Studies on the Residual Stress and Strain Gradients in Poly-SiGe Nanocantilevers

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Abstract - One of the fundamental structural requirements for Micro/Nano-ElectroMechanical (M/NEM) devices is low strain gradient. Measurement of strain gradients is time consuming, therefore finding a simple and fast method is necessary. In this paper, a comparative study of the strain gradients in poly-SiGe nanocantilevers measured experimentally and obtained using finite element modelling (FEM) approach is reported. Arrays of nanocantilevers were fabricated from 100 nm thick poly-SiGe films via lithography. Then, strain gradients were calculated from the tip deflections and cantilevers’ lengths. In the modelling study, similar cantilevers were modelled with COMSOL Multiphysics as superposition of smaller layers in which each layer sustained local stress obtained from stress evolution study. Results showed that the average strain gradients obtained from the experimental and FEM studies differ by ~5% and ~6% for film A and B, respectively with standard deviations lying between ±0.004 and ±0.009/µm. While this study established that stress gradient is responsible for the calculated strain gradient, it also emphasises that both parameters are proportional.

Keywords: Poly-SiGe, Strain gradient, FEM, COMSOL.

1 INTRODUCTION

Several technological devices such as gyroscopes, bolometers, low frequency comb drives, high frequency resonators, and micromirrors among others are now being fabricated with polycrystalline silicon germanium (poly-SiGe) films (Sedky, 2006; Witvrouw, et al., 2005; Stoffels, et al., 2010; Heck, et al., 2010; Haspeslagh, et al., 2008). These applications become feasible because poly-SiGe films can be deposited at low temperature (<450°C) which is particularly important when Micro/Nano-ElectroMechanical System (M/NEMS) is monolithically integrated with its driving electronic components in the MEMS-last approach (Sedky, 2006; Witvrouw, et al., 2005). The fundamental requirements for excellent poly-SiGe M/NEMS structural layers, such as low tensile stress, low stress gradient and low sheet resistance are achievable by effectively identifying the process regime most suitable for the deposition of these films. To achieve low strain gradient and low temperature deposition, the process variables can be optimized to deliver a simultaneous optimal response of all the desired film properties (Asafa et al, 2013).

Strain gradient is one of the most important parameters influencing performance of M/NEMS devices (Witvrouw, et al., 2005). The effect of stress gradient across film thickness can be explained by assuming the structural layer as a superposition of smaller layers with each layer sustaining its corresponding local stress (Stoffels, et al., 2010). Excessive strain gradient causes a released structure to bend upward or downward. This alters the dynamic and reliability characteristics of devices made therefrom (Sedky, 2006; Witvrouw, et al., 2005; Stoffels, et al., 2010). In bioresonators for example, excessive downward bending can lead to stiction and causes a change in resonance frequency. For applications such as resonators, excessive upward bending may negatively affect the pull-in and pull-out voltages as well as the resonance frequency (Witvrouw, et al., 2005).

Strain gradients are computed from the tip deflections and lengths of free-standing cantilevers which are fabricated by lithography (Asafa et al, 2013, Asafa et al, 2014). However, this method requires a lot of time since several processing steps are required coupled with complexity in deflection measurement. An alternative approach is to use finite element modelling to estimate the tip deflection based on the measured residual stresses across the film thickness. This approach saves time, and often guarantees near accurate results. In this method, local stresses are computed from stress evolution study of finite layers of poly-SiGe film. The structural layer is then considered as a superposition of the finite layers with each layer sustaining its local stress. This paper therefore compares the strain gradients obtained from experimental and FEM studies of Poly-SiGe nanocantilevers.

2 METHODOLOGY

2.1 EXPERIMENTAL TECHNIQUE

Two recipes - A and B - of poly-SiGe films were used for stress evolution study. These recipes were selected by the grey-Taguchi optimization technique as reported elsewhere (Asafa et al, 2013). The deposition conditions used are presented in Table 1. The films were deposited on SiO2/Si(100) substrate using an Applied Materials Centura low pressure chemical vapour deposition (LPCVD) system. By varying the deposition time, thicknesses of the deposited films were varied accordingly. The film’s thickness and the residual stress were characterized by Scanning Electron Microscopy (SEM, FEI Nova 200) and stress measurement (Frontier Semiconductor, FSM 128L), respectively.

To determine the strain gradients, 100 nm thick films were deposited on SiO2/Si(100) substrate using both recipes. Then, lithography was used to fabricate arrays of nanocantilevers following the procedure depicted in Fig. 1 (Asafa, 2013). The sacrificial layer was a patterned SiO2 layer which was later removed by using vapour HF to create freestanding nanostructures. The actual length L and the tip deflection Δ of a few nanocantilevers were

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obtained from SEM and AFM images, respectively (Asafa et al, 2013). The strain gradient $\Gamma$ was calculated from Equation (1).

$$\Gamma = \frac{2\delta}{L^2}$$

Subsequently, the tip deflections and the strain gradients from the two films were compared.

### 2.2 Finite Element Modelling (FEM)

Finite element models were constructed and implemented in COMSOL Multiphysics platform (COMSOL, 2013). The 100 nm thick nanocantilevers were modelled as superposition of smaller layers using the data obtained from the stress evolution study. The 3-D geometry of the nanocantilevers is shown in Fig. 2. The layers formed a ‘union’ without interfacial boundary conditions and were meshed using the ‘physics-controlled mesh’ sequence. The material properties were specified with an assumption of linear isotropic condition in which single values for $E$, $\nu$, and $\alpha$ were provided. The elastic modulus $E$ was chosen to be 130 GPa (Asafa et al, 2014) while the Poisson’s ratio $\nu$ was 0.22 (Hopcroft, Nix, & Kenny, 2010). Local stress was used as the input parameter in the model since the cantilever deflection was due to the intrinsic stress (see section 3 for details). The stress was imposed as the initial stress of Linear Elastic Material model. The tip deflection was obtained from the FEM results and the strain gradients were calculated therefrom. The strain gradients so obtained were compared to those of the experiments.

### 3 Results and Discussion

#### 3.1 Stress Evolution

The evolution of intrinsic stresses in the films is shown in Fig. 3. Since the films were deposited at 415°C and characterized at room temperature (20°C), the thermal stress component (computed as ~181 MPa from the temperature difference and thermal expansion coefficient of Poly-SiGe) was deducted from the measured total stress. The intrinsic stress evolved from an initial highly compressive stress regime to a less compressive stress state and stabilized thereafter (see the change of sign on the vertical axis of Fig. 3a). This behaviour slightly differs for materials such as Au, Ag, and Cu which exhibit Type I behaviour (Freund & Suresh, 2003; Evans & Hutchinson, 2009; Abermann, 1990; Thompson, 2000).

Because poly-SiGe has low adatom mobility and low surface and grain boundary diffusivities at low temperature, the tendency for adatom movement into the grain boundary is insignificant (Asafa et al, 2014). This might be responsible for the constant intrinsic stress observed as the film thickens (Sheldon, et al., 2005; Asafa et al, 2014). In addition, no substantial stress change is expected for grains with columnar shape compared to those with lateral shape (Chason et al, 2012).

Table 1: Deposition conditions used for stress evolution study (Asafa et al, 2013)

| Recipe | $T_{dep}$ | $SiH_4$ | $GeH_4$ | CP | $B_2H_6$ | $H_2$ | HH | Time |
|--------|-----------|---------|---------|----|----------|-------|----|------|
| A      | 415       | 8       | 180     | 60 | 18       | 500   | 60 | 470  |
| B      | 415       | 8       | 180     | 65 | 11       | 500   | 50 | 500  |

$T_{dep}$ = deposition temperature, CP = chamber pressure, HH = header/shower head spacing, *10 % in hydrogen, *1 % in hydrogen

Fig. 1: Fabrication sequence for the nanocantilevers: (a) 800 nm thick SiO$_2$ layer deposited by LPCVD (b) lithographic definition of the anchor (c) LPCVD deposition of ~100 nm thick poly-SiGe film (d, e) lithographic definition of the cantilever (f, g) sacrificial SiO$_2$ is removed in hydrofluoric acid. (NB: all dimensions are in nm).
For the films, the phenomena leading to the initial highly compressive stress state have been extensively discussed in the literature. Among them are island growth and coalescence of the neighbouring islands as they minimize the surface energy at the expense of elastic deformations (Cammarata et al., 2000; Gaspar et al., 2010; Hoffman, 1976). When islands grow and coalescence, the grain boundary also grows generating average local tensile stress in a short time. Surface effects such capillarity (Nix & Clement, 1999), atomic peening (Thornton & Hoffman, 1989) and surface stress (Floro, et al., 1997) can also be responsible for island pre-coalescence compressive stress state. Unlike type I and type II materials, the tensile stresses generated during coalescence process for poly-SiGe films are insufficient to bring the average stress to a tensile state.

3.2 LOCAL STRESSES
The instantaneous stress presents in each discrete layer of the film assuming the film to be a superposition of layers with each layer sustaining its corresponding intrinsic stress is termed local stress. Since the stress is biaxial which is confined to direction normal to the grain boundary (Chason et al, 2012), change in the local stress across the film thickness leads to the strain gradient which causes a released structure to deflect upward or downward. The local stress $\sigma_{h_i-h_{i-1}}$ due to an added layer $(h_i-h_{i-1})$ can be calculated from Equation (2).

$$
\sigma_{h_i-h_{i-1}} = \frac{\sigma_i}{h_{i-1}} h_i - \frac{\sigma_{i-1}}{h_{i-1}} h_{i-1} = \frac{1}{h_{i-1}} \{\sigma_i h_i - \sigma_{i-1} h_{i-1}\} 
$$

(2)

where $h_{i-1}$ and $h_i$ are the previous and current thickness, respectively which are associated with the corresponding average stresses of $\sigma_{i-1}$ and $\sigma_i$. Equation (2) implies that the consistency of stress-thickness of discrete layers and that of the equivalent stack must be satisfied. According to Chason et al (2012), the consistency equation for N number of local layers is given by Eq. (3).

$$
\sigma h_f = (h_i - h_{i-1}) \sum_{i=1}^{N} \sigma_{i}(h_i-h_{i-1})
$$

(3)

Figure 3 (b) shows how the local stresses evolve with discrete layers in both films. The local stresses are generally less compressive for the film A than for the film B except for the thin slightly tensile layers observed. These local stresses are due to the curvature changes as more film is deposited. Consequently, the local stress-thickness products are negative. It is also observed that the top layer is more compressive for film B than film A thereby induces more negative strain gradient in film B. Similarly, for a film thickness of 100 nm, most layers are under compressive stress with lower magnitude for film B. It will be of interest if similar difference in the strain gradients of the nanocantilevers made from these films is observed.

3.3 EXPERIMENTAL AND THEORETICAL STRAIN GRADIENTS
Figure 4 shows arrays of free-standing nanocantilevers fabricated lithographically from films A and B. Besides the influence of stiction, the cantilevers are completely released from the underlying oxide layer (Fig. 4c). The length of the cantilevers has a range of 0.8 - 5 µm while the spacing in-between two neighboring cantilevers is constant (~200 nm). The tip deflections were measured from SEM images (Fig. 4) while the strain gradients were calculated according to Eq. (1). For the modeling study, the strain gradients were obtained from the seven superimposed discrete layers. Each layer sustained its corresponding intrinsic stress as measured from stress evolution study (Fig. 2). The local thickness and the corresponding local stresses are indicated in Fig. 3(b). Due to the variation in the local stresses across the stack, the structural layers deflected downward (Fig. 5). Based on the calculated local stresses (Fig. 3b), the results of the FEM are compared with those of the experiments (Fig.6).
For film A, the experimental average strain gradient is -0.02±0.004 /µm while FEM gives -0.019±0.002 /µm. This implies a downward deflection of 10 nm for 1 µm long, 100 nm thick nanocantilevers. Also, the experimental average strain gradient for film B is -0.083±0.009/µm while FEM gives -0.078±0.007 /µm. These results imply that the strain gradient in film A is about 4 times lower than film B. The large difference in the strain gradients is due to the corresponding difference in the stress gradients (Fig. 4). For film A, the local stresses are more uniform compared to film B. In addition, the local stresses are far less compressive thereby reduce the film curvatures. This shows a clear trend between the stress gradients and the strain gradients across the films. With the stress gradient, it is possible to compare, albeit relatively, the anticipated strain gradients in different released structures.

The FEM results are very similar to those obtained from the experimental studies (Fig. 6). These results indicate that the calculated values of the local stresses are close to their actual values. To further confirm that the stress gradient is responsible for the observed strain gradient, FEM of 100 nm thick layer (Fig. 7a) is subjected to the average residual stress of the stack (-155 MPa). The observed tip deflection (Fig. 7b) is very insignificant compared to that of the superimposed layers (Fig. 5). This implies that the local stress is more relevant in describing strain gradient compared to the average stress of the stack.
4 Conclusion

A comparative study of experimental and finite element modelling approaches to strain gradient measurement for poly-SiGe nanocantilevers is reported. A careful estimation of strain gradients from the two approaches produces similar values for the two films considered. The average strain gradients obtained from experimental and finite element studies were -0.02±0.004/μm and -0.019±0.002/μm, respectively for film A and -0.083±0.009/μm and -0.078±0.007/μm for film B. These values are indications of the differences in the local stresses of the two films as measured through the stress evolution study.

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