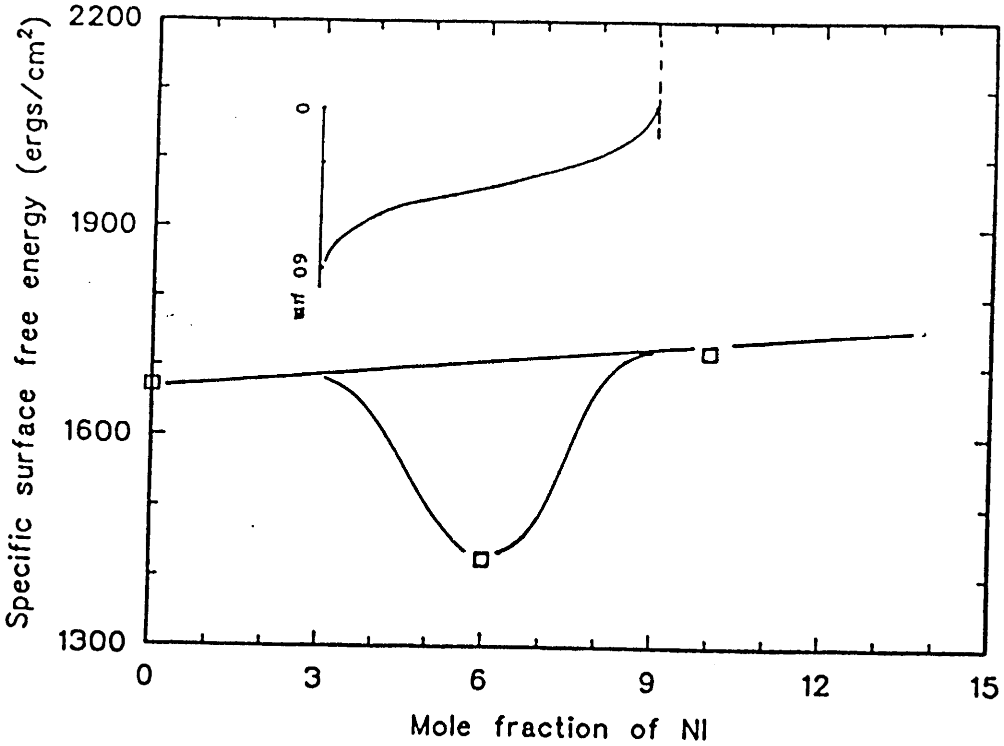


Fig. 4 - The influence of compositional gradients on the specific surface free energy calculated for a cored copper-nickel alloy.

fluctuation or the higher the compositional gradient the lower the value of the specific surface free energy.

With the results of Figure 4 as a base, the predicted change in the stress intensity factor for ideal brittle fracture in a stress corrosion cracking environment was calculated and is illustrated in Figure 5. Notice that as the segregation decreases, as seen by the decrease in the compositional amplitude, the stress intensity factor increases. These results may suggest that heat treatment of weldments and castings will not only relieve the residual stresses, but also reduce the compositional gradients.

DUCTILE FRACTURE

The presence of microsegregation can affect ductile fracture mechanisms at both low and high temperatures. With respect to low temperature deformation mechanisms, the local composition controls the stacking fault energy, which in FCC materials controls dislocation structure and movement. For example, fatigue of compositionally uniform alloys has been found to be related to the magnitude of its stacking fault energy (11,12). If the stacking fault energy is high, the dislocations can easily cross slip around obstacles and thereby promote slip band formation and have a significant plastic zone at the crack tip. This type of slip band behavior has been called "wavy" and has been reported (13) to lower the fatigue resistance. Low stacking fault energies make cross slip more difficult and constrict the dislocation motion to planar flow. This type of slip band behavior has been classified as "planar" and may hinder the fatigue process.

The influence of the compositional gradients on the formation of stacking faults, and thus on fatigue, can be evaluated following the procedures discussed above for stress corrosion cracking. Specifically the stacking fault energy in a compositional gradient can be expressed as the sum of the stacking fault energy of an alloy in the homogeneous condition (14), $\gamma_{SF}(\text{hom})$, and the increase in the energy due to the compositionally non uniform condition. Thus, the stacking fault energy for a heterogeneous system can be expressed as:

$$\gamma_{sf}(\text{het}) = \gamma_{sf}(\text{hom}) + 2\, N_v \int_0^{x_{sf}} G\, \left(\frac{dc}{dx}\right)^2 dx \qquad (6)$$

The second term is described using the Cahn-Hilliard expression (Eq. 2), x_{sf} is the width of the stacking fault, and (dc/dx) is the compositional gradient through the stacking fault region.

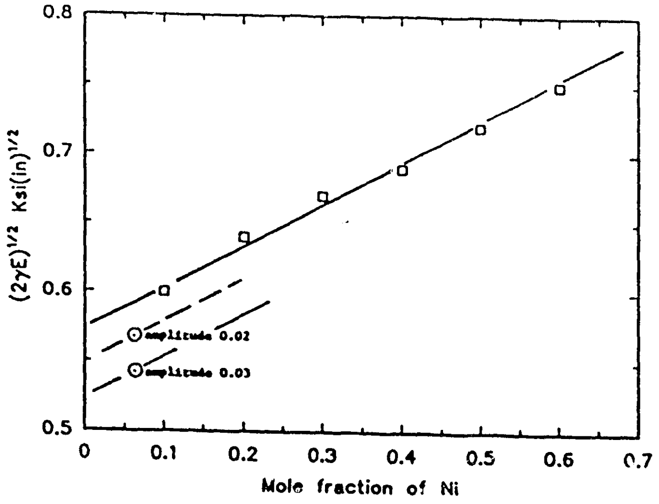


Fig. 5 - The effect of nickel mole fraction in a copper-nickel alloy on material properties $(2\gamma E)^{1/2}$. Calculations are presented for a fully homogenized condition and for two amplitudes of a sinusoidal composition profile.

Equation 6 describes how both the stacking faulty energy and the energy associated with the segregation change the reference energy state of the material. This is illustrated in Figure 6.

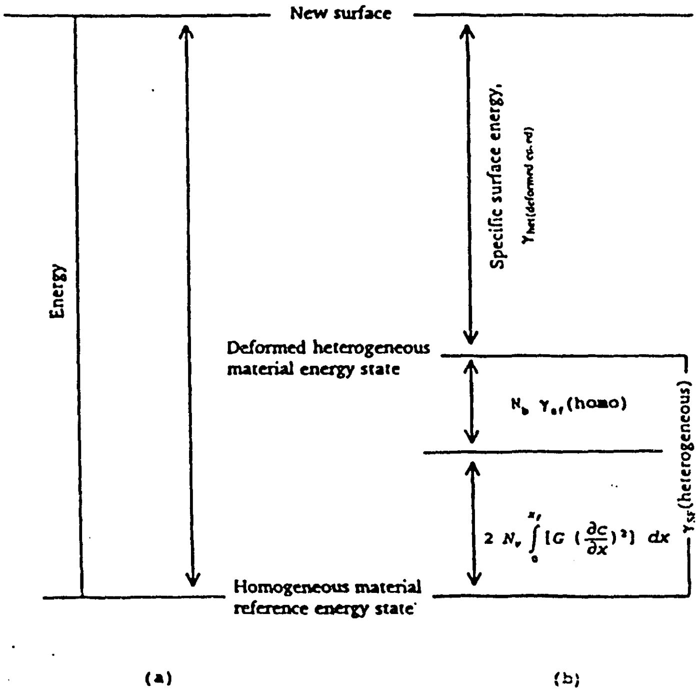


Fig. 6 - (a) Energy to create surface in a homogeneous material. (b) Energy to create surface in a segregated and deformed material.

Notice that both terms lower the specific surface free energy and enhance the susceptibility for fracture.

It is apparent based on this model that the stacking fault energy varies across the cored metal and that the locations of the steepest compositional gradients are most likely to produce extremes in stacking fault energy. These locations are predicted to have the least fatigue resistance and would be the preferred site for fatigue crack propagation.

The applicability of Eq. 6 was considered in an analysis of the path of preferred crack propagation in a copper-6.4 wt. pct. nickel casting. Fatigue crack growth was measured with compact tension samples with notches oriented to induce crack growth parallel to the solidification direction. The fatigue crack path was evaluated with both light and scanning electron microscopy. In addition, the as-cast segregation in the area of the fatigue crack was measured with energy dispersive spectroscopy (EDS). Selected results from the previous analysis are presented in Figures 7 and 8. Figure 7 shows a scanning electron micrograph of the fracture surface which indicates that fatigue crack growth occurred by a combination of intergranular and transgranular mechanisms. The variation in nickel content on a traverse across the fatigue crack (as measured on a mounted and polished sample which was stopped during the stable growth zone) is presented in Figure 8. Significant variations in nickel content are shown and the crack location is shown to correlate with the location of the highest composition gradient. The correlation between crack growth and compositional gradient supports the analysis which indicates that fatigue crack growth resistance is directly related to the local compositional gradient, and thus the local stacking fault energy.

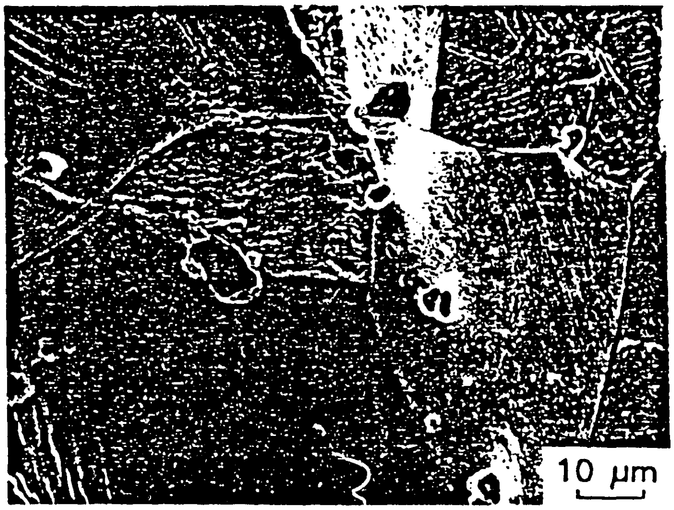


Fig. 7 - Fracture surface of the fatigue precracked test showing a mixture between transgranular and intergranular fracture (SEM micrograph).

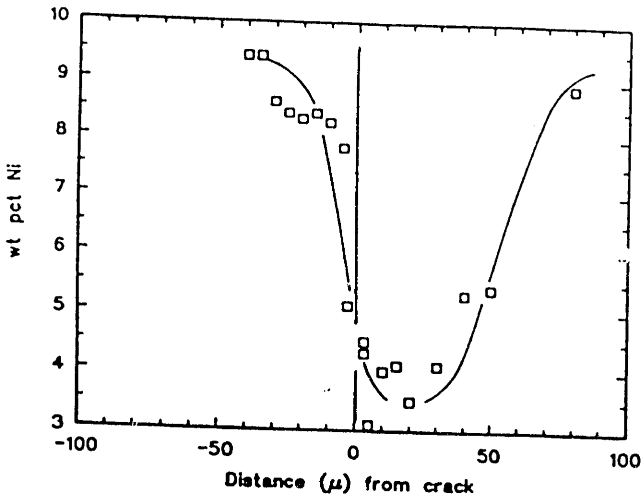


Fig. 8 - The variation of nickel content across a fatigue crack (located at the zero position) in a compact test specimen of an as-cast copper + 6.4 wt pct nickel alloy. Notice cracking occurs in region with compositional gradient.

SUMMARY

Many high temperature materials are based on complex alloy systems which exhibit significant microsegregation on solidification. The serviceability of weldments and castings of these materials may depend on the magnitudes of the local gradients. In this paper an analysis based on fundamental thermodynamic principles in the Cahn-Hillard analysis is presented to account for the effects of local compositional gradients. Analyses of both brittle and ductile fracture mechanisms are presented and shown to depend directly on the magnitudes of the local gradients. Based on a comparison of the predictions with experimental data it is concluded that the Cahn-Hillard analysis can be used to account for specific surface energy changes in surface energy driven deformation and fracture mechanisms. While the examples considered concentrate on low temperature fracture mechanisms, composition gradients are known (4,15-18) to directly affect high temperature properties, and thus it is anticipated that the analysis presented here can be extended to high temperature deformation and fracture mechanisms.

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