Thin Solid Films 522 (2012) 26–29

Contents lists available at SciVerse ScienceDirect

Thin Solid Films

journal homepage: www.elsevier.com/locate/tsf

# Study of microstructure deflections and film/substrate curvature under generalized stress fields and mechanical properties

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ARTICLE INFO

Available online 10 February 2012

*Keywords:*
Stress
Hetero epitaxy
Micro-structures

ABSTRACT

In this article we use a recently developed analytical stress theory to describe hetero-epitaxial growths, extending the analysis capability in case of extreme conditions of strongly nonlinear dependence of the local strain field and of the elastic properties (Young modulus) on the film thickness. We apply this extended theory to study the heteroepitaxial growth of cubic silicon carbide on silicon (100).



## 1. Introduction

Conductive, dielectric, semiconducting, piezoelectric and ferroelectric thin films are extensively used for micro and nano electromechanical systems (MEMS and NEMS) applications. Two important parameters affect their properties, namely the residual stress/strain and the elastic properties of the film. Presently, it is very difficult to predict these parameters directly from the growth process, therefore extended analysis of the grown films are essential for both process development and process monitoring. Many suggestions for stress measurements in thin films have been made over the past several decades. The conventional method involves measuring the wafer curvature to calculate the average defective stress using the Stoney equation [1–3]. Other approaches include X-ray diffraction [4] or analysis of the deflections of specifically designed surface machined microstructures [5–8]. In this last technique the microstructures, released after locally removing the underlying substrate, deform by increasing or decreasing their dimensions to minimize the total elastic energy. The residual local strain can be derived on the basis of these deformations. Several microstructures have been proposed [9], though it has been recently demonstrated that planar rotators (*PR*) [6,7] are superior in that allow for a simultaneous determination of both the in-plane and out-of-plane deflections and, thus, a deeper knowledge of the residual strain field which, in turn, is connected to the initial, defect related, strain field. On the other hand, the elastic properties of the films can be measured among the others, through nano-indentation [10], bulge tests [11] or micro-machined resonance frequencies [12,13].

Recently it has been found, through the analysis of cantilever natural resonance frequencies, that the Young modulus of cubic silicon carbide films (3C-SiC) hetero-epitaxially grown on silicon (100) [13] changes along the film thickness ranging from $E_{SiC}$~210 GPa for a ~2 μm thick film to $E_{SiC}$~420 GPa for a ~3.5 μm one. Furthermore, for the same film, it was observed a strong reduction of the out-of-plane deflection of the micro-machined cantilevers as function of the film thickness thus suggesting a non-linear variation of the defective strain within the film [6].

In this article we analyze the observed deflections incorporating the variation of the Young module in the theoretical model.

## 2. Stress theory for macro and micro deflections

To correlate the observed macro deflections in the wafer and the deflections of the microstructures to the initial defective strain $\varepsilon_{def}(z)$ and to the variation of the Young modulus we begin by considering the total elastic energy with respect to the strain fields, both at the macro and micro levels:

$$U_{wafer}\left(\delta_{wafer}\right) = \int_{-h_{sub}}^{h_{film}} M(z)\varepsilon_{res}^2(z)dz \quad U_{micro}(\delta_{micro}) = \int_0^{h_{film}} M(z)\varepsilon_{fin}^2(z)dz \tag{1}$$

where $h_{sub}$ and $h_{film}$ are the substrate and the film thicknesses, with the origin of the system ($z=0$) chosen at the substrate/film interface. $M(z)=E(z)/(1-\upsilon(z))$ is the biaxial modulus, $E(z)$ is the Young modulus, which can vary along the film thickness, and $\upsilon(z)$ is the Poisson's ratio of the substrate (for $z<0$) and film (for $z>0$), respectively (we assume the following values $E_{Si}=130GPa$, $\upsilon_{Si}=0.278$ [14] and $\upsilon_{SiC}=0.23$ [15]). $\varepsilon_{res}(z)$ and $\varepsilon_{fin}(z)$ are the residual strains after the first (wafer bowing) and second (microstructure deflection) relaxations.

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0040-6090/$ – see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.tsf.2012.02.014

In the Kirchoff hypothesis (i.e., lateral dimensions much greater than system thickness) we can assume linear relations [16]:

$$\varepsilon_{res}(z) = \varepsilon_{def}(z) - K_{macro}z + \varepsilon_{macro} \qquad \varepsilon_{fin}(z) = \varepsilon_{res}(z) - K_{micro}z + \varepsilon_{micro} \quad (2)$$

with $K_{macro}(K_{micro})$ and $\varepsilon_{macro}(\varepsilon_{micro})$ being the curvature and in-plane-strain of the heterosystem (microstructures). The final (experimentally observed) deflections can be obtained by the minimization of the total elastic energies $U$ with respect to all the allowed displacements ($K_{macro}$, $\varepsilon_{macro}$, $K_{micro}$, $\varepsilon_{micro}$). Solving the system of equations we get:

$$\left.\begin{aligned} \bar{K}_{macro} &= \left[\frac{\Delta_2}{\Delta_1}X_1 - X'_1\right] / \left(\frac{\Delta_2\Delta_2}{\Delta_1} - \Delta_3\right) \\ \delta_z &= 2L^2(\bar{K}_{macro} + \bar{K}_{micro}) \\ \delta_x &= \frac{2LL_C}{L_O} < \varepsilon_{fin}(z) - \varepsilon_{res}(z) >= -\frac{2LL_C}{L_O}\frac{X_2}{\Theta_1} \end{aligned}\right\} \quad (3)$$

with

$$\left.\begin{aligned} \bar{K}_{micro} &= \left(\frac{\Theta_2}{\Theta_1}X_2 - X'_2\right) / \left(\frac{\Theta_2\Theta_2}{\Theta_1} - \Theta_3\right) \\ X_2 &= Y_1 - \bar{K}_{macro}\Theta_2 + \bar{\varepsilon}_{macro}\Theta_1 X'_2 = Y'_1 - \bar{K}_{macro}\Theta_3 + \bar{\varepsilon}_{macro}\Theta_2 \end{aligned}\right\} \quad (4)$$

and

$$\left.\begin{aligned} \Theta_1 &= \int_0^{h_{film}} M_{film}(z)dz \qquad \Delta_1 = \int_{-h_{sub}}^{h_{film}} M_i(z)dz \\ \Theta_3 &= \int_0^{h_{film}} z^2 M_{film}(z)dz \qquad \Delta_3 = \int_{-h_{sub}}^{h_{film}} z^2 M_i(z)dz \\ \Theta_2 &= \int_0^{h_{film}} zM_{film}(z)dz \qquad \Delta_2 = \int_{-h_{sub}}^{h_{film}} zM_i(z)dz \end{aligned}\right\} \quad (5)$$

$$\left.\begin{aligned} X_1 &= \int_{-h_{sub}}^{h_{film}} M_i(z)\varepsilon_{def}(z)dz \qquad Y_1 = \int_0^{h_{film}} M_{film}(z)\varepsilon_{def}(z)dz \\ X'_1 &= \int_{-h_{sub}}^{h_{film}} zM_i(z)\varepsilon_{def}(z)dz \qquad Y'_1 = \int_0^{h_{film}} M_{film}(z)\varepsilon_{def}(z)dz \end{aligned}\right\} \quad (6)$$

Using Eqs. (3)–(6) we can calculate the final deflections ($K_{macro}$, $\delta_x$, $\delta_z$) in terms of the initial defective strain field $\varepsilon_{def}(z)$ including the impact of a variable young's modulus $E_{SiC}(z)$ through the integrals in Eqs. (5) and (6).

It is worth noting that, although the equations governing the model are numerous and relate the initial defective strain $\varepsilon_{def}(z)$ to the deflection rather than the deflections to the strain, i.e. they are formulated in an implicit form, the presented model can be easily implemented and solved iteratively in any computer by solving the integrals in Eqs. (5) and (6) and finding the $\varepsilon_{def}(z)$ function that give rise to final deflections ($K_{macro}$, $\delta_x$, $\delta_z$) consistent with the observed ones.

Following ref. [7,8] we consider a constrained/defective stress described by a power law function:

$$\sigma_{def}(z) = \left(\frac{E_{film}(z)}{1 - \upsilon_{film}}\right)Az^B \qquad z > 0 \quad (8)$$

where A and B are fitting parameters. The power law function was found to be the best one to describe the evolution of stacking fault film density in the heteroepitaxial growth of SiC/Si(100) [6,7,17]. $E_{film}(z)$ is chosen following Fig. 3 of ref. [13] and assuming the following functional expression:

$$E_{film}(z) = \begin{cases} 217\,[GPa] & 0<z<2\mu m \\ \left\{166\left(z/10^{-6}\right) - 110\right\}[\text{GPa}] & 2\mu m \le z \le 4\mu m \\ 427\,[GPa] & 4\mu m<z \end{cases} \quad (9)$$

the latter ($E_{film}(z) = 427$ GPa) being close to the ab-initio value for an ideal, defect free, crystal [15].

To study the impact of the variation of the Young modulus on the final deflections we compare the calculated macro and micro deflections with the one obtained assuming a constant $E_{SiC}$ equal either to the minimal experimental value ($E_{SiC}(z) = E_{SiC}(2\mu m) = 217GPa$) or to the maximal one $E_{SiC}(z) = E_{SiC}(4\mu m) = 427GPa$.

As can be seen in Fig. 1, the assumption of a variable $E_{SiC}(z)$ has a strong impact on the wafer curvature whereas it only slightly changes the micro (in-plane and out-of-plane) deflections. These results are

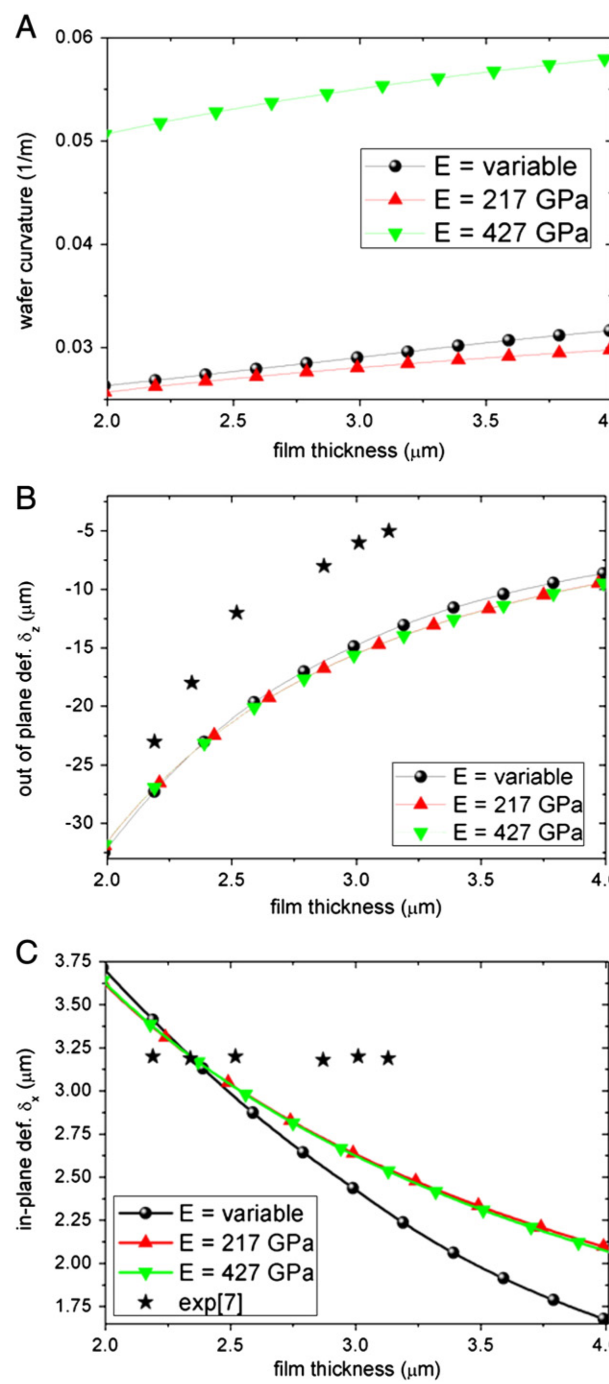


**Fig. 1.** Macro (A) and micro (B and C) deflections as a function of film thickness assuming two possible constant ($E_{SiC} = 217$ GPa and $E_{SiC} = 427$ GPa) or variable (following ref. [13], Eq. (9)) Young modules. The parameters $A$ and $B$ of Eq. (8) were chosen so that $\delta_z(h_{film} = 2.19\mu m) = -24\mu m$ and $\delta_x(h_{film} = 2.19\mu m) = 3.2\mu m$ with $L_O = 10\mu m$, $L = 300\mu m$, $L_C = 160\mu m$, $h_{film} = 2.19\mu m$ and $h_{sub} = 525\mu m$. Consistent with ref. [6] (star points in $B$ and $C$).