



Modeling a distribution of point defects as misfitting inclusions in stressed solids



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ABSTRACT

The chemical equilibrium distribution of point defects modeled as non-overlapping, spherical inclusions with purely positive dilatational eigenstrain in an isotropically elastic solid is derived. The compressive self-stress inside existing inclusions must be excluded from the stress dependence of the equilibrium concentration of the point defects, because it does no work when a new inclusion is introduced. On the other hand, a tensile image stress field must be included to satisfy the boundary conditions in a finite solid. Through the image stress, existing inclusions promote the introduction of additional inclusions. This is contrary to the prevailing approach in the literature in which the equilibrium point defect concentration depends on a homogenized stress field that includes the compressive self-stress. The shear stress field generated by the equilibrium distribution of such inclusions is proved to be proportional to the pre-existing stress field in the solid, provided that the magnitude of the latter is small, so that a solid containing an equilibrium concentration of point defects can be described by a set of effective elastic constants in the small-stress limit.

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1. Introduction

Solid solutions are a ubiquitous feature of metallic systems. They can arise through alloying to enhance mechanical properties, by the introduction of solutes during manufacturing or processing, or via attack by highly permeable contaminants (e.g. hydrogen). The interaction between solutes and other material defects, such as dislocations, can lead to significant changes in the mechanical properties of metals. These interactions can yield desirable effects, as in the case of solid solution strengthening, or undesirable effects, as with hydrogen embrittlement. Possessing a strong theoretical basis for understanding and evaluating the behavior of solid solutions is therefore a necessity for the materials community (Fleischer, 1964; Hirth, 1980; Haasen, 1996).

One key aspect that determines the character of these interactions is the distribution of solutes at chemical equilibrium. Consider a solid containing a set of pre-existing, non-solute defects, such as dislocations or precipitates, which generate a field of internal stresses. Now introduce solutes into the solid. The equilibrium solute distribution depends on the pre-existing stress field. The solutes also generate their own stress fields, whose character depends on the nature of the solutes and the lattice sites they occupy. We will focus on solutes that generate spherically symmetric stress fields, as in the case of octahedral interstitials in face-centered-cubic (FCC) metals. These solute stress fields produce thermodynamic

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forces on the pre-existing defects, which may, for instance, assist rearrangements of the dislocation structure. If solute diffusion is sufficiently fast, then we may assume the solutes to be in the equilibrium distribution for any instantaneous dislocation configuration. If solute diffusion is not fast enough, then the solute diffusion and dislocation microstructure evolution equations may need to be solved together. Even in this case, the equilibrium solute distribution corresponding to the instantaneous dislocation configuration is still of fundamental importance as it provides a reference state relative to which the solute chemical potential and the driving force for diffusion can be defined.

A common approximation for this problem is to model each point defect as an Eshelby inclusion with a spherical shape and purely dilatational eigenstrain (Eshelby, 1954, 1961) (we will use the terms solute, point defect, and inclusion interchangeably in this work). Often, in order to simplify the analysis both the inclusion and surrounding matrix are treated as elastically isotropic with identical elastic constants. Even though real point defects in crystals introduce additional effects not captured by this simple misfitting inclusion model (modulus effects, electronic effects, etc.), the above approximations provide a valuable starting point for understanding the behavior of point defects and are invoked in this work as well. A significant advantage of this model is that explicit analytical solutions exist for the stress/strain fields and elastic energy of a spherical dilatational inclusion in an infinite solid and, under certain circumstances, in a finite solid. The simplicity of this model makes it easier to expose any potential errors in our intuitive reasoning concerning the solute-defect interaction problem, while such errors can easily be masked in a more complicated model that includes many effects and adjustable parameters.

There have been two predominant approaches presented in the literature for analyzing the problem of a distribution of misfitting inclusions. Both utilize the Eshelby inclusion model to calculate the stress field due to a distribution of point defects, and both use the condition of chemical equilibrium to determine the defect distribution. The difference between the approaches lies in two seemingly small but vital details of the analysis. The first approach, which we will call Approach I, excludes what we will refer to as the *self-stress* of the inclusions, but accounts for the so-called *image stresses* that arise to satisfy the traction-free boundary conditions of the solid. In this paper, we refer to the self-stress as the purely hydrostatic stress found *inside* of each inclusion. The logic behind excluding the self-stress is that because inclusions cannot overlap, the self-stress of existing inclusions is not experienced by the next inclusion to be introduced into the solid, and hence irrelevant to the condition of chemical equilibrium. In contrast, the second approach termed Approach II, ignores the image stress and includes the spatially homogenized self-stress of the inclusions in calculating the equilibrium distribution. Approach II considers the overall stress state of the solid to be a smeared-out homogenization of the stresses both internal and external to the inclusions.

The question of whether Approach I or II is correct has had a long history. The notion of accounting for self-stress was first introduced by Cottrell (1948) and Cottrell and Bilby (1949), who argued that point defects would lessen the hydrostatic tension beneath the glide plane of an edge dislocation and lead to a saturation of the solute concentration, a thesis that requires the self-stress to be included in the equilibrium analysis. But this argument was made before the pioneering work of Eshelby (1954, 1961), who showed that the interaction energy for two dilatational inclusions in an infinite isotropic solid is zero.¹ Based on this result, Thomson (1958) and Hirth and Lothe (1968) excluded the homogenized self-stress field from their analyses. Furthermore, Eshelby (1954) and Hirth and Lothe (1968) pointed out that the presence of a free surface would introduce a position-independent interaction between misfitting defects through the image stresses. So, by the end of the 1960s, after two decades of work focused on discrete atomic point defects on a crystalline lattice, it was widely agreed that the homogenized self-stress field should be excluded and image stresses included in analyzing point defects in stressed solids.² We have called this Approach I. But beginning in the early 1970s, in a series of highly cited papers, Larché and Cahn (1973, 1982, 1985) developed a continuum approach to point defect equilibrium that resulted in the re-introduction of the homogenized self-stress and removal of the image stresses. Through this choice they were able to develop an elegant theory that brought the mechanics of point defects into a rigorous thermodynamic framework. The framework developed by Larché and Cahn, which we have called Approach II, has been adopted by others in recent years, including Sofronis (1995), Sofronis and Birnbaum (1995), Chateau et al. (2002), and Delafosse (2012).

With the present paper we wish to conclusively demonstrate that Approach I provides the correct model for understanding the chemo-mechanical equilibrium of solid solution systems. We will present a detailed derivation of the approach and show that in order to have self-consistency, the homogenized self-stress field must be excluded and the image stresses need to be accounted for. Some authors have stated that Approach I is valid only in the limit of dilute solutions (Sofronis, 1995), and we will demonstrate that to the contrary, it is valid both in the dilute limit and beyond. We will then prove analytically that the shear stress induced by a solute atmosphere in equilibrium with the pre-existing stress field is proportional (component by component) to the pre-existing stress, in the limit of small pre-existing stress. As a result, the solid and solutes together behave as a new solid with a set of effective elastic constants, in the limit of small stress. This idea was first presented by Larché and Cahn (1973), but without a proof for the case of non-uniform stress fields. Their expressions were also approximate because the image stresses were ignored. Finally, we will provide a series of numerical results of a solute atmosphere around an edge dislocation to visualize and corroborate our analytic expressions and to contrast the differences between Approaches I and II.

¹ This result is also reproduced in a number of classic texts, such as Khachaturyan (1983) and Mura (1987), and is sometimes referred to as Crum's theorem.

² The self-stress is also effectively removed in the continuum theory used by Siems (1970) and Wagner and Horner (1974).

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