Modeling of Intrinsic Stress Effects in Deposited Thin Films

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Abstract: Simulation of intrinsic stress effects in deposited thin layers is an important aspect, especially for cantilever fabrication, because after removal of the sacrificial layer the intrinsic stress leads to an undesirable and uncontrolled deflection of the cantilever.

Keywords: Simulation, Intrinsic Stress in Thin Films, Cantilever

INTRODUCTION

Thin film deposition is a widely used technique for the fabrication of MEMS (Micro-Electro-Mechanical Systems) devices. This technique is required to manufacture free-standing structures which can induce or sense a mechanical movement. During the deposition of new thin layers an intrinsic stress is generated. After removal of the underlying sacrificial layer, the deposited layer which is an important component of the MEMS device, is left free-standing. As a consequence, the process induced stress can relax and deform the deposited layer in an undesirable way.

PHYSICAL ASPECTS

The investigation of stress effects in thin films is focused on the deposition of SiGe on sacrificial layers. In the first phase of this process, islands with varying crystal orientation are formed and grow isotropically. The radial growth of the material islands mainly depends on the Si-Ge ratio, the substrate temperature, and the silane (SiH_4) and germane (GeH_4) flow. In the course of further deposition these islands start to coalescence, which forces the islands to grow in the height instead in a direction parallel to the substrate surface. The islands are consequentially transformed from an island shape to a grain-like shape. The orientation of the crystal structure in a single grain is independent of its neighbors. Due to the amorphous substrate, it is not possible to evolve a perfect crystal structure in the first atom layers [1]. Another aspect is that the deposition takes place at elevated temperatures. When the temperature decreases to room temperature, the volumes of the grains decrease and the stresses at the grain boundaries increase. The main sources of intrinsic stresses are [2, 3]: coalescence of the grain boundaries, misfit stresses, rearrangement of the atoms, grain growth, and annihilation of excess vacancies. Different process conditions and physical phenomena make it convenient to describe the previously described sources of stress in *initial mode* and *transient mode* microstructure models. The initial mode of the thin film growth model considers development of the first grain layer (see Figure 1). The dominant stress components in this case are caused by coalescence of the grain boundaries and misfit stresses. As transient mode we consider a situation where more than one grain layer is deposited (see Figure 2). The stress build-up in the transient mode is caused by the grain growth and non-equilibrium vacancy dynamics. We use predictions of a level set based simulation [4] to obtain the grain size distribution from the bottom to the top of a polycrystalline film.

MODELING AND SIMULATION

The goal of this work is the integration of microstructure models which describe strain development due to grain dynamics in a macroscopic mechanical formulation. This strain loads the mechanical problem which provides a distribution of the mechanical stress and enables the calculation of displacements in the MEMS structure. The approach developed in this work is applied to the experimental setting presented in [5]. In this experiment a 10 μm thick SiGe film was deposited on an oxide sacrificial layer. After removal of this sacrificial layer the deflection of the free 1 mm long cantilever was measured at different thicknesses down to 1 μm. The smaller thicknesses were made by thinning. It was observed that the deflection increases exponentially with reduced thicknesses. The intrinsic strain curve for this film (see Figure 3), which is qualitatively predicted by the model, was calibrated according to measurement results. The highest strain (gradient) is at the bottom of the film which explains the very large deflections for thin cantilevers under the aspect that the elastic line, which is located in midway, is moving with the cantilever thickness. This strain curve was used to simulate the cantilever deflections for various thicknesses. The simulated cantilever deflections show good agreement with the experimentally determined deflections (see Figure 4). Figure 5 presents the results of the three-dimensional cantilever deflection simulation without thinning. The deposited thin film with the intrinsic stress is presented in Figure 5a. The distribution of the peak stress values is displayed by the red areas. After removing the sacrificial layer, the cantilever is released (Figure 5b) and the stress can relax by deflection of the free standing cantilever. Therefore the high stress areas are reduced.

ACKNOWLEDGMENT

This work has been supported by the European Community *PROMENADE* IST-2002-2.3.1.2 project.

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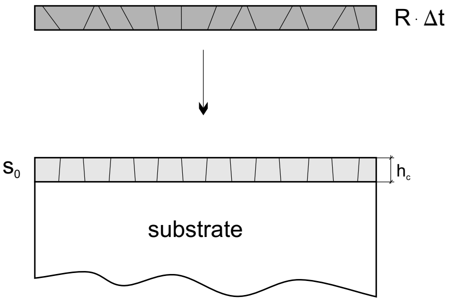

Figure 1: Initial mode. R is the deposition rate and h_c the film thickness immediate after grain formation.

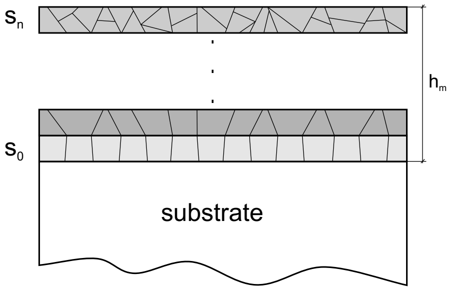

Figure 2: Grains formed in the initial mode continue development in transient mode.

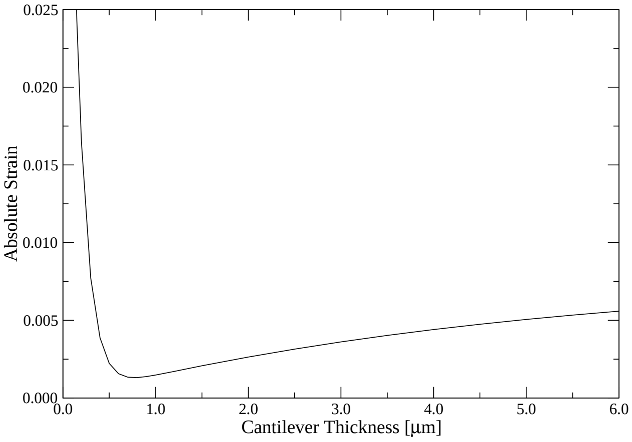

Figure 3: The run of strain curve through the thickness of the deposited thin film.

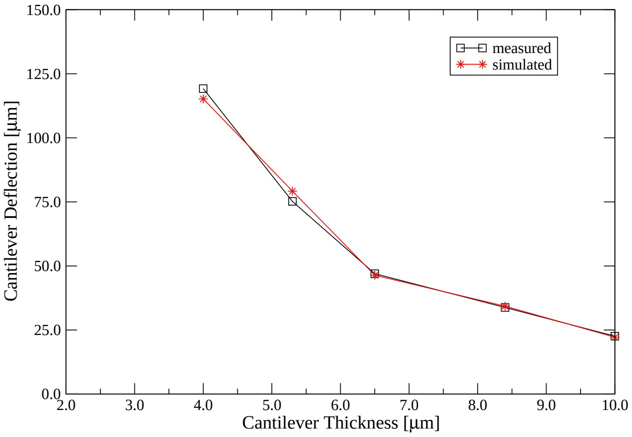

Figure 4: Comparison between the measured and the simulated cantilever deflections for different thicknesses.

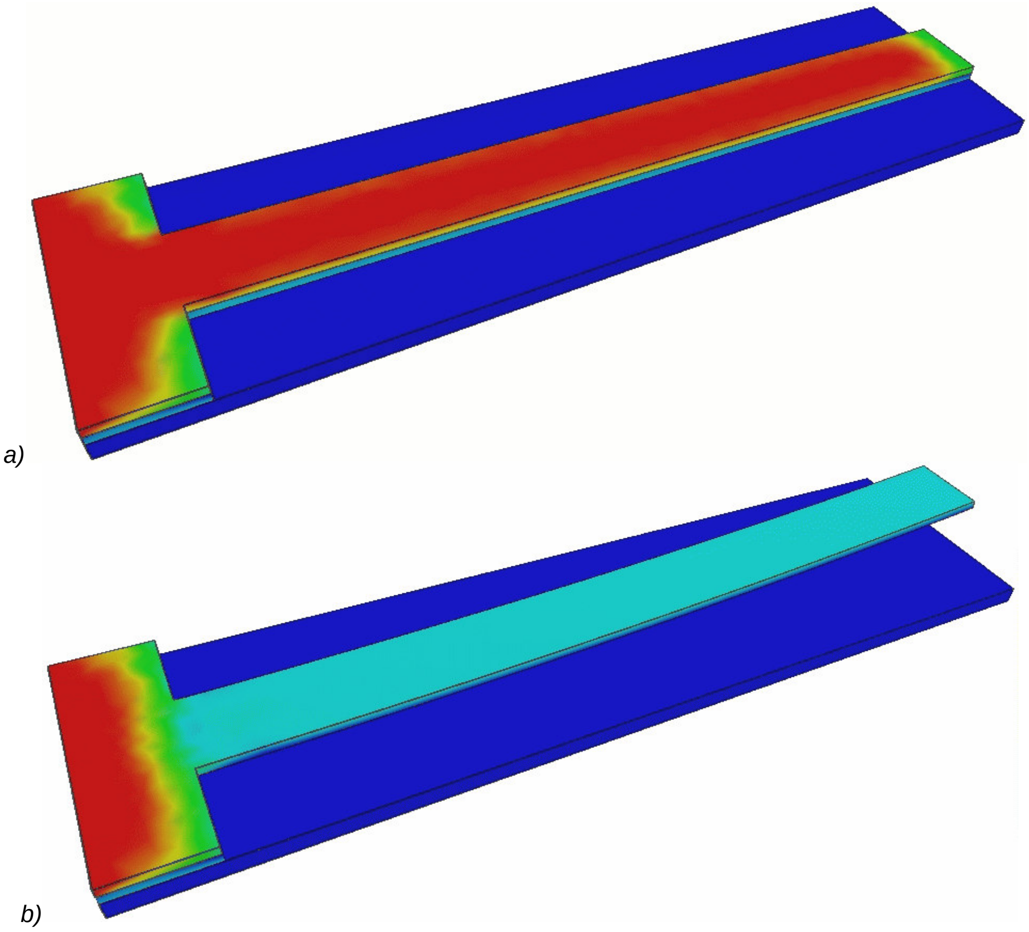

Figure 5: Stress distribution for the fixed a) and released b) 1 mm long cantilever. High stress areas are marked with red color. The build-up of intrinsic stresses induces the cantilever deflection.