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Invariant slow manifolds of an Atomic Force Microscope system under the effects of Lennard-Jones forces and a slow harmonic base motion

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ABSTRACT

We study the nonlinear vibrations of an AFM system, modeled as a linear mass-spring-damper system, under the Lennard-Jones forces and an imposed harmonic base displacement. The frequency of this latter is very low with respect to the natural fundamental frequency of the system. The invariant slow manifolds of the system are approximated and their bifurcations are investigated. It is shown that two dynamic saddle-node bifurcations, during one period of the base oscillation, of the contact and the noncontact invariant slow manifolds are responsible for triggering the tapping mode. It is also shown that these dynamic bifurcations govern the contact time between the probe and the sample during the tapping mode.

1. Introduction

The Atomic Force Microscope (AFM) [1] is one of the scanning probe microscopes. It is a nano-scale tool for manipulation and characterization in nanosciences. An AFM can be employed in a broad spectrum of applications such as imaging, nanolithography, electronics, semi-conductors, materials, manufacturing, polymers, chemical and biological analysis, see for instance [2,3] for more applications. Atomic force microscopy is based mainly on a vibrating microcantilever with a nano-scale tip that interacts with a sample surface via short- and long-range intermolecular forces. An enhanced understanding of these vibrations is central to the correct interpretation of the AFM outputs. Indeed, different intermolecular, surface and macroscopic effects give rise to interactions with distinctive distance dependencies. In the absence of external fields, the dominant forces are van der Waals interactions, short-range repulsive interactions, adhesion and capillarity forces [4]. In the present paper, a Lennard-Jones force is used to model the tip-surface highly nonlinear interactions and a linear lumped-parameters model is used to model the cantilever.

The nonlinear dynamics of single-degree-of-freedom system models under the Lennard-Jones (LJ) interactions and harmonic external and/or parametric forcings, mainly near the fundamental resonance, were investigated by many authors, see the review paper [5] and references therein. Sarid et al. [6] used a model with Lennard-Jones and repulsive indentation forces acting between tip and sample to determine numerically characteristics of the tapping mode. Ashhab et al. [7] used the Melnikov method to analytically determine chaotic behaviors when the mass is excited by a sinusoidal force. For the same system, Basso et al. [8] showed numerically that the main root to chaos is period doubling cascades. San Paulo and Garcia [9]

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showed, using the virial theorem, that the resonance curve is heavily distorted by the strength and character of the interaction forces. Indeed, attractive forces tend to pull the resonance curve to lower frequencies while repulsive forces drive the curve to higher frequencies. The competition between attractive and repulsive interactions may give rise to a multivalued resonance curve which implies the coexistence of several steady-state oscillations. Rützel et al. [10], studied a discretized model of a microcantilever subject to resonant harmonic base displacements. They showed, using mainly continuation techniques, that the forced periodic motions of the probe tip destabilize through a sequence of period-doubling bifurcations. Hu and Chen [11] investigated bifurcation diagrams and Poincaré sections, for a particular initial gap, in the case of one and two term truncation Galerkin method. Sasaki et al. [12] studied the dynamics of a mass spring system under two types of the tip-surface interactions: Lennard-Jones and the hard-wall potentials. They found various strange behaviors such as quasiperiodic oscillations, fractional resonance and the coexistence of the dynamic touching mode and the nontouching mode in the case of the hard-wall potential.

In addition to theoretical investigations, several experimental studies were conducted [13–17]. Gleyzes et al. [13] observed experimentally bistable behavior near the principal resonance of a vibrating tip close to a solid surface. This bistable behavior may lead to artifacts such as unpredictable jumps. These latter may cause problems when one tries to use a feedback loop to maintain the tip-surface interaction at a constant level and could complicate the acquisition and the interpretation of a topographic image. They concluded that the best solution to avoiding artifacts is to work at a frequency lower (respectively higher) than the resonance frequency for repulsive (attractive) forces. Burnham et al. [14] observed experimentally subharmonics and chaos in the dynamics of a micro-cantilever-tip sample interaction in tapping mode (in their experiment the sample was excited harmonically). Martin et al. [15] vibrated the tip at a resonant frequency and moved it repeatedly toward and away from the surface, at a low frequency. This technique allowed the simultaneous measurement of interaction forces and surface profile. Stark et al. [16] demonstrated experimentally that the transition from an oscillatory state dominated by a net attractive force to the state dominated by repulsive interactions is accompanied by the enhanced generation of higher harmonics. The higher harmonics are a consequence of the nonlinear interaction and are amplified to significant amplitudes by the eigenmodes of the cantilever. Haugstadt and Jones [17] showed, using heterogeneous films of polyvinyl alcohol, that when driving slightly below the free resonance frequency at moderate amplitudes, the tip-sample interaction jumps between non-contact and intermittent contact or tapping mode.

It is worth pointing out that the tapping mode AFM [18] was the dominant imaging mode for most scanning probe microscopes during the last decade. It is based mainly on resonant excitations of the cantilever with a feedback loop keeping the cantilever vibration amplitude constant. This mode minimizes the shear forces, present in the contact mode, that can be destructive to the tip and samples. It overcomes some deficiencies of the noncontact mode by improving the resolution and enabling the measurement of mechanical properties [19]. However, operating the cantilever near its resonances can cause complex dynamics due to the nonlinearities. As a remedy nonresonant tapping mode techniques are used. Thus, AFM with low frequency excitation compared to the fundamental natural frequency of the cantilever is used, for instance, in the pulsed-force mode AFM [20] and the peak-force AFM [21]. Indeed, the low frequency excitation leads to lower the tapping force causing limited tip-sample contact areas and minimizing the loss of resolution. Consequently, this mode is non-destructive to tips and samples, especially the biological ones. Moreover, it avoids complicated dynamics of the cantilever, likely to occur, near resonances. Marti et al. [22] used pulsed-force mode AFM to measure the nanomechanical properties of cancer cells. Heu et al. [23] used peak-force mode to study chemically induced changes in the cellular mechanical properties of a human epidermal cell line. Abadias et al. [24] applied the AFM in peak-force mode to obtain topographic and mechanical characteristics of Siloxane–Hydrogel soft contact lenses. The study was carried out in liquid using cantilevers of silicon nitride of low spring constant (0.1–1 Nm^{-1}) and of natural frequency in liquid between 2 and 20 kHz.

The present work is focused on the dynamics of an AFM system under Lennard-Jones forces and a very slow harmonic base displacement. Consequently, the system can be viewed as a fast-slow system with two time scales dynamics: one ruled by the natural frequency of the system and the other by the low frequency of the base displacement. We will show that solutions of the system follow the stable invariant slow manifolds. For more information on the fast-slow systems see for instance [25,26]. In fact, two stable invariant slow manifolds coexist, one corresponds to the contact mode and the other to the noncontact mode. These two stable slow manifolds undergo dynamic saddle-node bifurcations (through the collision with an unstable slow manifold) when the amplitude of the base displacement is varied. These dynamic bifurcations rule the operational mode of the AFM: contact, noncontact and tapping modes, respectively.

The present paper is organized as follows: in Section 2 the problem is formulated and changes of variables are performed to apply the theory of slow manifolds. Then, investigations of the static equilibria and the corresponding natural frequencies are performed. In Section 3, The slow manifolds are determined and the dynamics of the forced vibrations are studied. The conditions of existence of the tapping mode and the contact duration are determined.

2. Mathematical modelling

A single-degree-of-freedom model depicted in Fig. 1 is utilized to represent a lumped-parameters model of an Atomic Force Microscope. The cantilever-tip-sample interaction is modeled by a Lennard-Jones force F_{LJ} between a sphere and a flat surface [4,7]. In spite of its simplicity, this interaction model captures generic properties present in the near-field interactions [10,27]. The microcantilever is modeled as a sphere of radius R and mass m, its equivalent spring rigidity and viscous damping coefficient are denoted k and c, respectively. The base of the microcantilever is excited by a piezoelectric actuator generating a vertical