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Prediction of Residual Stress Distribution in Multi-Stacked Thin Film by Curvature Measurement and Iterative FEA

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In this study, residual stress distribution in multi-stacked film by MEMS (Micro-Electro Mechanical System) process is predicted using Finite Element method (FEM). We develop a finite element program for residual stress analysis (RESA) in multi-stacked film. The RESA predicts the distribution of residual stress field in multi-stacked film. Curvatures of multi-stacked film and single layers which consist of the multi-stacked film are used as the input to the RESA. To measure those curvatures is easier than to measure a distribution of residual stress. To verify the RESA, mean stresses and stress gradients of single and multilayers are measured. The mean stresses are calculated from curvatures of deposited wafer by using Stoney's equation. The stress gradients are calculated from the vertical deflection at the end of cantilever beam. To measure the mean stress of each layer in multi-stacked film, we measure the curvature of wafer with the left film after etching layer by layer in multi-stacked film.

Key Words : MEMS, Residual Stress, Stress Distribution, Multi-stacked Film, Stress Gradient

1. Introduction

Micro-Electro Mechanical systems (MEMS) is made of surface and bulk micromachining or LIGA process. These processes are main sources of residual stresses development. Residual stresses are the main factor that reduces the reliability of MEMS devices. The amount of residual stress is a function of the growth and deposition conditions and post processing steps. Residual stresses can have a beneficial or detrimental effect on the fracture properties of the structure, by inhibiting or promoting crack propagation in film or substrate (Johansson et al., 1989). Furthermore, various mechanical relaxation of internal stresses can have rather a drastic influence on the morphology of ductile film (Smith et al., 1991) and the residual stress field in multi-stacked films is very important to determine the mechanical behavior of micro-machined structures (Park et al., 2004). For the application of micromachine, the precise distribution of residual stress is essential. However, the distribution of residual stress in multi-stacked films is very difficult to measure or predict precisely. In general, the curvature of the wafer with thin film is measured. And then mean stress in thin film on wafer is calculated from it. Further, to measure a stress gradient of the film, MEMS process for making a structure such as cantilever beam are needed.

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Therefore, a variety of methods have been developed to measure residual stresses in thin films (Bromley et al., 1983 ; Guckel et al., 1985 ; Lin et al., 1997 ; Guo et al., 2000 ; Chen et al., 2002). They have mostly proposed methods for measuring a mean residual stress. Recently, several researchers have studied on stress distribution in thin films (Schreck et al., 2000 ; Poladian et al., 2000 ; Suhir, 2000). Victor Moagur et al. have presented the stress analysis of a multi-stacked micro-machined cantilever using commercial finite element software.

In this study, a finite element program for residual stress analysis (RESA) in multi-stacked film is developed. The developed program estimates residual stress distribution in multi-stacked film and the deflection of a cantilever beam of single and multi-stacked thin film. The results by the program are compared with experimental investigation. The program needs curvatures of multi-stacked and single layers that consist of multilayer as the inputs. Measurement of curvature of multi-stacked and each single layer is easier than measurement of stress distribution in multi-stacked film. To verify the program, we fabricated cantilever beam with the same multilayer configuration. And to measure the mean stress of each layer in multi-stacked film, we measure curvature of wafer before and after etching each layer.

2. Process of Films Deposition and a Cantilever Beam

The fabrication processes of each film are as follows. A double-side polished silicon wafers with (100) surface are used as a substrate. It is 500 μm thickness and 4 inches diameter. For 1.0 μm silicon dioxide films, silicon wafers are cleaned and oxidized for 3 hours at 1050℃. The 1.2 μm thick polysilicon films are deposited by low-pressure chemical vapor deposition (LPCVD) process at 585℃ and then they are highly doped with phosphorus using $POCl_3$ source resulting in resistivity of 400 $\mu\Omega$/cm for 30 min. at 950℃. The 0.44 μm thick silicon nitride films are also deposited by low-pressure chemical vapor deposition (LPCVD) process for 2 hours at 785℃. The 1 μm tetra-ethyl-ortho-silicate (TEOS) oxide films are formed by plasma enhanced chemical vapor deposition (PECVD) at 390℃. It is deposited in the order of 1.0 μm silicon dioxide film on substrate, 1.2 μm poly-silicon film, 0.44 μm silicon nitride film and 1 μm TEOS oxide film to make the multi-stacked film. The film was used in inkjet print head.

A MEMS structure can be curled up or down due to non-uniform distribution of residual stress through thickness. Each film is deposited as mentioned above. Cantilever beams of each film are fabricated, as shown in Fig. 1. Each film is deposited on (100) silicon wafer and patterned in shape of cantilever beam (Fig. 1(a)). Photoresist (PR) is coated to protect cantilever pattern and then an etching window is formed on silicon wafer (Fig. 1(b)). The silicon wafer is etched using XeF_2 as an isotropic etching gas (Fig. 1 (c)) and at that time, etching duration controlled length of cantilever. The silicon wafer is ashed using O_2 plasma to remove PR (Fig. 1(d)). Figure 2 is SEM showing the cantilever beams fabricated. All free-standing cantilever beams are

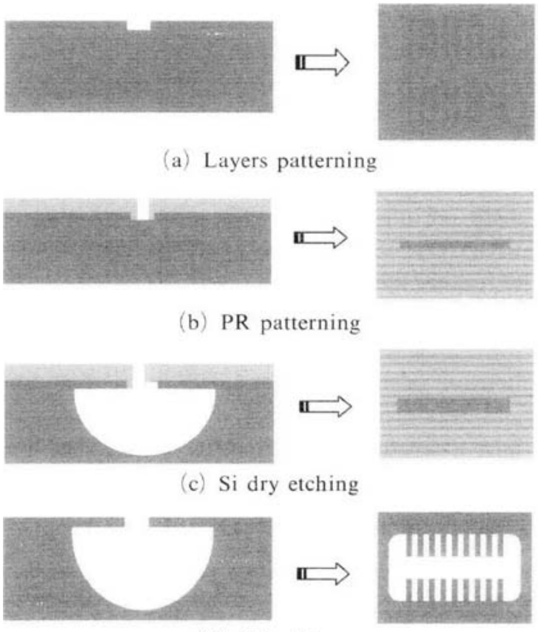
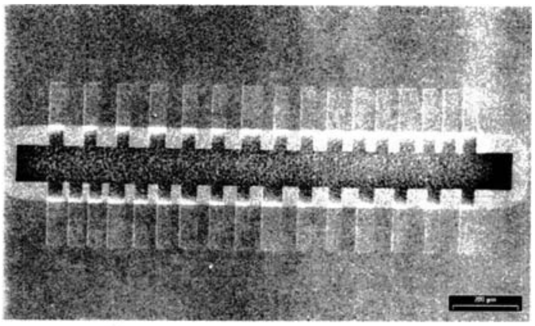
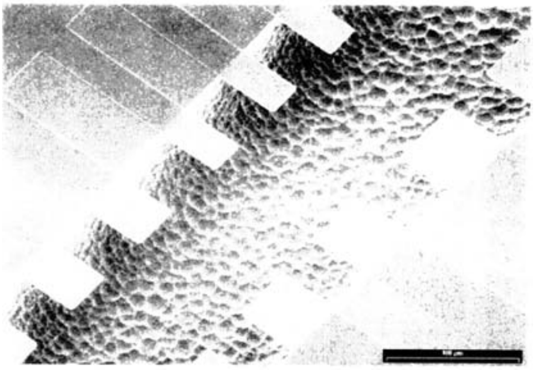

(a) Layers patterning
(b) PR patterning
(c) Si dry etching
(d) PR ashing

Fig. 1 Microcantilever beam fabrication process



(a) Top view of cantilever beams



(b) Magnified view of cantilever beams

Fig. 2 SEM image of multilayer film microcantilever beam

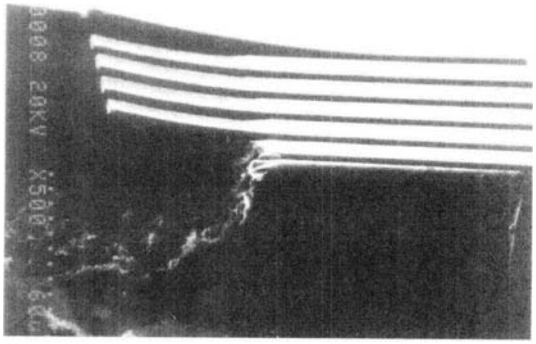


Fig. 3 SEM image of free-standing cantilever beams curling up

curled up, as shown in Fig. 3.

3. Measurement of Residual Stress

The stress of a thin film on top of substrate can be calculated by Stoney's equation (Hoffman, 1966)

$$\sigma_r = -\frac{E}{6(1-\nu)}\frac{t_s^2}{t_f}\left(\frac{1}{R_f}-\frac{1}{R_o}\right) \quad (1)$$

where R_o is the radius of curvature of the bare substrate after the thin film is etched off, R_f is the radius of curvature of the film on the substrate. E and ν are the Young's modulus and Poisson's ratio of the single crystal silicon substrate, respectively, and t_s, and t_f are, respectively, the thickness of the substrate and the film. Equation (1) assumes that both the film and the substrate are isotropic and the film is much thinner than the substrate.

Because the deposited film induce a curvature of the wafer, if a film of interest is deposited on the substrate, curvature studies are commonly used for determining the mean residual stress in the film.

The curvatures are measured with a TENCOR FLX 2300 profilometer. We also measure curvatures after removing. However, the curvatures of multi-stacked films are measured after removing each film. TEOS layer in multi-stacked film was etched by reactive ion etching in CF_4. This process has low selectivity to silicon nitride. Silicon nitride layer in multi-stacked film is peeled by reactive ion etching in SF_6. This process has also low selectivity to polysilicon. Polysilicon layer in multi-stacked film is etched by reactive ion etching in SF_4. This process has high selectivity to silicon dioxide. Silicon dioxide is removed by wet etching in HF. This process has high selectivity to silicon. Therefore, residual stresses of TEOS, silicon nitride and polysilicon layer measured in multi-stacked film have some error due to low selectivity.

4. Development of a Finite Element Program

Figure 4 shows the algorithm of RESA. This program finds the residual stress fields by finite element method. During iteration, it calculates the radius of a wafer or films. Radius obtained from FEM is compared with experimental radius. When the difference between the radius obtained from experiment and the calculated radius is be-

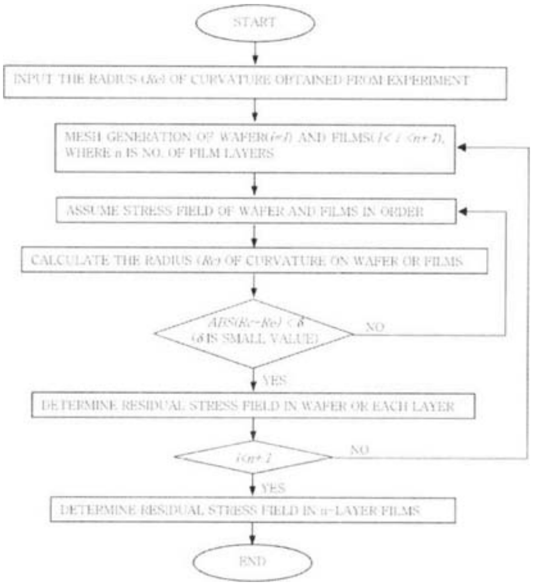


Fig. 4 Algorithm of residual stress analysis in multilayer film

low clearance, stress is determined. In the algorithm, R_e is the radius of curvature obtained by measurement and Rc is the radius of curvature calculated by simulation. The residual stress analysis in multilayer film is described in the following procedure. The mesh generation of the first layer is carried out and the stress field in the layer is assumed. The calculated radius of curvature of the layer is determined from FEA. If the difference between the calculated and the experimental radius of curvature is within tolerance, the residual stress field in a layer is determined. If not, the assumed stress field is redefined and the above procedure is repeated. After the stress field of a layer is obtained, the calculation is going to the next layer and is repeated. The finite element code used for RESA in this study is developed by modifying a general elastic finite element code of Owen and Fawkes (Owen and Fawkes, 1983). Small deformation theory is used in this code. Material properties used for the analysis are shown in Table 1.

Table 1 Material properties and thickness

Film	Young's Modulus (GPa)	Poisson's Ratio	Thickness (μm)
Si (100)	169	0.07	500
Poly-Si	160	0.226	1 17
Si_3N_4	380	0.24	0.44
SiO_2	73	0.17	0.98
TEOS	70	0.17	0.95

5. Residual Stress Distribution

Table 2 indicates results obtained from RESA about single layer film. Stresses in experiment are obtained from radii of the film using the Stoney's equation. Stresses in FEM are determined when the calculated radius by FEM shows the same value with experimental radius. FEM results show a good agreement with the stresses obtained from experiment.

Table 3 presents results of multi-stacked films. After stacking several layers on a wafer, we mea-

Table 2 Experimental and finite element analysis results of single layer

Film	Experiment		FEM	Error (%)
	Curvature, R (m)	Stress (MPa)	Stress (MPa)	
SiO_2	−38.429	−310.9	−308	0.93
	−36.917	−313.5	−310.5	0.96
Poly-Si	58.504	−3.5	−3.47	0.86
	102.684	−18.7	−18.63	0.37
Si_3N_4	11.926	1270.2	1263.2	0.55
	11.886	1255.1	1248.4	0.53
TEOS	−44.274	−272.8	−270.2	0.95

Table 3 Experimental and finite element analysis results of multilayer film

Film	Experiment		FEM	Error (%)
	Curvature, R (m)	Stress (MPa)	Stress (MPa)	
Multilayer	36.81	31.40	−	−
TEOS	42.41	28.58	28.4	0.63
Si_3N_4	−22.84	1159.26	1155.2	0.35
Poly-Si	−38.04	−113.26	−113.2	0.05
SiO_2	299.56	−299.51	−299.2	0.10

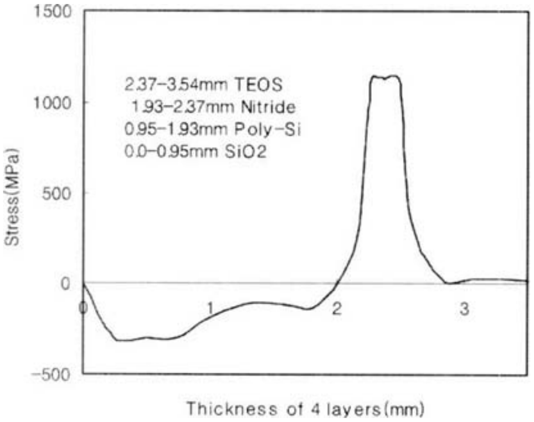


Fig. 5 Predicted residual stress distribution in multilayer film

sure the curvature of the wafer with the multi-stacked film. After etching layer by layer, we also measure the curvature of the wafer. These values are to be compared with the radius calculated by FEM. Stress in every film by FEM shows the almost same values in experiment. The residual stress in Si_3N_4 layer represents almost 1159 MPa in tension, which shows a similar trend with single layer result of 1255 MPa in tension from Stoney's equation. SiO_2 also indicates a little difference between single layer and multilayer results. But the residual stresses of polysilicon and TEOS layers in multilayers show a large difference with the ones in single layer as shown in Table 2. It can be found that the residual stress value in single layer cannot predict the residual stress field in multilayers because of thermal mismatch between two materials and intrinsic problem while deposition process.

Table 4 Curvatures of multilayer film (unit : m)

Measurement	As Received, $R_{(as-rec)}$	Before Etching, R_f	After Etching, R_o
Case 1	−20.21	30.46	53.02
Case 2	−23.31	36.81	80.10

Table 5 Residual stress of multi-layer film (unit : MPa)

Film	Measurement			FEM
	Case 1	Case 2	Single layer	
Multilayer film	31.4	29.87	−	−
TEOS	28.58	29.86	−279.3	26.2
Si_3N_4	1159.26	1149.5	1262.7	1154
Poly-Si	−113.26	−115.3	−11.1	−114
SiO_2	−299.51	−299.56	−312.2	−299

Figure 5 shows FEM results that are the residual stress distribution obtained from curvature measured by peeling the each layer from multilayers. The sum of residual stress through the whole thickness in multilayer can be obtained from area integration of figure. The mean residual stress is 31.05 MPa in tension. It can be predicted that the deflection direction of cantilever beam will be positive. The tension value of nitride layer has mostly influenced on the whole layers. In the Table 4, the $R_{(as-rec)}$ is the curvature of bare wafer before a film is deposited and R_f is the curvature of wafer after a film or multilayer is deposited. The R_o is the curvature of wafer after the deposited films are peeled. Table 4 shows that there is the differences between the $R_{(as-rec)}$, −20.21 m and −23.31 m, and the R_o, 53.02 m and 80.1 m, respectively. It is presumed that the difference is occurred by the deposition process.

Therefore, to calculate the residual stress field as shown in Fig. 5, it is needed to correct the discrepancy between R_o and $R_{(as-rec)}$.

Table 5 indicates various residual stress fields of multi-stacked films. In the case of multilayer film, residual stress was measured in twice using two wafers. Case 1 and Case 2 are residual stresses obtained by etching process as mentioned above. Single layer values mean the residual stresses obtained from each layer values as indicated in Table 2. Prediction values are calculated by the average of Case 1 and Case 2 and the compensation of stresses calculated considering the difference between R_o and $R_{(as-rec)}$.

6. Prediction of Deflection at Cantilever Beam

We developed the method to determine the

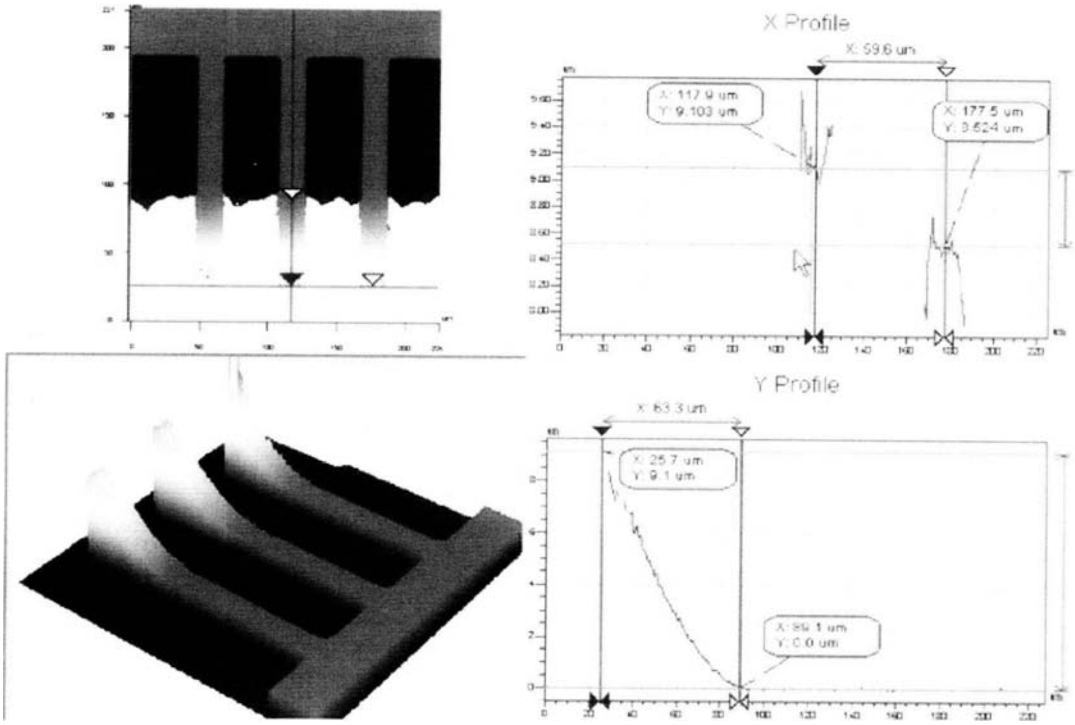


Fig. 6 Measurement of vertical deflection of a cantilever beam

residual stress in multilayers using RESA. The prediction of deflection in MEMS devices such as a cantilever beam is important to design micro system structure. The residual stress field in multilayer is essential to predict the precise deflection in a cantilever beam. Therefore, the RESA developed for predicting a residual stress distribution in multilayer was used to predict the deflection of a cantilever beam.

The amounts of the vertical deflection of cantilever beams are measured using Wyko 3D Optical Profiler as shown in Fig. 6. A cantilever beam's geometries used in this study are 20 μm long, 72 μm width and 3.54 μm thick. The vertical deflection obtained from this experiment indicates 9.1 μm. Figure 7 shows the comparisons of vertical deflection of cantilever beams. Every deflection calculated by FEM shows positive value and the prediction result is similar to experimentally measured result. It can be concluded from the above results that prediction method in this study is very useful to predict the vertical deflection in cantilever beam of a multi-stacked layer.

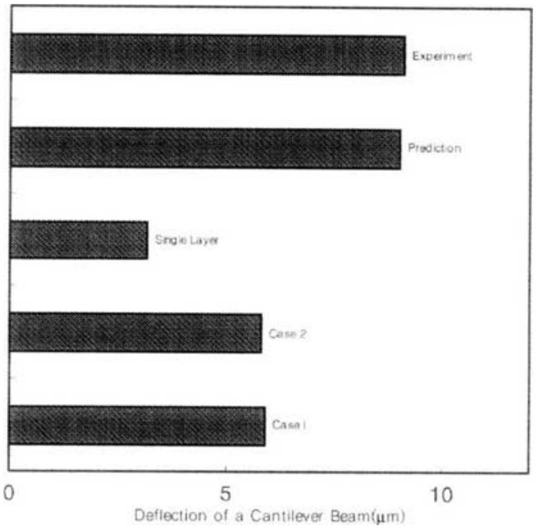


Fig. 7 Comparisons of vertical deflection in a cantilever beam

The FEM analysis is considered an alternative, powerful technique for precisely predicting deflection and residual stress field in multilayers.

7. Conclusions

In this study, a finite element program for predicting a residual stress field in multi-stacked film is developed. The developed program estimates residual stress distribution in multi-stacked film and the deflection of a cantilever beam of single or multi-stacked thin film. The results by the developed program are compared with experimental investigation. The mean residual stresses and stress gradients of silicon dioxide, polysilicon, silicon nitride, and TEOS films are measured. And also the mean residual stresses and stress gradients of the multi-stacked film which is deposited in the order of silicon dioxide, polysilicon, silicon nitride and TEOS, are measured. The tension value of nitride layer in the residual stress field of multilayer has mostly influenced on the whole layers. Every deflection calculated by FE analysis shows positive value and the result of prediction is similar to experimentally measured result. Prediction method in this study is very useful to assess the integrity of MEMS devices such as a cantilever beam made from multi-stacked film.

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