



From coherent to incoherent mismatched interfaces: A generalized continuum formulation of surface stresses

Rémi Dingreville ^{a,*}, Abdelmalek Hallil ^b, Stéphane Berbenni ^c

^a Sandia National Laboratories, Albuquerque, NM 87185, USA

^b Laboratoire des Sciences de l'Ingénieur pour l'Environnement (LaSIE), Université de La Rochelle, Avenue Michel Crépeau, 17042 La Rochelle Cedex 1, France

^c Laboratoire d'Étude des Microstructures et de Mécanique des Matériaux, LEM3, UMR CNRS 7239, Université de Lorraine, Ile du Saulcy, 57045 Metz, France

ARTICLE INFO

Article history:

Received 20 January 2014

Received in revised form

22 May 2014

Accepted 2 August 2014

Available online 19 August 2014

Keywords:

Surface stresses

Interface properties

Mismatch

Grain boundaries

Generalized Shuttleworth relationship

ABSTRACT

The equilibrium of coherent and incoherent mismatched interfaces is reformulated in the context of continuum mechanics based on the Gibbs dividing surface concept. Two surface stresses are introduced: a coherent surface stress and an incoherent surface stress, as well as a transverse excess strain. The coherent surface stress and the transverse excess strain represent the thermodynamic driving forces of stretching the interface while the incoherent surface stress represents the driving force of stretching one crystal while holding the other fixed and thereby altering the structure of the interface. These three quantities fully characterize the elastic behavior of coherent and incoherent interfaces as a function of the in-plane strain, the transverse stress and the mismatch strain. The isotropic case is developed in detail and particular attention is paid to the case of interfacial thermo-elasticity. This exercise provides an insight on the physical significance of the interfacial elastic constants introduced in the formulation and illustrates the obvious coupling between the interface structure and its associated thermodynamics quantities. Finally, an example based on atomistic simulations of Cu/Cu₂O interfaces is given to demonstrate the relevance of the generalized interfacial formulation and to emphasize the dependence of the interfacial thermodynamic quantities on the incoherency strain with an actual material system.

© 2014 Elsevier Ltd. All rights reserved.

1. Introduction

The physical and chemical properties of materials are greatly influenced by the presence of surrounding surfaces and interfaces, whether interfaces are in the form of grain boundaries separating two grains or in the case of a bicrystal between two dissimilar materials (phase boundaries). Interfacial stress and interfacial energy are quantities that play key roles in the thermodynamics of solid surfaces by providing a continuum description of the underlying atomistic complexity of interfaces. Through various constitutive interfacial models, the thermodynamics of interfaces has proven to be an important factor governing the behavior of material systems separated by an interface or for which the surface to volume ratio is significant (Povstenko, 1993; Cammarata, 1994; Nix and Gao, 1998; Miller and Shenoy, 2000; Sharma et al., 2003; Dingreville et al., 2005; Duan et al., 2005; Chen et al., 2007; Duan and Karimhaloo, 2007).

* Corresponding author.

E-mail address: rdingre@sandia.gov (R. Dingreville).

Indeed, atoms near an interface experience a different local environment than atoms in the bulk of a material. In the direction normal to a surface or an interface, the periodicity of the atomic lattice loses its translational symmetry over several atomic layers as demonstrated for example by atomistic simulations (Dingreville and Qu, 2007, 2009; Mi et al., 2008). In the case of an interface between two dissimilar materials, at least one phase must be elastically stretched due to the lattice mismatch between both phases resulting in the formation of defects such as dislocations or vacancies. Similarly, as a consequence, the equilibrium position and energy of atoms located in the vicinity of an interface are, in general, somewhat different from their bulk counterparts. Both the translational and the in-plane atomic shuffling near the interface contribute to a change in the total energy of the interfacial system. The excess energy associated with atoms near an interface is called *interfacial excess energy*.

For incoherent interfaces (e.g. those between two adjacent phases), relaxation of lattice mismatches may result in the formation of peculiar interfacial structures furthering the “excess thermodynamic state” over the bulk configuration. The state of interfacial coherency depends on the physical and the chemical nature between both phases but is also inherently dependent on external factors such as the temperature or the stress field. Qualitatively, the contacting phases possess mismatching lattice constants. For a coherent interface, the mismatch is completely accommodated by straining both phases. In the case of a semi-coherent interface, localized misfit dislocations are assumed to be responsible for compensating uniform far-field elastic fields, while an incoherent interface is the result of two rigid semi-infinite media in rigid contact (Romanov et al., 1998; Romanov and Wagner, 2001).

There are commonly three approaches adopted to study the properties of interfaces: (i) the diffuse interface model, (ii) the interphase model and (iii) the dividing interface/sharp interface model. In the case of the diffuse interface, interfacial properties are described by a smooth, but rapid transition of the various fields (e.g., concentration or elastic fields) describing the interfacial properties (Leo et al., 1998; Hu and Chen, 2002). The interphase approach treats the interface in a classical thermodynamic fashion, namely an arbitrarily defined finite volume is attributed to the interphase region (hence treated as a three-dimensional material system) and is assigned thermodynamic properties in a classical manner (Lipinski et al., 2006; Duan et al., 2007; Berbenni and Cherkaoui, 2010). Finally, the concepts of dividing surface, interfacial excess energy and interfacial stress are not new and were initially introduced by Gibbs (1928). In this paradigm, the surface contributions to the thermodynamic quantities are defined as the excesses over the values that would be obtained if the bulk phases retained their properties constant up to a two-dimensional imaginary dividing surface embedded in a three-dimensional continuum. In other words, the interface (not interphase) is a mathematical surface of zero thickness over which the thermodynamic properties change discontinuously from one bulk phase to the other. The excess amount is associated only with the dividing surface. This Gibbsian conceptual approach has been widely studied in the fields of physics and chemistry (Shuttleworth, 1950; Herring, 1951; Vermaak et al., 1968; Gurtin and Murdoch, 1975; Cahn and Larché, 1982; Nozières and Wolf, 1988; Cammarata and Sieradzki, 1994; Cammarata, 1994, 1997; Steigmann and Ogden, 1997; Gurtin et al., 1998; Nix and Gao, 1998; Cammarata et al., 2000; Sander, 2003; Müller and Saúl, 2004; Dingreville and Qu, 2008; Marichev, 2011; Mi and Kouris, 2014). Despite minor differences in the formulations, all interfacial models consist of the definition of an interfacial strain and the definition of an interfacial constitutive behavior linking the interfacial strain to the interface excess stress (also commonly called “*surface stress*”). Apart from a few exceptions, theories based on such two-dimensional framework cannot account for the flexural stiffness (Nozières and Wolf, 1988; Steigmann and Ogden, 1997, 1999; Gao et al., 2014) nor can they describe the transverse behavior of real material interfaces or account for the interfacial mismatch. Fairly recently, for a coherent interface in an elastic solid, the so-called Shuttleworth or Shuttleworth–Herring relation (Shuttleworth, 1950; Herring, 1951) relating the interfacial excess energy Γ to the surface stress Σ^S has been generalized by Dingreville and Qu (2008) to account for the three-dimensional nature of the interface in a Gibbsian context such that

$$\Sigma^S = \left. \frac{\partial \Gamma}{\partial \epsilon^S} \right|_{\sigma^\perp} + \sigma^\perp \cdot \underline{\underline{H}}, \quad (1)$$

where the surface stress Σ^S is not only a function of the interface in-plane strain ϵ^S (which is the case in the original Shuttleworth relation) but also a function of the transverse stress σ^\perp . The third-order interfacial tensor $\underline{\underline{H}}$ measures the inherent Poisson’s effect in the transverse direction of the interface. However, in the case of a semi-coherent or a incoherent interface, as discussed by Cahn and Larché (1982), it is necessary to define two strain and stress measures to describe the general deformation at the interface, rendering Eq. (1) inadequate since both phases can in principle be stretched independently along the interface.

The present work proposes the use of the Gibbs dividing surface thermodynamic framework to develop generalized expressions for interfacial excess stresses and interfacial excess energy and to account for their variations with respect to the in-plane surface strain, the transverse stress and the interface mismatch strain. Our goal is to unambiguously define interface stresses and the interfacial excess strain in order to understand the connection between the interface thermodynamic quantities and the interface kinetic quantities to arrive at a generalized Shuttleworth relation for mismatched interfaces. In essence, our approach is close to that of Cahn and Larché (1982); in fact, we mostly render their formulation more general and systematic.

The paper is organized as follows. Section 2 starts with the definitions of the interfacial kinematics. In Sections 3 and 4, we propose a generalized formulation of the Shuttleworth relationship when a structural mismatch is present at the interface. Explicit expressions of the interfacial tensors are derived in the special case of an incoherent interface between two dissimilar isotropic solids. The connection between the structural mismatch and elastic properties of interfaces is

Download English Version:

<https://daneshyari.com/en/article/7178173>

Download Persian Version:

<https://daneshyari.com/article/7178173>

[Daneshyari.com](https://daneshyari.com)