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Evaluation of adhesion in microsystems using equivalent rough surfaces modeled with spherical caps

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ABSTRACT

The correct evaluation of adhesion energy is a challenging task and even more difficulties are found when dealing with real-life surfaces in Micro-Electro-Mechanical Systems (MEMS). In this paper, we devise an effective tool for such a computation, on the basis of an innovative, yet simple, geometrical model for the description of rough surfaces by means of spherical caps. A mechanical model is devised for the adhesive contact of spherical surfaces: the model accounts for the presence of elastic and plastic deformation and introduces the effects of both van der Waals forces and capillary attraction. The correctness of the geometrical description has been checked with reference to several measurements on realistic surfaces. The obtained results, in terms of adhesion energy, have been compared with experimental data, which are available in the literature. The agreement between measurements and numerical outcomes is satisfactory and by far better than for previously proposed models.

1. Introduction

The reliability of microsystems (or Micro-Electro-Mechanical Systems (MEMS)) is a topic of paramount importance for technological advances: proper design and fabrication of micro-devices must ensure the perfect functioning both in standard exercise conditions and in extreme situations (e.g. accidental drop, mechanical and electrical shock, harsh environment, etc.). Among the various dangerous situations, spontaneous adhesion can seriously jeopardize the reliability of micro-electro-mechanical systems. In view of the high surface-to-volume ratio of MEMS, the adhesive forces between parts in contact may exceed the elastic restoring force: in this case, the components remain stuck to each other and the micro-machine could be completely unusable. The aforementioned scenario is often addressed to in the literature as “stiction failure”, where the word “stiction” is a neologism coined from “static friction”.

A large part of the available literature on stiction is devoted to experimental investigations. DelRio et al. (2005), DelRio et al. (2007), de Boer (2007) have developed a reliable procedure to correlate, through a fracture mechanics methodology, the interferometric measurement of the detached length in cantilevers to the adhesive surface energy. Bachmann et al. (2006) approached the problem in a different way, by performing pull-in tests on silicon suspended discs. Recently in Basu et al. (2007), the pull-out behavior has been exploited for an indirect measurement of adhesive forces through optical and electrostatic data.

Many efforts have been also devoted to the computational prediction of adhesion. It has been shown in Cho and Park (2004) that the problem of adhesive spheres could be solved in a genuine Finite Element (FE) environment, by modeling the elastic parts through conventional finite elements and performing a contact analysis. More recently in Sauer (2010), the Lennard-Jones interatomic potential has been used in FE analysis to obtain an innovative formulation of frictionless contact problem. The stochastic nature of the actual rough surface has been considered in many papers, most of which, see e.g. Hariri et al. (2007), are based on simplified models of elastic–plastic deformation. In Wu et al. (2011) a multi-scale approach has been considered for adhesion in dry conditions. In van Spengen et al. (2002) a simpler model has been adopted, in the sense that rigid-plastic behavior of asperities has been considered and that adhesive forces have been estimated on the basis of the average surface separation.

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DelRio et al. (2008) have presented a comprehensive numerical procedure in which the two surfaces are represented as a plane contacting a collection of spherical surfaces with an equivalent Gaussian height distribution. They extended previous models to explore the effects of surface topographical correlations, plasticity and disjoining pressure on the capillary adhesion due to adsorbed water layers. In particular the presence of adsorbed water layers on the hydrophilic polysilicon surfaces only slightly modifies the asperity geometry but seems to have an important role in the capillary adhesion process which is highly sensitive to the form of asperities.

The previous research of our group in the field of adhesion phenomena in MEMS has been devoted to the development of refined computational tools to obtain a realistic estimate of adhesion energy in different conditions and their experimental validation. In Ardito et al. (2013b) representative areas of the two contacting rough surfaces have been numerically reproduced respecting as closely as possible the statistical properties of the real geometry. We have considered a non-linear finite element model, enriched by the presence of adhesive forces. Among the various causes of adhesion, we have considered the van der Waals and capillary forces, which are prevalent in the typical applications of MEMS. Some encouraging results have been obtained, showing good agreement with previous experimental data. New experiments have been conceived in Ardito et al. (2013a), in order to obtain an autonomous measure of adhesion energy.

One of the major issue of the procedure proposed in Ardito et al. (2013b) was the computational burden, which impeded the study of significant portions of the rough surface. Moreover, simplified techniques like the Proximity Force Approximation – PFA, seems to be mandatory for computing adhesive forces between generic surfaces. For instance, even though in Ardito et al. (2014) a full FEM procedure has been developed for the simulation of meniscus formation between arbitrary asperities, this can be hardly applied to realistic surfaces with many asperities.

Therefore, we started the development of a simplified method in which the roughness of both surfaces is modeled with spherical asperities, with the aim of exploiting known accurate (or even exact) results for adhesive forces between spherical caps, like the "neck" or "gorge" type of approximation (Lian et al., 1993, Willett et al., 2000) for capillary forces. In the present paper a new algorithm is proposed to obtain an equivalent surface made of spherical caps with the same statistical properties of the real situation. A further advantage of using spherical caps is represented by the possibility to apply analytical formulae in order to simulate the mechanical behaviour of asperities. In this way, we develop a new simulation procedure, which combines the elastic–plastic deformation of the asperities and the formulae that represent the adhesive behavior. The proposed procedure allows us to obtain the traction–separation curve, even for large portions of the rough surfaces, with a negligible computational effort.

The paper is organized as follows. First, the models for adhesive forces between spherical caps are presented. In the subsequent section, we consider the analytical formulae for elastic–plastic contact and their modifications in order to include the adhesive effects. Then, the algorithm for achieving the equivalent rough surface is delineated, with emphasis on some examples and on the assessment of statistical significance. We put everything together to obtain the adhesion energy, via integration of the traction–separation curves. Numerical results compare well to experimental outcomes, with encouraging perspectives. In the conclusive section, we discuss the approximations involved in the procedure.

2. Simplified model for adhesion forces between spherical particles

Adhesion between surfaces is a complex phenomenon, which is caused by several physical and chemical interactions and depends on several features of the problem at hand. In the present paper, we focus on the most important attractive forces for the case of MEMS surfaces: van der Waals attraction and capillary effect. It is worth noting that there are other sources of adhesion, such as parasitic electrostatic forces (van Spengen et al., 2004) and hydrogen bonding (Legtenberg et al., 1994). The presented model could be easily extended to encompass such additional forces, if necessary for the specific problem.

In the next two sub-sections, we propose a short summary of the basic features for van der Waals forces and capillary effect, with the aim of providing a sound basis for the approximate formulae which will be used in the computation of the adhesive force.

2.1. Van der Waals forces

Van der Waals forces represent the main source of attraction between non-polar atoms or molecules, in the absence of chemical bonds. The essential aspect of van der Waals forces can be summarized as follows: effectiveness from interatomic spacing (more or less 0.2 nm) up to distances of the order of 10 nm; change of sign depending on the material properties (usually attractive force, but can change in repulsive); anisotropic behavior in some cases of interactions; "non-additivity", due to the fact that the dispersion force between two atoms is affected by the presence of a third atom.

In spite of the last observation (see comments in Israelachvili (2011)), the van der Waals force is usually computed by simple integration of the atom-to-atom potential, which depends on the distance d between the atoms (or molecules) and is governed by the Hamaker constant A. In the case of silicon one finds $A \approx 27 \cdot 10^{-20}$ J. An interesting representation of the atom-to-atom interactions can be obtained by using the Lennard-Jones potential (Jones, 1924), which captures the mild attraction ($6th$ power) of surfaces as they approach one another and the strong repulsion ($12th$ power), or steric forces, when they come too close to one another.

The distributed force consequent to van der Waals interactions can be computed in the framework of the so-called *Proximity Force Approximation* (PFA) (DelRio et al., 2005). Each point on a surface is endowed with a portion of area and interacts with a corresponding point on the opposite surface. The van der Waals force is then computed by introducing the following load per unit surface (based on Lennard-Jones potential) on the portion of surface connected to each point

$$q_{vdW}(\rho) = \frac{A g_f}{6\pi [d(\rho) + d_0]^3} \left[\left(\frac{d_0}{d(\rho) + d_0} \right)^6 - 1 \right] \tag{1}$$

where ρ is the lateral position on the surface, d_0 is the equilibrium separation, which for silicon reads $d_0 = 0.149$ nm, and g_f is a function based on the separation distance that describes the transition between normal and retarded vdW attraction (Anandarajah and Chen, 1995). The overall force is obtained by a summation of the contributions provided by all the points, given by q_{vdW} multiplied by the surface connected to the points.

The PFA is widely accepted for van der Waals interactions in the case of surfaces with arbitrary morphology: if a mathematical description of the surface roughness is available, the overall force is obtained by a suitable discretization and by the computation of the