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## Snap transitions in adhesion

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## Abstract

Equilibrium adhesion states are analyzed for nonlinear spherical caps adhered to a rigid substrate under the influence of adhesive tractions that depend on the local separation between the shell and substrate. Transitions between bistable snapped-in and snapped-out configurations are predicted as a function of four nondimensional parameters representing the adhesive energy, the undeformed shell curvature, the range of the adhesive interactions, and the magnitude of an externally applied load. Nonuniform energy and traction fields associated with free-edge boundary conditions are calculated to better understand localized phenomena such as the diffusion of impurities into a bonded interface and the diffusion of receptors in the cell membrane. The linear Griffith approximations commonly used in the literature are shown to be limited to shells with a small height to thickness ratio and short-range adhesive and elastic energies. An important implication of the latter analysis is the theoretical prediction of the pull-off force, which is shown to depend not only on the interface properties, but also on the geometric and material parameters of the shell and on both the magnitude and type of external loading.

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## 1. Introduction

The adhesion of thin shell structures either to other shells or to substrates plays an important role in many micro- and nano-mechanical systems in engineering and biology. Geometric nonlinearities associated with finite shell deformations and the highly nonlinear nature of the adhesive interactions complicates our understanding of these important systems. In this paper bistable (static) equilibrium states are studied to develop a more fundamental understanding of nonuniform adhesion. Specifically, this paper investigates the adhesion of spherical caps interacting nonlinearly with a rigid substrate through an adhesion law that is derived from Lennard–Jones interactions. Bulk adhesion parameters are described that represent the strength and range of the adhesive forces. These parameters are taken to describe the cumulative interactions between the surfaces, including electrostatic forces, Van der Waals forces, steric repulsion, and the specific forces of fixed surface groups. Theoretical (Muller et al., 1983; Israelachvilli and Jacob, 1985; Maugis, 2000) and

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experimental (Israelachvili and Tabor, 1972; Klein, 1982; Leckband et al., 1992, 1994; Wong et al., 1997; Leckband and Israelachvili, 2001) support for the adopted adhesion law is available in the literature.

Nonlinear shallow shell theory is used to study the elastic deformations of the shell structures (Reissner, 1950; Budiansky, 1959; Sanders, 1963; Niordson, 1985). An important implication of the free-edge boundary conditions considered in this analysis is the inadmissibility of perfectly bonded configurations, which also are excluded by compatibility in the case of closed vessels. The coupling between shell bending and stretching, as captured with nonlinear shallow shell theory, is shown to play a particularly important role in adhesion, which typically involves the deformation of curved shell surfaces into nearly planar configurations. Such configurations cannot be achieved with a length preserving (isometric) mapping when the undeformed shell surface has a nonzero Gaussian curvature (Stoker, 1969). Nonlinear effects associated with this coupling are important once the magnitude of the normal displacement approaches half the shell thickness (Reissner, 1950), which can occur for adhesion if the reference shell height is greater than or equal to the shell thickness.

The vast majority of prior work on the adhesion of elastic bodies assumes the adhesive energy of the system is directly proportional to the area of an ideally bonded region (Seifert, 1991; Mastragelo and Hsu, 1993a, b; Sackmann and Bruinsma, 2002; Turner and Spearing, 2002; Freund and Yuan, 2004; Graf et al., 2006). Since this is analogous to the approach taken by Griffith in studies of brittle fracture (Griffith, 1921), this estimate of the adhesive energy is referred to as a Griffith approximation. Kinematical conditions on the displacement field required to ensure compatibility between the bonded and unbonded surface regions result in a separation profile with discontinuous derivatives of second order and higher at the adhesion front, which implies a jump in bending-moment that has not been justified physically. Several steps have been taken to treat the adhesive energy in a more general way. For example, Seifert (1991) studied the adhesion of inextensible, two-dimensional (cylindrical) membranes to a rigid half-space by minimizing the sum of the Helfrich bending energy (Helfrich, 1973) and the adhesive energy. In that work the adhesive energy is treated both by Griffith approximations and by considering a finite range adhesive potential that has a dependence on the local separation between the membrane and half-space. In the limit of short-range interactions and moderate to large adhesive energy, the computed vesicle shapes of both formulations agree well. More recently, Komura et al. (2005) modeled a spherical shell as a network of tethered springs and determined adhered states by minimizing a discrete energy functional that includes stretching of the springs, an approximate description of bending resistance, and an adhesive potential that depends on the local separation between the nodal points and a rigid half-space (Tamura et al., 2004). In addition, they use that analysis to infer continuum properties by comparison with *linear* measures of strain. Unlike these prior works, the analysis in this paper accounts for nonlinear coupling between the bending and stretching deformations of a continuum shell and finite-range adhesion interactions.

Shell analysis is applicable to wafer bonding, the adhesion of metallic nanocaps (Love et al., 2002; Charnay et al., 2003; Chen et al., 2004), the adhesion of lipid vesicles with finite shear resistance (Evans and Skalak, 1980; Secomb, 1988; Boal, 2002), in micro-mechanical structures (Maboudian and Howe, 1997), and to approximately model the adhesion induced deformation of biological cells. In the latter case, it is important to note that the cell membranes of eukaryotic cells are stiffened by transmembrane proteins and are supported by a filamentous structure called the actin cortex (Boulbitch et al., 2000; Lang et al., 2000; Pesen and Hoh, 2005), while different structures support the membranes of prokaryotic cells (e.g. bacteria) (Boal, 2002). Therefore, in the context of living cells the shell structural and material properties should be associated with the effective behavior of the cell membrane and attached protein networks. Force generation associated with active structural reorganization (Dobereiner et al., 2004; Reinhart-King et al., 2005) accompanies the adhesion of many living cells over long time periods, which may limit the applicability of elastic analyses in studies of these cell types. However, the initial stages of adhesion that occur without structural reorganization are important in their own right. In particular, the traction forces exerted during initial contact are believed to trigger the assembly of focal adhesion complexes, which in turn initiate the mechanical signals required for actin polymerization and myosin driven contraction (Galbraith et al., 2002). Furthermore, the nonuniform distributions of adhesive energy and tractions presented in this paper are a general characteristic of adhesion whenever the interacting surfaces are not perfectly bonded over their entire domain.

Although the mechano-chemical coupling that occurs in the presence of mobile chemical species is not explicitly considered in this analysis, the presented results have some general implications for the coupled system. Most notably, the spatially nonuniform energy fields that are a feature of mechanical equilibrium also

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