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Mechano-chemical coupling in the adhesion of thin-shell structures

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ABSTRACT

Nonlinear coupling between mechanical and chemical fields at material interfaces can result in complex phenomena that include segregation-driven interface strengthening or weakening and bistability. Spatial nonuniformity of those fields is driven by elastic stresses that develop in the conforming bodies and from surface topography that is the result of patterning or inherent roughness. In this paper, equilibrium states are analyzed as a function of geometrical, material, and chemical properties to understand coupling mechanisms that impact interface strength. In particular, a theoretical model is presented for the finite deformations of a shallow spherical cap adhering to a rigid substrate that is either flat or has topography. The adhesive interactions are taken to be a continuous function of the local shell–substrate separation and the local concentrations of strengthening or weakening chemical species. Equilibrium states characterized by contact radii and energies are presented as a function of the average concentration of surface species (closed system) and the ambient chemical potential (open system). Bistable equilibria, snap transitions, and nonuniform energy, traction, and concentration fields are salient features of the numerical solutions. Interface separation under edge loading conditions is also investigated to determine the geometrical, material, chemical, and rate of the pull-off load and the work of separation. Additionally, adhesion to substrates with sinusoidal topography is analyzed to investigate the impact of patterning or inherent roughness. Important predictions of the later analysis are topography-induced segregation patterns and bistability.

1. Introduction

Adhesion is a complex process that involves nonlinear coupling between mechanical and chemical fields, in addition to physical forces that bridge from the molecular to continuum scale. Nonconforming geometries and surface dissimilarities both contribute to the development of elastic restoring forces that balance adhesive tractions acting between the bodies. Surface dissimilarities arise due to roughness, waviness, patterning, and crystal orientations. Thin elastic bodies are prone to puckering, wrinkling, and other buckling-type phenomena, which further complicate adhesion analyses of these structures. For geometries with dimensions approaching the micrometer and nanometer size, the finite range of the adhesive interactions and the surface topography can have a significant influence on the bulk deformations of the bodies. Additionally, chemical processes, e.g. segregation of species, can result in nonuniform adhesive properties that influence the overall adhesive state. Interplay between these competing effects is particularly of interest in wafer bonding (Conrad et al., 1996; Turner and Spearing, 2002; Christiansen et al., 2006; Reiche, 2006), in design of microelectronic devices

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(Maboudian and Howe, 1997), adhesion of microcapsules (Graf et al., 2006), and in biological cell adhesion (Sackmann and Bruinsma, 2002; Freund and Lin, 2004; Lim and Donahue, 2007).

The mechano-chemical coupling between nonuniform mechanical and chemical fields is investigated theoretically in this paper over a wide range of geometrical and material parameters. Finite shell deformations, finite-range adhesive tractions, and effects of chemical segregation are considered. In particular, the model system is comprised of a shallow spherical cap that interacts adhesively with a rigid substrate in the presence of strengthening and weakening mobile chemical species. Both closed and open chemical systems are considered. The adhering surface of the shell is taken to have a free energy that depends on temperature, local chemical concentrations, and the local shell–substrate separation. The adhesive tractions and chemical potential, which are defined from an interfacial free energy, enter the governing equations for mechanical and chemical equilibria, respectively. Axisymmetric shell deformations are studied using nonlinear shallow-shell equations that account for finite shell kinematics (Reissner, 1958; Budiansky, 1959; Sanders, 1963; Budiansky, 1968). These equations are known to predict snap and buckling phenomena that result from finite, elastic deformations (Koiter, 1967; Thompson and Hunt, 1973; Budiansky, 1974; Springman and Bassani, 2008). For flat plates and shallow caps, these nonlinear effects are generally important once the maximum normal displacement approaches half the shell thickness (Levy, 1949; Reissner, 1958; Springman and Bassani, 2008).

In addition to more traditional engineering applications, the current model may be adapted to explain the *initial stages* in the adhesion of biological cells (Dobereiner et al., 2004; Dubin-Thaler et al., 2004; Reinhart-King et al., 2005; Sengupta et al., 2006), which are known to be dominated by *passive driving forces* such as elastic restoring forces and adhesive interactions (Sackmann and Bruinsma, 2002; Pierres et al., 2003; Sengupta et al., 2006). In this context, the geometrical and material properties of the shell are taken to represent the effective properties of the lipid membrane and attached protein networks. The later stages of adhesion may be dominated by cytoskeleton reorganization and *active* myosin-driven force generation, in which case the mechanical properties are time varying. An important note is that, unlike isolated fluid lipid membranes, the cell membranes of eukaryotic cells are reinforced by an attached actin cortex (Boulbitch et al., 2000; Lang et al., 2000; Alberts et al., 2002; Pesen and Hoh, 2005) and other protein networks (Alberts et al., 2002), which provide resistance against shearing deformations.

A thorough study of a deformable elastic cap adhering to a rigid substrate under the action of a finite-range adhesive potential has recently been published (Springman and Bassani, 2008). Snap transitions between curved and flat configurations are predicted as a function of geometrical and material properties in that analysis. In particular, the ratio between characteristic measures of the adhesive and elastic energies is found to play a prominent role. Additionally, findings from that investigation demonstrate that: (i) Griffith-type assumptions for adhesive interactions break down for weak adhesion (small contact area) or for long-range interactions, (ii) linear kinematics break down for large curvatures and strong interactions, and (iii) the pull-off load and work of separation depend strongly on the type of loading and the stored elastic energy in the adhered state, particularly for large curvature shells undergoing finite deformations.

Building on Springman and Bassani (2008) the analysis in this paper investigates: (i) the influence of chemical segregation on the bistable solution regimes predicted for uniform adhesive properties, (ii) the dependence of the pull-off load and the work of separation on species redistribution, and (iii) the emergence of segregation patterns and bistable equilibria that result from substrate topography. The remainder of this introduction highlights related studies on various aspects of this complete analysis. In general, very few studies to date have considered the full coupling of finite deformations and chemically dependent adhesive interactions, particularly over wide parameter ranges that include bistable regimes.

Most prior *shell* adhesion studies adopt an adhesive contact potential, which assumes that the total adhesive energy is proportional to the area of a perfectly bonded interfacial region (Turner and Spearing, 2002; Graf et al., 2006), analogous to Griffith's treatment of brittle fracture (Griffith, 1920) and studies of adhesive contact (e.g. see Greenwood, 1997, or Maugis, 2000, for review). Similarly, adhesive contact potentials are the standard approach to study adhesion of lipid vesicle that deform according to Helfrich vesicle theory (Helfrich, 1973; Seifert and Lipowsky, 1990; Lipowsky, 1991; Sackmann and Bruinsma, 2002), as opposed to classical shell theory. An important study of this nature by Freund and Lin (2004) addresses the dynamics of segregation-driven adhesion in 1D using linear bending theory and an adhesive contact potential.

Finite-range adhesive potentials have been used in several prior studies of shell and membrane adhesion that are similar to the phenomenological descriptions adopted in this paper. Notable investigations include the use of finite-range adhesive potentials to study adhesion of lipid vesicles (Seifert, 1991) and a tethered spring network used to model an elastic shell (Tamura et al., 2004; Komura et al., 2005), both of which are discussed briefly in Springman and Bassani (2008). Additionally, a finite-range, double-welled adhesive potential has been used to identify nucleation criteria for adhesion of a Helfrich membrane with flat reference geometry and fixed edges (Zhang and Wang, 2008). Adhesion of a hyperelastic vesicle containing a liquid of fixed volume has been studied using finite-element methods in conjunction with a finite-range and chemistry-dependent adhesion law (Zhang et al., 2007).

There have been numerous studies of interfacial chemical processes that neglect deformations of the adhering bodies, and these are limited cases that may apply locally to processes of detachment or pull-off considered in this paper. For example, thermodynamic models have been used to investigate impurity-driven embrittlement of flat interfaces under uniformly applied load (Hirth and Rice, 1980; Mishin et al., 2002). Separation between a rigid sphere and rigid plate has been investigated by considering the dynamics of receptor and ligand cross-bridging (Vijayendran et al., 1998). Recently,