An *in situ* growth method for property control of LPCVD polysilicon film

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Polysilicon films deposited by low-pressure chemical vapor deposition (LPCVD) exhibit large residual stress and stress gradient, depending on the deposition condition. An *in situ* growth method based on multi-layer concept is presented to control the property for as-deposited polysilicon. A 3-μm thick polysilicon film with nine layers structure is demonstrated under the detailed analysis of multi-layer theory and material characteristic of polysilicon. The results show that a 3-μm-thick polysilicon film with 8-MPa overall residual tensile stress and 2.125-MPa/μm stress gradient through the film thickness is fabricated successfully.

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Polysilicon is the most widely used structural material for surface-micromachined micro-electro-mechanical system (MEMS) devices. It is typically deposited by low-pressure chemical vapor deposition (LPCVD) using thermal decomposition of saline[1]. There exists large residual stress in the as-deposited polysilicon films and large residual stress gradient through the film thickness, which depend largely on the deposition condition and can be detrimental to devices[2,3]. For example, the performance of devices for optical application can be seriously affected by the defocus and diffraction aberration due to stress and stress gradient of the polysilicon film, when the device is composed of polysilicon[4]. Doping and ion beam machining have been used to reduce residual stress and residual stress gradient, but both of them are performed by introducing external factors and require some special equipment, thus restricting their application[5,6]. In this paper, an *in situ* growth method based on multi-layer concept is presented for controlling the property of polysilicon film deposited by LPCVD. It is realized by depositing multi-layer polysilicon films with tensile and compressive stress alternately in the same equipment.

The multi-layer film has been widely used in the region of composite material[7−10]. Each individual layer is composed of different material respectively, which displays excellent property in one aspect. So this multi-layer composite material can be provided with prominent property in multi-aspect through the combination of them. It is this combination that we expect, through which polysilicon film with less residual stress and stress gradient can be obtained.

There actually exists complicated interaction at the interface between different layers, which is influenced by many factors such as deposition condition, thus making it difficult to analyze exactly. Considering that the object discussed in this paper is composed of material with the same composition, the characteristic of the multi-layer is simply treated as the superposition of that of individual layer. Since the beam-type structure is mostly used in MEMS, a three-layer structure for beam shown in Fig. 1 is demonstrated for illustrating the working theory.

Provided that the stress in the first and third layers is tensile, while that of the second layer is compressive, the thicknesses of them are t_1, t_2 and t_3 respectively, the widths of them are all w, and the variation of stress through the film thickness is linear and positive as discussed in the following text. So the stress distribution through the film thickness can be given by[11]

$$P(t) = \begin{cases} P_1 + \frac{P_2-P_1}{t_1}t & 0 \le t \le t_1 \\ P_3 + \frac{P_4-P_3}{t_2}(t-t_1) & t_1 < t \le t_1+t_2 \\ P_5 + \frac{P_6-P_5}{t_3}(t-t_1-t_2) & t_1+t_2 < t \\ & \le t_1+t_2+t_3 \end{cases}, \tag{1}$$

where P_1, P_3 and P_5 are the stresses at the beginning of film deposition, while P_2, P_4 and P_6 are the stresses at the end of deposition, and $(P_2 - P_1)/t_1 = (P_6 - P_5)/t_3$, $(P_4 - P_3)/t_2$ are the stress gradient of tensile stress and compressive stress respectively.

From Eq. (1), the stress distribution can be plotted as shown in Fig. 2.

The net stress of the multi-layer film can be expressed as[11]

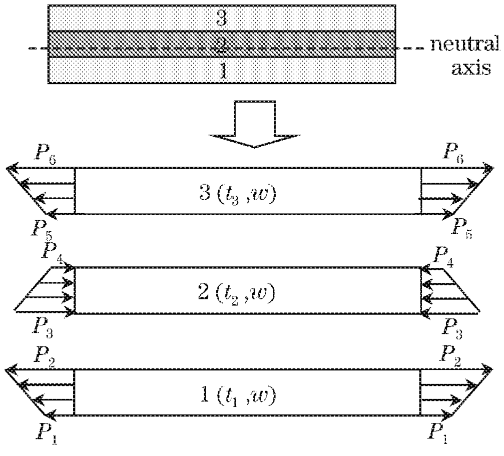

Fig. 1. Schematic of a three-layer structure.

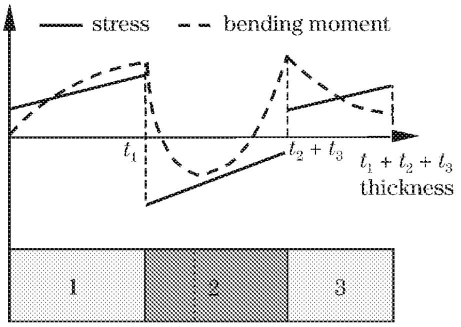

Fig. 2. Three-layer stress and bending moment distribution through the film thickness.

$$P_{\mathrm{total}} = \left(\frac{P_1 + P_2}{2}t_1 + \frac{P_5 + P_6}{2}t_3 - \frac{P_3 + P_4}{2}t_2\right) / (t_1 + t_2 + t_3). \tag{2}$$

The multi-layer film can display zero overall residual stress when the numerator term of Eq. (2) equals to zero. It is corresponding to the case that the equivalent forces caused by the stresses of different layers are balanced by each other, whose directions are parallel with the film surface. In addition, the equivalent stress gradient through the film thickness can be calculated from the bending moment applied on the neutral axis of the multi-layer structure. When the multi-layer structure is composed of the material with same composition, the neutral axis is located at the mid point of the thickness of the whole film. In the case of three-layer structure, it is divided into three different regions for analysis, and the bending moment is given as follows[11].

1) $0 \leq t \leq t_1$,

$$M(t) = \int_0^t \left(P_1 + \frac{P_2 - P_1}{t_1}t\right) \cdot w \cdot \left(\frac{t_1 + t_2 + t_3}{2} - t\right) \mathrm{d}t.$$

2) $t_1 < t \leq (t_1 + t_2)$,

$$M(t) = \int_0^{t_1} \left(P_1 + \frac{P_2 - P_1}{t_1}t\right) \cdot w \cdot \left(\frac{t_1 + t_2 + t_3}{2} - t\right) \mathrm{d}t + \int_{t_1}^{t} \left[P_3 + \frac{P_4 - P_3}{t_2}(t - t_1)\right] \cdot w \cdot \left(\frac{t_1 + t_2 + t_3}{2} - t\right) \mathrm{d}t.$$

3) $(t_1 + t_2) < t \leq (t_1 + t_2 + t_3)$,

$$\begin{aligned} M(t) = {} & \int_0^{t_1} \left(P_1 + \frac{P_2 - P_1}{t_1}t\right) \cdot w \cdot \left(\frac{t_1 + t_2 + t_3}{2} - t\right) \mathrm{d}t \\ & + \int_{t_1}^{t_1+t_2} \left[P_3 + \frac{P_4 - P_3}{t_2}(t - t_1)\right] \cdot w \\ & \cdot \left(\frac{t_1 + t_2 + t_3}{2} - t\right) \mathrm{d}t \\ & - \int_{t_1+t_2}^{t} \left[P_5 + \frac{P_6 - P_5}{t_3}(t - t_1 - t_2)\right] \cdot w \\ & \cdot \left(t - \frac{t_1 + t_2 + t_3}{2}\right) \mathrm{d}t. \end{aligned}$$

So the eventual bending moment of the whole film is expressed as

$$M_{\mathrm{total}} = M(t_1 + t_2 + t_3). \tag{3}$$

As the stress distribution, the variation of the bending moment along the thickness can also be shown in Fig. 2 from the equations mentioned above.

For a monolithic layer film with the same thickness and width as those of the multi-layer film above, if the stress gradient Γ through the thickness is assumed to be constant, the bending moment applied onto the neutral axis can be given by[11]

$$M = \Gamma \cdot w \cdot (t_1 + t_2 + t_3)^3/12.$$

As a result, the equivalent stress gradient through the whole thickness of the multi-layer film can be obtained by substituting M_{total} for M, i.e.

$$M_{\mathrm{total}} = \Gamma \cdot w \cdot (t_1 + t_2 + t_3)^3/12, \tag{4}$$

where t_1, t_2, t_3, and w are all known for a particular polysilicon film, and M_{total} can be obtained by measuring the deflection at the tip of a cantilever beam composed of this polysilicon.

From the discussion above, it can be seen that there are two possible ways to control the property for the as-deposited film. The first one is to adjust the residual stress of each individual layer, which can be realized by controlling the deposition temperature. But in view of the stability and reproducibility, the deposition parameters are always set to be relatively constant, which in turn restricts the adjust range. In the case of the polysilicon deposition by LPCVD, the most used temperatures in our experiment are 575 and 610 °C respectively. The other one is to adjust the relative thickness of each individual layer. It can be achieved by simply changing the deposition time for each layer. So this method has larger flexibility. Through reasonable design for the thickness, it can be expected that the multi-layer film with small stress and stress gradient can be fabricated.

The residual stresses in the polysilicon films vary with the microstructure, which is dependent on the deposition condition. In general, the films display fine ellipsoidally shaped grains at intermediate temperatures (560−600 °C) and contain columnar (110)-textured grains with a thin fine-grained nucleation layer at the interface between film and substrate at higher temperatures (600−700 °C), and the residual stresses in the as-deposited polysilicon films are tensile and compressive respectively. The residual stress of a 1-μm-thick polysilicon film coating the whole wafer surface as a function of the deposition temperature is shown in Fig. 3, which is obtained by curvature measurement technology.

In the case of the polysilicon film deposited between 560−600 °C, the film is amorphous at the beginning of deposition. With the deposition proceeding, the nucleation and crystal growth initiate at the film-substrate interface and then expand toward outside. As a result, the volume of film decreases, causing the tensile stress. However, the compressive stress of the polysilicon film deposited between 600−700 °C is caused by excess interstitial atoms such as oxygen or hydrogen depositing in

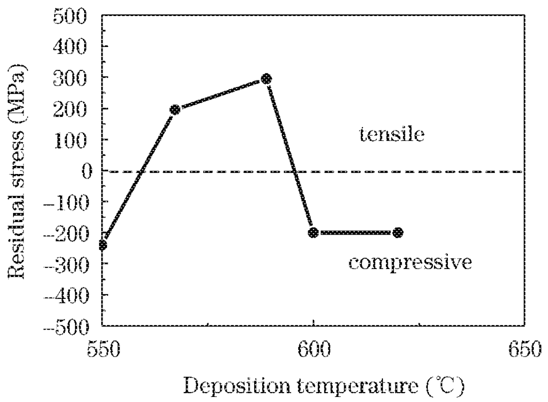

Fig. 3. Stress in polysilicon film as a function of deposition temperature.

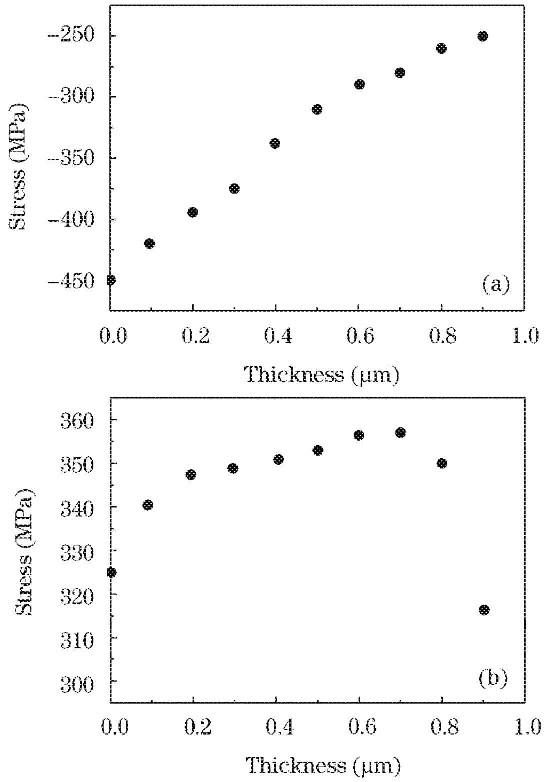

Fig. 4. The stress in polysilicon films with different stress type as a function of film thickness. (a): Compressive stress; (b): tensile stress.

the developing grain boundaries.

To determine the stress distribution for the film, a thicker polysilicon film is deposited on the whole wafer first and then successively thinned by etching. After some intervals of etching, average stresses of films with different thickness are measured respectively and shown in Fig. 4.

Figure 4(a) shows that the columnar compressive film deposited at 610 °C is highly stressed at the film-substrate interface, with the compressive stress decreasing as the film thickness increases. On the other hand, the fine-grained tensile film deposited at 575 °C exhibits more complicated variation. At the beginning of etching, the tensile stress increases with the decreasing film thickness and reaches a maximum peak. After this point, the tensile stress begins to decrease as the film thickness decreases further (see Fig. 4(b)). It can be explained that the compressive stress in film approaching to the growth interface due to the amorphous microstructure, can partly counteracts the tensile stress within the lower film, thus, the average tensile stress of the whole film increases with the decreasing thickness of amorphous film, and the time when the maximum tensile stress is obtained corresponds to the thoroughly removal of amorphous film. Through subsequently annealed at 610 °C for complete crystallization, it can be eliminated. With the tensile stress decreasing as the film thickness decreases further, the fine-grained tensile film deposited at 575 °C is less tensile at the film-substrate interface.

Since the property of polysilicon film fabricated under a particular condition is relatively fixed whatever its shape is[12], the stress and stress gradient in equations above for beam-type structure can also be obtained from Fig. 4.

A 3-μm-thick polysilicon film is studied in our work. In order to obtain 3-μm-thick polysilicon film with zero residual stress and stress gradient, a nine-layer structure is designed. Combining values of stress shown in Fig. 4 with Eqs. (2) and 3, the relative thicknesses of each individual layer are designed to be 0.20, 0.32, 0.44, 0.32, 0.44, 0.32, 0.44, 0.32, and 0.20 μm respectively.

The substrate used was 4-in [100] silicon wafer. The polysilicon film was deposited by LPCVD. A nine-layer 3-μm-thick polysilicon film was deposited at 575 and 610 °C alternatively, with the outmost layer being tensile. Following the deposition of each individual layer, the silane flow was shut off and the reactor was adjusted and stabilized at a new deposition temperature before the silane was reintroduced. From the empirical growth rate, the particular thickness of each individual layer can be controlled by the deposition time. The transmission electron microscope (TEM) micrograph of the cross section of this nine-layer polysilicon film was shown in Fig. 5. The curvature measurement of silicon wafer shows that the multi-layer film exhibits a 8-MPa residual tensile stress, which is significantly smaller than that of the one-layer film with the same thickness deposited at either 575 or 610 °C.

The same substrate was used for stress gradient experiment. A 2-μm-thick silicon dioxide film was first deposited at 680 °C by LPCVD using tetraethyl orthosilicate (TEOS) at a flow rate of 100 sccm and a pressure of 350 mTorr. The oxide was patterned with buffer

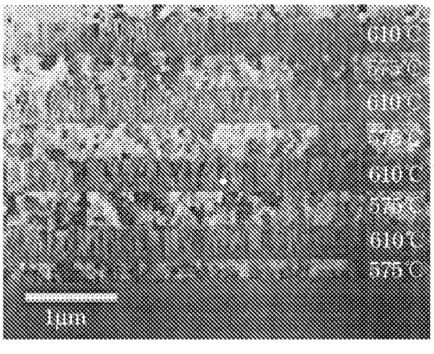

Fig. 5. The TEM micrograph of the cross-section of nine-layer polysilicon structure.

hydrofluoric acid (HF) to define anchors, followed by the same 3-μm-thick nine-layer polysilicon film deposition as above. The polysilicon was then patterned into cantilever beam with 400 μm long, 4 μm wide by using SF_6/He-based reactive ion etching (RIE). Finally, the beam was released by removing the residual oxide in buffered hydrofluric acid (BHF). The deflection at the tip of the beam was measured with interferometry. Since the relation between the deflection x and the bending moment M applied to the cantilever beam can be given by[11]

$$x = \frac{M \cdot l^2}{2EI}, \tag{5}$$

where l is the length of beam, E and I are Young's modulus and moment of inertia respectively.

From Eqs. (4) and (5), the relationship between the equivalent stress gradient of the polysilicon film and the deflection at the end of the beam can be given by

$$\Gamma = 2.125x, \tag{6}$$

where Γ is stress gradient, x is the deflection at the tip of the beam, and their units are MPa/μ m and μm respectively.

When substituting deflection measurement into equation, the equivalent stress gradient can be obtained. The result shows an upward 1-μm deflection at the tip of the beam, indicating a positive stress gradient of 2.125 MPa/μm.

Though these results are not exactly zero as expected, which are mainly caused by ignoring the interaction at interface between layers as mentioned above, this method is also proved to be an effective way to produce polysilicon film with near-zero results of stress and stress gradient.

The multi-layer structure can fabricate polysilicon film with low stress and stress gradient. It is achieved by depositing tensile film and compressive film alternatively. From the results, it can be seen that a 3-μm-thick polysilicon film with nine-layer structure exhibits 8-MPa residual tensile stress and 2.125-MPa/μm stress gradient, which are significantly smaller than those of the one-layer film with the same thickness. This method can also be readily used for the as-deposited films with different thickness.

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