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Investigation of Intrinsic Stress Effects in Cantilever Structures

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***Abstract*— We present a method for the prediction of intrinsic stress in poly-SiGe thin films. The simulation of intrinsic stress effects in deposited thin film is an important issue, especially for the cantilever fabrication, because after removal of the sacrificial layer the intrinsic stress leads to an undesirable and uncontrolled deflection of the cantilever. The developed methodology to treat thin film stress is applied to analyze fabricated cantilever structures and the simulation results are compared with experiments.**

INTRODUCTION

Thin film deposition is a widely used technique for the fabrication of free-standing MEMS structures which can induce or sense a mechanical movement. During the deposition process of new thin layers and afterwards an intrinsic stress is generated. In subsequent process steps the underlying sacrificial layer is removed and the (stressed) deposited layer is left free-standing. As a consequence the process induced stress can relax and deform the deposited layer in an undesirable way.

Polycrystalline silicon-germanium (poly-SiGe) has been promoted as an attractive material suitable as structural layer for several MEMS applications [1]. Poly-SiGe is a good alternative to polycrystalline silicon (poly-Si), because it has similar properties. The same good mechanical and electrical properties can be obtained with poly-SiGe at much lower temperatures (down to 400 °C) as compared to poly-Si (above 800 °C). These low processing temperatures enable post-processing MEMS on the top of CMOS without significant changes in the existing CMOS fabrication processes. The sacrificial layer is usually made of silicon dioxide (SiO_2) (see Fig. 1), because this material can be etched with a high selectivity towards the structural layer by the use of hydrogen fluoride (HF).

Different aspects of the connection between microstructure and stress have been investigated in the past 30 years. The focus was mostly on some specific grain-grain boundary configurations in several stages of microstructure evolution [2]. As a result there are numerous models based on continuum mechanics, which are only applicable for simple situations. On the other hand side complex models for describing the morphology of microstructural evolution, which culminate in multi-level set models of grain evolution [3], have been developed. These models can reproduce the realistic grain boundary network in a high degree, but they do not include stress [4]. 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.

CANTILEVER DEFLECTION PROBLEM

The effects of intrinsic stress in free-standing MEMS structures can be demonstrated most plausibly with the cantilever deflection problem. Fig. 1 shows the schematic structure of a free-standing cantilever, where the SiGe structural layer is deposited on the SiO_2 sacrificial layer. In this case it is assumed that there is no stress gradient in the SiGe film, and so no deformation of the released cantilever occurs.

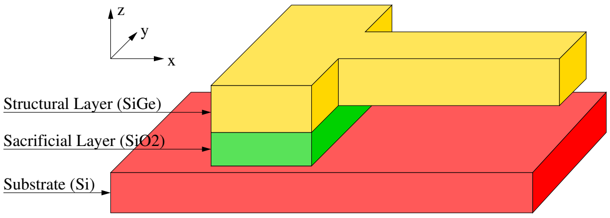

Fig. 1: Structure of a free-standing cantilever without stress gradient.

But in practice the structural layer can not be deposited stress free. Therefore, an unwanted deflection in the free-standing cantilever occurs. Such a deflection of a 400 μm long and 10 μm thick fabricated cantilever is shown in Fig. 2.

For an assumed linear stress gradient Γ over thickness and a rectangular cross-section of the beam (see Fig. 1), the deflection $\delta(x)$ at position x is

$$\delta(x) = \frac{Mx^2}{2EI} = \frac{\Gamma}{2E}x^2, \qquad (1)$$

where E is the Young modulus, M is the bending moment, and I is the moment of inertia. This means that for a constant Γ the deflection at the end of the cantilever ($x = l$) increases quadratically with length l.

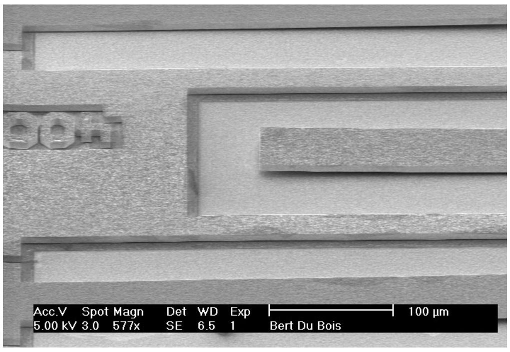

Fig. 2: Cantilever deflection.

The bending of the released cantilever depends on the stress distribution over the layer thickness before release. Fig. 3 shows three possible forms of stress distribution and gradients in the fixed cantilever in the left hand side and the corresponding direction of deflection in the right hand side. In this context only the stress above and under the neutral bending line is responsible for the direction of the deflection. The stress causes forces which result in the bending moments regarding

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the neutral bending line which is always located in the middle of the cantilever. If the sum of the moments under the neutral bending line is larger than the above one, the deflection is upward, otherwise downward.

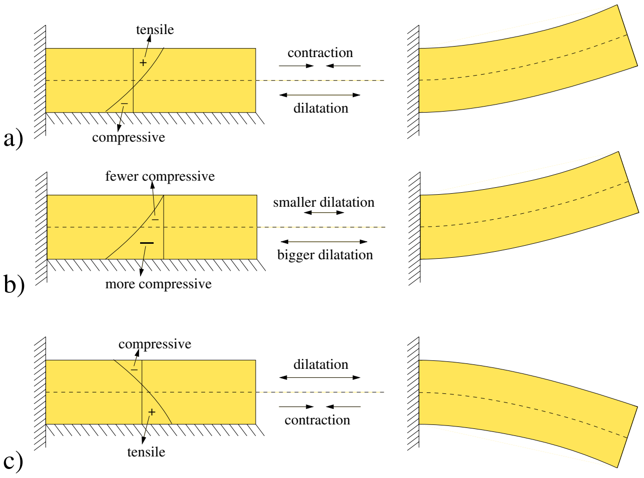

Fig. 3: Various stress distributions and gradients in the fixed cantilever and their regarding deflections after release.

INTRINSIC STRESS SOURCES

In the first phase of the SiGe deposition process, islands with varying crystal orientation are formed and grow isotropically. These individual islands which first form on a substrate usually exhibit compressive stress [5]. In the course of further deposition the 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 subsequently transformed from an island shape to a grain-like shape.

For the stress aspect the deposition process plays a key role. The stress gradient and the average stress in the SiGe film depend on the Si-Ge ratio which can be controlled by the silane (SiH_4) and germane (GeH_4) flow, the substrate temperature, and the deposition technique which is usually CVD (chemical vapor deposition) or PECVD (plasma enhanced CVD).

Beside the first formed islands, the intrinsic stress observed in thin films has the following main sources [2]:

- *Coalescence of Grain Boundaries:*

In the early stage of the film growth the individual grain islands grow until they make contact to adjacent islands. The isolated islands have a relatively high surface energy γ_s compared to the relatively low energy γ_i between the island interfaces. Therefore, the net free energy in the system can be reduced by replacing the surfaces by interfaces. If the gaps between the islands are small enough, cohesion begins to develop between the islands, and the system can lower its net free energy by closing up these gaps. In the course of zipping up the interfaces, the participating islands become elastically strained and a tensile stress is generated [6]. The average intrinsic stress caused by coalescence in the film with thickness h_c is

$$\sigma_{xx}^{\text{in}} = \sigma_{yy}^{\text{in}} = \frac{2\pi\gamma}{3h_c}, \qquad \sigma_{zz}^{\text{in}} = 0, \tag{2}$$

where γ is the surface energy of the contacting spheres.

- *Misfit Stress:*

Innately the lattice constants for the thin film a_s and the substrate a_f normally are different. Because of the deposition process the crystal lattice of the thin film and the substrate are forced to line up perfectly at the interface and stress arises. The influence of these misfit stresses is only significant in the initial phase of thin film deposition [7] because of the local lattice adaption at the interface area. The lattice adaption is characterized by the misfit parameter [8]

$$m = 2\frac{a_f - a_s}{a_f + a_s}, \tag{3}$$

The nonzero components of the misfit stress tensor are

$$\sigma_{xx}^{\text{in}} = \sigma_{yy}^{\text{in}} = \frac{E\,m}{1-\nu^2}, \qquad \sigma_{zz}^{in} = \nu\sigma_{xx}^{\text{in}}. \tag{4}$$

- *Grain Growth:*

Due to the elimination of grain boundaries a minimum in the total energy of the system can be obtained. So grain growth means that the volumes of the individual grains become larger and the number of grains and their boundaries decrease. Since grain boundaries are less dense than the grain lattice [9], the elimination of grain boundaries leads to a densification of the film and therefore to a build-up of tensile stress. The intrinsic tensile stress associated with the grain growth is

$$\sigma_{xx}^{\text{in}} = \sigma_{yy}^{\text{in}} = \sigma_{zz}^{\text{in}} = \frac{2E}{1-\nu}\Big(\frac{1}{L_1} - \frac{1}{L_2}\Big)\Delta a, \tag{5}$$

where Δa is the excess volume per unit area of the grain boundary. L_1 and L_2 are the the average grain diameters before and after grain growth.

- *Annihilation of Excess Vacancies:*

The annihilation and the dynamics of the crystal vacancies produce a local volume change which leads to stresses in the deposited film. When vacancies annihilate at a grain boundary there is a gap. In order to close the gap there is a motion of the crystals towards each other. This would produce a planar contraction of the film, if it is not attached to the substrate. Since the substrate prevents the contraction, a tensile stress is built-up [2], which is given by

$$\sigma_{xx}^{\text{in}} = \sigma_{yy}^{\text{in}} = \sigma_{zz}^{\text{in}} = \frac{E}{1-\nu}\frac{\Delta C_v(\Omega_a - \Omega_v)}{3}, \tag{6}$$

where Ω_v is the vacancy volume, Ω_a is the atomic volume and ΔC_v is the number of vacancies which annihilate per unit volume.

- *Insertion of Excess Atoms:*

It is assumend that the film growth process can add atoms to the film in two ways [10]. Most of the material is added on the top surface by traditional crystal growth mechanisms, where each layer of atoms is deposited onto the underlying crystalline lattice. The second mechanism is the insertion of excess atoms into the grain boundaries, which creates a compressive stress in the film [11].

$$\sigma_{xx}^{\text{in}} = \sigma_{yy}^{\text{in}} = \sigma_{zz}^{\text{in}} = \frac{E}{1-\nu}\frac{\Delta C_i\,\Omega_e}{3}, \tag{7}$$

where Ω_e is the excess atom volume and ΔC_i is the number of excess atoms which are inserted per unit volume.

- *Thermal Stress:*

This stress is caused by the different thermal expansion coefficients of the thin film and the substrate in case of a temperature change after deposition and the fact that at least always a part of the film's base area is attached to the substrate. Therefore thermal stress develops during cooling down to ambient temperature. The developed intrinsic stress due to thermal mismatch is

$$\sigma_{xx}^{\text{in}} = \sigma_{yy}^{\text{in}} = \sigma_{zz}^{\text{in}} = B\alpha(T - T_0), \tag{8}$$

where $B = (3\lambda + 2\mu)/3$ is the bulk modulus, α is the thermal expansion coefficient, and T_0 is the room temperature.

STRESS DISTRIBUTION AND RELAXATION

As example for a positive stress gradient in thin films (see Fig. 3a)), where only tensile stress was assumed, the stress distributions for a 1 mm long and 10 μm thick cantilever structure were simulated. As long as the cantilever is attached to the underlying SiO_2-layer, the deposited SiGe film is under stress and the cantilever can not deform. Due to the positive stress gradient the highest tensile stress, marked with red color, is on the top of the fixed cantilever as demonstrated in Fig. 4a).

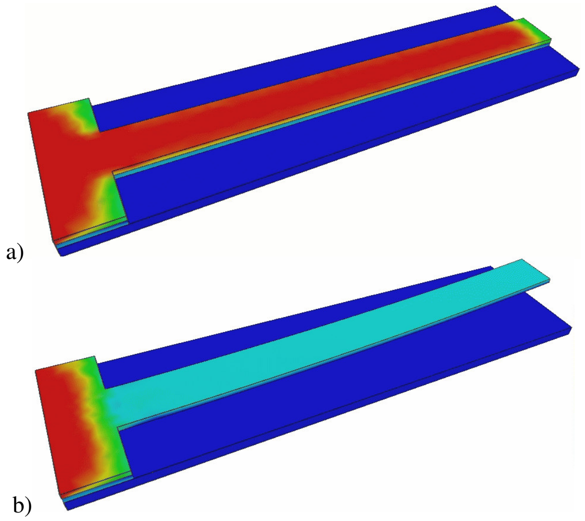

Fig. 4: Stress distribution for the fixed a) and released b) 1 mm long cantilever. High stress areas are marked with red color.

After removal of the sacrificial SiO_2-layer by etching, the SiGe beam is free standing. Now the cantilever can deform and the stress is relaxed, as shown in Fig. 4b). The intrinsic stress in the deposited SiGe layer is the driving force for the cantilever deflection.

MODELING AND SIMULATION

The developed methodology to treat thin film stress, which takes the different intrinsic stress sources into account, is applied to an experimental setting [12]. In this experiment a 10 μm thick multilayer SiGe film was deposited on an oxide sacrificial layer. Since the SiO_2 layer is amorphous, no misfit stress can arise here. The cross section of this investigated cantilever structure is shown in Fig. 5. The SiGe multilayer film starts with a very thin PECVD seedlayer (95 nm), which works as nucleation layer, followed by a 370 nm thick CVD layer which helps to crystallize the top PECVD layer.

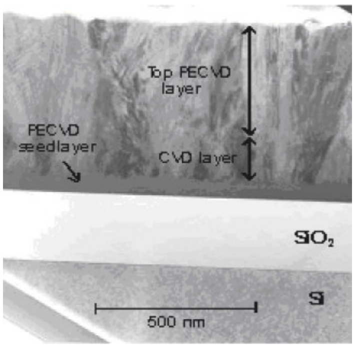

Fig. 5: Cross section of the poly-SiGe multilayer [13].

After removal of this sacrificial layer, the deflection of the free 1 mm long cantilever was measured at different thicknesses from 10 down to 1 μm. The smaller thicknesses were made by thinning. It was observed that the deflection increases exponentially with reduced thickness.

The intrinsic strain curve for this SiGe multilayer film (see Fig. 6), which is qualitatively predicted by the different stress sources, was calibrated according to the measurement results.

The highest intrinsic compressive strain value with 0.08 is at the bottom of the SiGe film. This can be explained with the compressive stress which comes from the insertion of excess atoms and the individual islands which first form on the sacrificial layer [5]. Thermal stress can be also compressive.

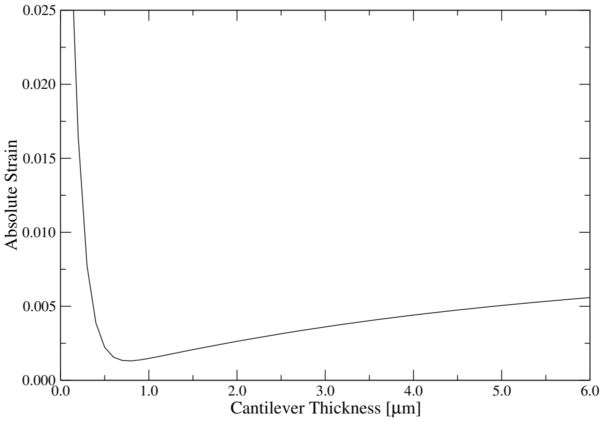

Fig. 6: Strain curve through the thickness of the SiGe multilayer film.

Within the next 800 nm of the film the strain plunges down to a minimum of 1.3×10^{-3} because of the tensile stress source in the deposited material, namely the coalescence of grain boundaries, the grain growth, and the excess vacancy annihilation. In the rest of the film there is a slow increase of the compressive part. For this phenomenon it is assumed that the grains tend to grow isotropically, but because of their neighbors they are prevented to extend in the plane and so they are forced to grow into the height instead, which leads to compressive stress.

The large compressive strain at the bottom of the SiGe film explains the very large deflections for thin cantilevers.

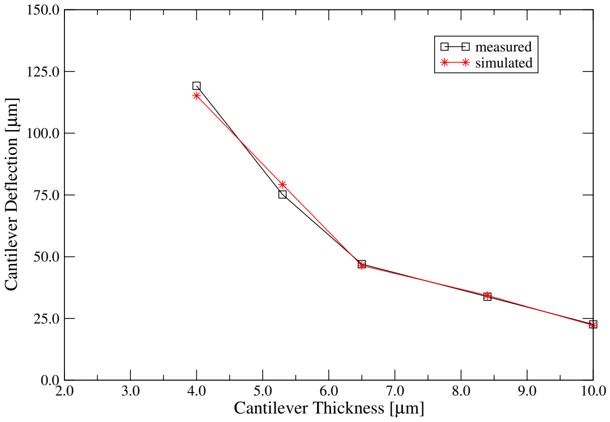

Fig. 7: Comparison between the measured [12] and the simulated cantilever deflections for different thicknesses.

At first the neutral bending line which is located midway, is moving with the cantilever thickness, and secondly the stiffness is decreased for thinner cantilevers. This strain curve was used to simulate the deflections for various thicknesses for the 1 mm long cantilever structure shown in Fig. 4. As demonstrated in Fig. 7, the simulated cantilever deflections show good agreement with the experimentally determined deflections.

EXAMPLE

As example for the simulation procedure a fabricated cantilever as shown in Fig. 8 is used. In this SEM picture which shows an array of unreleased cantilevers with different lengths, the SiGe is already etched so that the side walls of the cantilevers lie free. The process has been stopped before the sacrificial layer is removed and thus the SiGe cantilevers are still fixed. The light material which separates and frames the cantilevers is also SiGe. In Fig. 8 the selected structure is marked with a yellow rectangle. This cantilever is 900 μm long, 50 μm wide, and 6 μm thick.

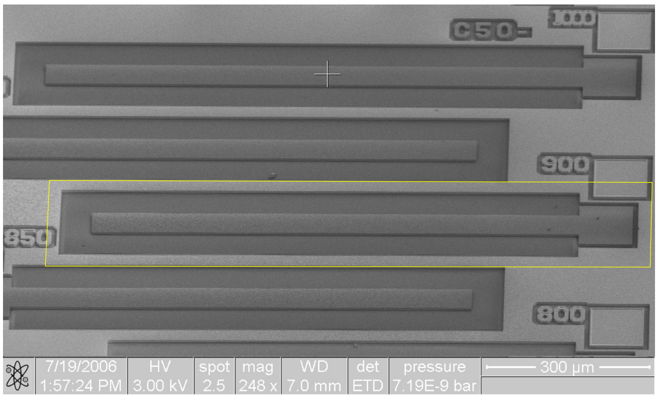

Fig. 8: Array of unreleased cantilevers.

Fig. 9 shows the initial structure for the simulation, where green is the Si substrate, blue is the SiGe frame, and red is the cantilever. The dimension of the simulated geometry with a floor space of $(1120 \times 220)\,\mu$m is identical with the yellow framed structure in Fig. 8. The strain curve (see Fig. 6) which was found with our thin film stress approach, loads the deflection problem for this example structure. The simulated deflection at the end of the 900 μm long and 6 μm thick cantilever is 44.6 μm. The structure after simulation with the deflected cantilever is displayed in Fig. 10.

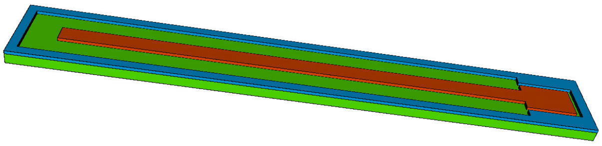

Fig. 9: Initial structure with unreleased cantilever.

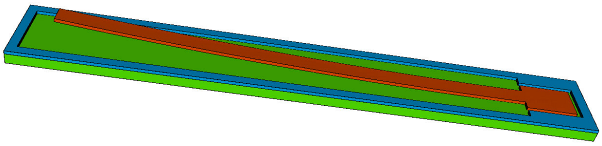

Fig. 10: Cantilever structure after simulated deflection.

CONCLUSION

A simulation concept which connects the microstructural mechanical properties in a deposited thin film with a macroscopic mechanical formulation was presented. An intrinsic strain curve which is qualitatively predicted by the different stress sources, was calibrated for a cantilever structure with a multilayer SiGe film. The calibrated curve leads to very good agreement of the simulated and the measured cantilever deflections. The stress effects in a fabricated cantilever structure were analyzed.

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