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Review

Celebrating the 100th anniversary of the Stoney equation for film stress: Developments from polycrystalline steel strips to single crystal silicon wafers

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ABSTRACT

Stress in a thin film on a flexible substrate induces a curvature of the substrate. Usually the substrate is orders of magnitude thicker than the film, leading to small and purely elastic deformation of the substrate. In this case, the Stoney equation yields the stress in the film from the measured curvature of the substrate. The Stoney equation contains thickness of film and substrate and the elastic properties of the substrate. Typically the elastic properties of the substrate are specified by E (Young's modulus), and ν (Poisson's ratio). E and ν provide a valid description for elastically isotropic substrates, e.g. polycrystalline steel strips, as used by Stoney in 1909.

Today the Stoney equation is still used for relating substrate curvature to film stress. However, in the majority of thin film stress measurements by means of substrate curvature, Si wafers are used as the substrate. Silicon wafers are cut from single crystals and are thereby elastically anisotropic. In the present paper, a modified form of the Stoney equation, well known for elastic isotropic substrates, is derived for Si(001) and Si(111) wafers, using the elastic stiffness constants of silicon, c_{ij}, instead of the orientation averaged values E and ν, which do not have a meaning for elastically anisotropic single crystal materials.

Curvature measurements of thin films on Si(001) and Si(111) wafers are presented. The difference in film-stress-induced curvature of Si(001) and Si(111) wafers is discussed.

Contents

1. Introduction

Thin films on a substrate are usually in a stressed state. A convenient method to study stress in thin films is to deposit these films on a flat substrate and observe the curvature of the substrate due

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to the stress in the film. The Stoney equation relates the curvature of the substrate to the stress in the film. A first requirement for application of the Stoney equation is that the substrate is thick compared to the thickness of the film, but still thin enough that it bends due to the stress in the film. A second requirement for application of the Stoney equation is that the film is in a state of plane stress, meaning that in the plane of the film the stress is independent of direction, or in tensor notation:

$$\vec{\vec{\sigma}}_f = \begin{pmatrix} \sigma_f & 0 & 0 \\ 0 & \sigma_f & 0 \\ 0 & 0 & 0 \end{pmatrix}. \qquad (1)$$

The formula relating the curvature of the substrate to the stress in the film is known as the Stoney equation. Various versions of the Stoney equation exist for various types of substrates. For elastic isotropic substrates, e.g. steel strips or glass slides, the Stoney equation reads [1–3]:

$$\sigma_f t_f = \frac{E_s h^2}{6(1-\nu_s)R}, \qquad (2)$$

with σ_f the in-plane stress component in the film, t_f the thickness of the film, E_s Young's modulus of the substrate, ν_s Poisson's ratio for the substrate, h the thickness of the substrate and R the radius of curvature of the initial flat substrate after deposition of the film.

For elastically anisotropic substrates, e.g. single crystal silicon wafers, versions of the Stoney equation also exist. For Si(001) wafers, the Stoney equation reads [2]:

$$\sigma_f t_f = \frac{h^2}{6(s_{11}^{Si} + s_{12}^{Si})R}, \qquad (3)$$

with s_{11}^{Si} and s_{12}^{Si} elements of the compliance tensor of silicon. The factor $1/(s_{11}^{Si}+s_{12}^{Si})$ is called the biaxial modulus (M) of Si(001). The numerical value is:

$$M_{(001)}^{Si} = \frac{1}{s_{11}^{Si} + s_{12}^{Si}} = 1.803(1) \cdot 10^{11}\ \text{Pa}. \qquad (4)$$

For Si(111) wafers the Stoney equation reads [2]:

$$\sigma_f t_f = \left(\frac{6}{4s_{11}^{Si} + 8s_{12}^{Si} + s_{44}^{Si}} \right) \frac{h^2}{6R}. \qquad (5)$$

The factor $6/(4s_{11}^{Si}+8s_{12}^{Si}+s_{44}^{Si})$ is called the biaxial modulus of Si(111). The numerical value is:

$$M_{111}^{Si} = \frac{6}{4s_{11}^{Si} + 8s_{12}^{Si} + s_{44}^{Si}} = 2.291(1) \cdot 10^{11}\ \text{Pa}. \qquad (6)$$

The values of s_{11}^{Si}, s_{12}^{Si}, and s_{44}^{Si} are presented in Section 3, below.

At present the substrates of choice for stress measurements by substrate deformation are almost exclusively silicon wafers. In fact, this is so common that the technique is known as the "wafer curvature method". It is therefore strange that while the majority of the substrates used are Si(001) wafers, requiring Eq. (3), most authors use Eq. (2) to analyze their results. We suspect that the application of the inappropriate formula stems from two causes:

* The initial work on stress in thin films was done on isotropic substrates [4,5]
* The correct formulas were presented without derivation [2], and because of their conceived complexity not appealing to a non-mechanical engineering audience.

In the present paper we will first give a historical overview of the work on stress measurements by observation of deformation of the substrate curvature and then present a derivation of Eqs. (3) and (5) for single crystal silicon wafers. Moreover, in Appendix A, we will demonstrate that Eqs. (3) and (5) reduce to Eq. (2) for isotropic substrates.

To convince the reader of the validity of Eqs. (3) and (5), we deposited two identical series of three tungsten films each on Si(001) and Si(111) substrates. Films identical in stress and thickness induce a different curvature in Si(001) and Si(111) wafers according to Eqs. (3) and (5), showing the need for these equations for silicon wafers instead of Eq. (2). We hope that henceforth Eq. (3) will be used to analyze stress in film on Si(001) wafers, since E and ν have no meaning for an elastically anisotropic material like silicon.

2. Historical overview

In 1909 Stoney published his seminal paper "The Tension of Metallic Films Deposited by Electrolysis" [4]. In that paper he derived an expression for the curvature of a steel strip due to the stress in a metallic coating applied to one side of the strip. This expression, like all subsequent versions of what has become known as the Stoney equation, was arrived at by requiring two equilibrium conditions. For a beam oriented along the x_1 direction, that bends in the x_3 direction, these conditions can be expressed as [6]:

$$F = \int \sigma_{11} dA = 0 \qquad (7)$$

$$M = \int \sigma_{11} x_3 dA = 0 \qquad (8)$$

with dA an element perpendicular to the x_1 direction. Eq. (7) states that the sum, F, of the longitudinal forces within the strip is zero, i.e., that the internal compressive forces are equal to the internal tensile forces. Eq. (8) states that at equilibrium the internal bending moment M of the strip is zero about any axis. (The bending moment M must not be confused with the biaxial modulus M_{hkl}). Using these conditions it is straightforward algebra to arrive at the expression published by Stoney:

$$\sigma_f t_f = \frac{E_s h^2}{6R}. \qquad (9)$$

Stoney erroneously assumed a uniaxial stress in the film instead of a biaxial stress. Even though the strip is considerably longer than wide, still the width of the strip is very much larger than the thickness of the film; therefore the stress in the film is bi-axial. Due to this oversight Stoney characterized the elastic behavior of the strip by E_s instead of $E_s/(1-\nu_s)$. Eq. (9) differs from Eq. (2) by a factor $1/(1-\nu_s)$. This factor stems from the difference between a uniaxial stress and a biaxial stress.

A steel strip consists of many grains. Therefore any elastic anisotropy is averaged out and the use of Eq. (2) is justified even though the individual grains in the strip may be elastically anisotropic. Such an averaging over randomly oriented crystals yields aggregated values for E and ν [7].

The first requirement in the derivation of the Stoney equation (Eqs. (2), (3), and (5)) is that the film is thin compared to the substrate. This requirement allows one to describe the mechanical action of the film on the substrate by a single quantity: the force per unit width (F/w) [8]. The left hand side of Eqs. (2), (3), and (5) is called the force per unit width; it is expressed in units N/m. For the case that the stress is not constant over the film thickness, the force per unit width is not the product of stress and film thickness, but the integral of the stress in the film over the thickness of the film [9]. Since for solution of the equilibrium Eqs. (7) and (8) the film is replaced by an "action" on one side of the substrate, the elastic properties of the film do not enter Eqs. (2), (3), and (5).

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Another consequence of the requirement that the film is thin compared to the substrate is that no distinction has to be made between deposition on a clamped substrate and a substrate that is free to bend. Assume deposition of a stressed film on a clamped substrate. After deposition, the substrate is released and will assume a curvature, thereby changing the strain of the film and lowering the absolute value of the stress in the film. Since the film is thin compared to the substrate, the curvature, and hence the strain and change in stress in the film will be small. In Appendix B this is elaborated.

Of course one can also solve Eqs. (7) and (8) for systems consisting of films and substrates with comparable thickness. This was done for a number of systems in a 1949 paper by Brenner and Senderoff [6]. In that article, however, it was still not realized that the stress in a film is typically biaxial and not uniaxial.

During the 1970's, Hoffman and Thornton studied stress in sputter deposited films. They analyzed their data by observing the curvature of glass slides by interferometry. In 1977 [5], they published a formula for the non-uniform curvature of a glass slide, caused by a non-uniform stress in the film. Eq. (2) can straightforwardly be derived from their formula.

In 1979, a derivation for the curvature of a steel strip due to a stressed film was presented by Perakh [10]. Also from this result, Eq. (2) can be obtained by straightforward algebra.

To our knowledge, the first occurrence of the Stoney equation in the form of Eq. (2) was in 1987, in a paper by Flinn, Gardner and Nix [1]. Only two years later Nix presented Eqs. (2), (3) and (5) [2] for isotropic substrates, Si(001) wafers and Si(111) wafers, respectively. The biaxial moduli of Si(001) and Si(111), that enter in Eqs. (3) and (5) had been published in 1972 by Brantley [11]. It is probably because the derivations of Eq. (3) and (5) were not given in the paper by Nix [2], that these equations have not caught on in the thin films community.

In the 1990's, it was realized that a round plate covered on one side with a stressed film will deform in an axially symmetric manner only for a small force per unit width. For a larger force per unit width, a cylindrical deformation is the energetically preferred solution [12–16]. The mode of deformation is determined by a parameter A [16]:

$$A = \sigma_f t_f \frac{D^2}{h^3}, \tag{10}$$

with D the diameter of the plate. For a silicon wafer with $D/h \geq 50$, the critical value is $A_c = 680$ GPa. For $A < 0.2\ A_c$ the Stoney equation is correct within 10%. For $0.2\ A_c < A < A_c$, the deformation of the wafer will be axially symmetric, but the curvature at the center of the plate will be significantly lower than the value predicted by the Stoney Equation. Vice versa, unguarded application of the Stoney equation in this regime will lead to an underestimation of the stress up to a factor of two. Finally, for $A > A_c$, bifurcation will occur with a large curvature in one direction and almost no curvature in the perpendicular direction. For 100 mm Si wafers, the requirement $A < 0.2\ A_c$ leads to maximum force per unit width for 90% accuracy of the Stoney Equation of:

$$(\sigma_f t_f)_{\max} = 1.9\ \text{GPa} \cdot \mu\text{m}. \tag{11}$$

With the exception of Thornton and Hoffman [5], in all papers reviewed so far the stress in the films has been assumed to be plane stress: $\sigma_{11} = \sigma_{22}$ and all other components of the stress tensor zero. In a large number of cases, the deposition equipment in which the films are deposited exhibits anisotropy. This anisotropy may lead to anisotropy in the microstructure of the film and hence to anisotropy in the stress. To tackle this problem, Zhao et al. [17] derived equations for the case where $\sigma_{11} \neq \sigma_{22}$.

In recent years, papers are still being published on the Stoney Equation, be it on the accuracy [18,19] or on special cases, e.g. the case where the stress in the film is position dependent [20], but more importantly, the equation is used extensively in the study of stresses in thin films.

3. The Stoney equation for a Si(001) wafer substrate

The substrate of choice for curvature measurements is often a silicon wafer with (001) orientation. In that case, Eq. (2) is not applicable since the elastic response of silicon is anisotropic. E and ν are direction dependent for a single crystal. The in-plane stiffness of a silicon (001) wafer depends on the direction, that is $E_{Si}[110] = 171$ GPa and $\nu_{Si}[110] = 0.06$ while $E_{Si}[100] = 130$ GPa and $\nu_{Si}[100] = 0.28$. [21,22]. In Fig. 1 a sketch of a 100 mm Si wafer is presented. The flat designates the $[1\bar{1}0]$ direction. For a Si(001) wafer, the [001] direction is normal to the wafer and the [001] and [010] directions coincide with the x_1- and x_2-axes. In the calculations for Si(001) wafers, we will use a coordinate system with the x_1- and x_2-axis as indicated in Fig. 1 and the x_3 axis perpendicular to the wafer. These directions coincide with the crystallographic axes of the silicon crystal.

3.1. Constitutive equation

We will derive the Stoney equation based on the constitutive equation for silicon, i.e. generalized Hooke's law, in tensor notation. Stress and stain are both tensors of rank two with nine components. Both tensors, however, are symmetric [23] and therefore each have only six distinct components. The tensor relating stress to strain has 81 components (9×9). Based on symmetry, this number reduces for a cubic crystal to only three distinct components [23]. For cubic materials, one arrives at

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & c_{12} & & & \\ c_{12} & c_{11} & c_{12} & & & \\ c_{12} & c_{12} & c_{11} & & & \\ & & & c_{44} & & \\ & & & & c_{44} & \\ & & & & & c_{44} \end{pmatrix} \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{pmatrix}, \tag{12}$$

where σ_{ij} are the components of the stress tensor, c_{11}, c_{12}, c_{44} are the elastic stiffness constants of silicon and ε_{ij} are the strains. The values of c_{11}, c_{12}, and c_{44} (see Table 1) have been determined in the 1960's [24,25] and are today still used as a touchstone for first principle calculations [26]. In this paper, we will drop the designation Si in the compliances and stiffness coefficients, so instead of c_{ij}^{Si} and s_{ij}^{Si} we will henceforth use c_{ij} and s_{ij}.

In Eq. (12) the stress components are expressed as a function of the strain components. It is equally well possible to express the strain

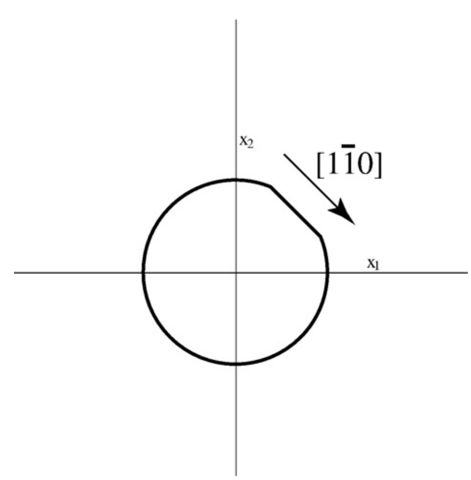

Fig. 1. A sketch of a 100 mm silicon wafer. The flat designates the crystal direction $[0\bar{1}1]$, both for Si(001) as well as for Si(111) wafers. For Si(001) wafers, [001] is normal to the wafer. For Si(111) wafers, [111] is perpendicular to the wafer.

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Table 1
Experimental values of the elastic stiffness constants of silicon in units of GPa

	c_{11} (GPa)	c_{12} (GPa)	c_{44} (GPa)
Ref. [24]	165.77	63.92	79.62
Ref. [25]	165.64	63.94	79.51

Table 2
Compliance constants of silicon in units of Pa^{-1}, calculated from the experimental values of the stiffness constants in Table 1

	s_{11} (Pa^{-1})	s_{12} (Pa^{-1})	s_{44} (Pa^{-1})
from Ref. [24]	$7.685\ 10^{-12}$	$-2.139\ 10^{-12}$	$1.256\ 10^{-11}$
from Ref. [25]	$7.691\ 10^{-12}$	$-2.142\ 10^{-12}$	$1.258\ 10^{-11}$

components in the stress components. In that case one employs the non-zero elements of the compliance tensor s_{11}, s_{12}, and s_{44}. Following the equations in ref. [27] it is straightforward to calculate the values of s_{11}, s_{12} and s_{44} from the values c_{11}, c_{12}, and c_{44}. For convenience of the reader the results are presented in Table 2.

3.2. Kinematics

Due to the stressed film, the silicon wafer will bend. For the case of a tensile stress in the film, the part of the wafer adjacent to the film will be contracted and the part of the wafer furthest away from the film will be elongated. Assume that in the wafer there is a neutral plane $\mathbf{u}^{(0)}$ that is neither expanded nor contracted. The situation is sketched in Fig. 2. The displacement of a point on the neutral plane perpendicular to the wafer is denoted by w. The components of the displacement of a point on the neutral plane in the plane of the wafer are small compared to w and are set to zero. Furthermore, we assume that the shape of the silicon wafer can be described by one unique curvature, hence:

$$u_1^{(0)} = u_2^{(0)} = 0, \quad (13a)$$

$$u_3^{(0)} = w(x_1, x_2) = ax_1^2 + ax_2^2. \quad (13b)$$

The curvature of the sample, κ, and the constant a are related to the radius of curvature, R, by:

$$\kappa = 2a = \frac{1}{R}. \quad (14)$$

In the section on experimental results, it will be shown that for 100 mm diameter wafers the assumption of a unique curvature is correct for all presented samples within 5%.

Since the wafer plus film are an isolated system, no stresses perpendicular to the substrate are possible at the surface, and since the moments are constant over the thickness of the wafer $\sigma_{13}=\sigma_{23}=\sigma_{33}=0$ [23,28]. Using Eq. (12), we arrive at:

$$\varepsilon_{13} = 0, \quad (15a)$$

$$\varepsilon_{23} = 0, \quad (15b)$$

$$\varepsilon_{33} = -\frac{c_{12}}{c_{11}}(\varepsilon_{11} + \varepsilon_{22}). \quad (15c)$$

The relation between strains, ε_{ij} and the displacement (vector) field $\mathbf{u}$ is [21]:

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right). \quad (16)$$

Combining Eqs. (15a) and (16) yields:

$$\frac{\partial u_1}{\partial x_3} = -\frac{\partial u_3}{\partial x_1}. \quad (17)$$

From Eq. (17), combined with Eq. (13b), we obtain:

$$\frac{\partial u_1}{\partial x_3} = -\frac{\partial w}{\partial x_1}. \quad (18)$$

Integrating Eq. (18) with respect to x_3 yields:

$$u_1 = -x_3 \frac{\partial w}{\partial x_1}. \quad (19)$$

Differentiating Eq. (19) with respect to x_1 and x_2 yields:

$$\varepsilon_{11} = -x_3 \frac{\partial^2 w}{\partial x_1^2} \quad (20)$$

and

$$\varepsilon_{12} = -x_3 \frac{\partial^2 w}{\partial x_1 \partial x_2}. \quad (21)$$

Starting from Eqs. (15b) and (16), we arrive at

$$\varepsilon_{22} = -x_3 \frac{\partial^2 w}{\partial x_3^2}. \quad (22)$$

From Eqs. (15c), (20), and (22), we obtain:

$$\varepsilon_{33} = x_3 \frac{c_{12}}{c_{11}}\left(\frac{\partial^2 w}{\partial x_1^2} + \frac{\partial^2 w}{\partial x_2^2}\right). \quad (23)$$

All strains in the silicon sample are now known:

$$\begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{pmatrix} = \begin{pmatrix} -2x_3 a \\ -2x_3 a \\ 4x_3 a \frac{c_{12}}{c_{11}} \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad (24)$$

From Eq. (12) we find σ_{11}, σ_{22}, and σ_{12}. Summing up, the stresses in the silicon are:

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix} = -2ax_3 \begin{pmatrix} c_{11} + c_{12} - \frac{2c_{12}c_{12}}{c_{11}} \\ c_{11} + c_{12} - \frac{2c_{12}c_{12}}{c_{11}} \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad (25)$$

The stress in the silicon wafer is an equiaxed biaxial stress, as would be expected from a plane stress in the film. Not a priori

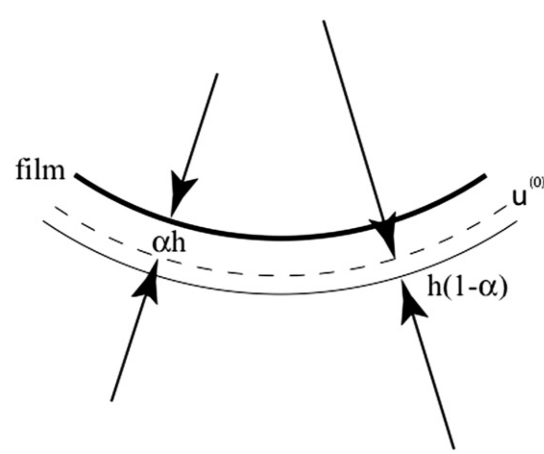

Fig. 2. The wafer is curved due to the stress in the film. A neutral surface, $\mathbf{u}^0$, that is neither compressed nor expanded is assumed, somewhere in the wafer.

expected, however, is the fact that the strain in the silicon wafer is rotationally symmetric (Eq. (24)). This is a consequence of the symmetry and orientation of the silicon crystal.

3.3. Equilibrium

The next step is to balance force and momentum of the film/substrate combination on any cross section of the film/substrate system [3]. The balance will yield the location of the neutral plane and the curvature of the sample. From the fact that Eq. (25) contains only σ_{11} and σ_{22}, the solution is straightforward. The in-plane stress in the silicon substrate, $\sigma_{//}$, with respect to the neutral plane is now given by:

$$\sigma_{//}(x_3) = \sigma_{11}(x_3) = \sigma_{22}(x_3) = -2ax_3\left(c_{11} + c_{12} - \frac{2c_{12}c_{12}}{c_{11}}\right). \quad (26)$$

Assume that the distance from the neutral plane to the film is αh (see Fig. 2). This yields the integration limits for the force- and momentum-balance.

$$\int_{h(\alpha-1)}^{\alpha h} \sigma_{//}(x_3)dx_3 + \sigma_f t_f = 0 \quad (27)$$

$$\int_{h(\alpha-1)}^{\alpha h} x_3\sigma_{//}(x_3)dx_3 + \alpha h\sigma_f t_f = 0. \quad (28)$$

Substitution of Eq. (26) and integration of Eqs. (27) and (28) yields:

$$ah^2(1-2\alpha)\left(c_{11} + c_{12} - \frac{2c_{12}c_{12}}{c_{11}}\right) + \sigma_f t_f = 0 \quad (29)$$

$$-\frac{2ah^3}{3}\left(c_{11} + c_{12} - \frac{2c_{12}c_{12}}{c_{11}}\right)(3\alpha^2 - 3\alpha + 1) + \alpha h\sigma_f t_f = 0. \quad (30)$$

Multiplying Eq. (29) by αh and subtracting it from Eq. (30) yields α=2/3.

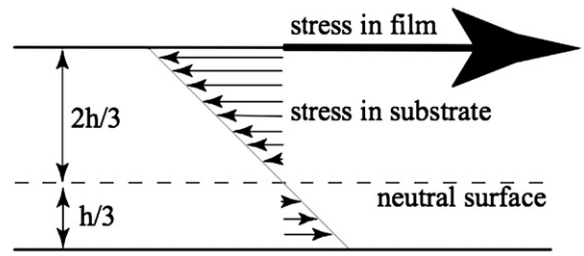

Fig. 3. Distribution of stresses in the film and wafer. The stress gradient in the wafer is caused by the simultaneous requirement of force and momentum equilibrium.

In Fig. 3, a schematic representation of the stresses in film and substrate is given. Inserting α=2/3 in Eq. (29) yields:

$$\sigma_f t_f = \frac{1}{3}ah^2\left(c_{11} + c_{12} - \frac{2c_{12}c_{12}}{c_{11}}\right). \quad (31)$$

Substitution of Eq. (14) in Eq. (31) yields:

$$\sigma_f t_f = \left(c_{11} + c_{12} - \frac{2c_{12}c_{12}}{c_{11}}\right)\frac{h^2}{6R}. \quad (32)$$

The stiffness constants c_{ij} can be expressed in terms of the compliance constants s_{ij} [27],

$$c_{11} + c_{12} - 2\frac{c_{12}c_{12}}{c_{11}} = \frac{1}{s_{11} + s_{12}}. \quad (33)$$

With this substitution, Eq. (32) now reads:

$$\sigma_f t_f = \frac{h^2}{6(s_{11} + s_{12})R}. \quad (3)$$

This is the Stoney equation for Si(001) wafers. The numerical value for $1/(s_{11}+s_{12})$ is $1.803(1)\times 10^{11}$ Nm^{-2}, based on the stiffness numbers reported in Refs. [24] and [25].

4. The Stoney equation for a Si(111) wafer substrate

In the derivation of the Stoney equation for Si(001), we had the constitutive equation in the same coordinate frame as the deformation. For Si(111) wafers, we have the deformation in the frame of the wafer and the constitutive equation in the frame of the crystal. Those two frames are rotated with respect to each other.

In order to describe the elastic deformation of a Si(111) wafer due to the force per unit width exerted by a stressed film, we first transform the constitutive equation to a rotated set of axes suitable for this problem. The unit vectors of this rotated set of axes are $\hat{\mathbf{e}}_i$, i=1,2,3. The unit vectors $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ are perpendicular to each other and lie in the plane of the Si(111) wafer and $\hat{\mathbf{e}}_3$ is perpendicular to the Si(111) wafer. For the calculation of the deformation of a Si(111) wafer, $\hat{\mathbf{e}}_1$ replaces x_1 in Fig. 1 and $\hat{\mathbf{e}}_2$ replaces x_2.

As new unit vectors, we choose:

$$\hat{\mathrm{e}}_1 = \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{pmatrix}, \quad \hat{\mathrm{e}}_2 = \begin{pmatrix} 1/\sqrt{6} \\ 1/\sqrt{6} \\ -2/\sqrt{6} \end{pmatrix}, \quad \hat{\mathrm{e}}_3 = \begin{pmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{pmatrix}. \quad (34)$$

All mutual dot products between these unit vectors are zero and the vector product of the first two yields the third, accounting for the right handedness of the new unit vectors.

The transformation matrix, T, from the set of axes $\mathbf{x}$ to the set of axes $\hat{\mathbf{x}}$ is:

$$T = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{6} & 1/\sqrt{3} \\ -1/\sqrt{2} & 1/\sqrt{6} & 1/\sqrt{3} \\ 0 & -2/\sqrt{6} & 1/\sqrt{3} \end{pmatrix}, \quad (35)$$

The inverse transformation is given by the transpose of T, T^t:

$$T^t = \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6} \\ 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \end{pmatrix}. \quad (36)$$

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Now assume a stress tensor $\hat{\overline{\overline{\sigma}}}$ in the rotated coordinate system. With the use of Eq. (37), we can calculate the stress in the original coordinate system:

$$\overline{\overline{\sigma}} = T \cdot \hat{\overline{\overline{\sigma}}} \cdot T^t.$$

We can now determine ε in the original coordinate system from Eq. (38) below, which is the inverse of Eq. (12).

$$\begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} & s_{12} & & & \\ s_{12} & s_{11} & s_{12} & & & \\ s_{12} & s_{12} & s_{11} & & & \\ & & & s_{44} & & \\ & & & & s_{44} & \\ & & & & & s_{44} \end{pmatrix} \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix}, \tag{38}$$

with s_{ij} the compliance constants. For cubic crystals, the compliance constants can readily be expressed in terms of the stiffness constants [27]:

$$s_{11} = \frac{c_{11} + c_{12}}{(c_{11} - c_{12})(c_{11} + 2c_{12})}, \quad s_{12} = \frac{-c_{12}}{(c_{11} - c_{12})(c_{11} + 2c_{12})}, \quad s_{44} = \frac{1}{c_{44}}. \tag{39}$$

Now, we obtain $\hat{\varepsilon}$ from ε by applying the following transformation,

$$\hat{\overline{\overline{\varepsilon}}} = T^t \cdot \overline{\overline{\varepsilon}} \cdot T. \tag{40}$$

Knowing all components of the strain tensor, $\hat{\overline{\overline{\varepsilon}}}$, for an assumed stress tensor, $\hat{\overline{\overline{\sigma}}}$, allows us to express $\hat{\overline{\overline{\varepsilon}}}$ as a function of $\hat{\overline{\overline{\sigma}}}$. This is done in the constitutive Eq. (41) below.

$$\begin{pmatrix} \hat{\varepsilon}_{11} \\ \hat{\varepsilon}_{22} \\ \hat{\varepsilon}_{33} \\ 2\hat{\varepsilon}_{23} \\ 2\hat{\varepsilon}_{13} \\ 2\hat{\varepsilon}_{12} \end{pmatrix} = \begin{pmatrix} \frac{s_{11}}{2} + \frac{s_{12}}{2} + \frac{s_{44}}{4} & \frac{s_{11}}{6} + \frac{5s_{12}}{6} - \frac{s_{44}}{12} & \frac{s_{11}}{3} + \frac{2s_{12}}{3} - \frac{s_{44}}{6} & \frac{s_{11}\sqrt{2}}{3} - \frac{s_{12}\sqrt{2}}{3} - \frac{s_{44}\sqrt{2}}{6} & 0 & 0 \\ \frac{s_{11}}{6} + \frac{5s_{12}}{6} - \frac{s_{44}}{12} & \frac{s_{11}}{2} + \frac{s_{12}}{2} + \frac{s_{44}}{4} & \frac{s_{11}}{3} + \frac{2s_{12}}{3} - \frac{s_{44}}{6} & -\frac{s_{11}\sqrt{2}}{3} + \frac{s_{12}\sqrt{2}}{3} + \frac{s_{44}\sqrt{2}}{6} & 0 & 0 \\ \frac{s_{11}}{3} + \frac{2s_{12}}{3} - \frac{s_{44}}{6} & \frac{s_{11}}{3} + \frac{2s_{12}}{3} - \frac{s_{44}}{6} & \frac{s_{11}}{3} + \frac{2s_{12}}{3} + \frac{s_{44}}{3} & 0 & 0 & 0 \\ \frac{s_{11}\sqrt{2}}{3} - \frac{s_{12}\sqrt{2}}{3} - \frac{s_{44}\sqrt{2}}{6} & -\frac{s_{11}\sqrt{2}}{3} + \frac{s_{12}\sqrt{2}}{3} + \frac{s_{44}\sqrt{2}}{6} & 0 & \frac{4s_{11}}{3} - \frac{4s_{12}}{3} + \frac{s_{44}}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{4s_{11}}{3} - \frac{4s_{12}}{3} + \frac{s_{44}}{3} & \frac{2s_{11}\sqrt{2}}{3} - \frac{2s_{12}\sqrt{2}}{3} - \frac{s_{44}\sqrt{2}}{3} \\ 0 & 0 & 0 & 0 & \frac{2s_{11}\sqrt{2}}{3} - \frac{2s_{12}\sqrt{2}}{3} - \frac{s_{44}\sqrt{2}}{3} & \frac{2s_{11}}{3} - \frac{2s_{12}}{3} + \frac{2s_{44}}{3} \end{pmatrix} \begin{pmatrix} \hat{\sigma}_{11} \\ \hat{\sigma}_{22} \\ \hat{\sigma}_{33} \\ \hat{\sigma}_{23} \\ \hat{\sigma}_{13} \\ \hat{\sigma}_{12} \end{pmatrix}. \tag{41}$$

In order to calculate the curvature of a Si(111) wafer due to a stressed film, we employ Eq. (41) and make use of the assumption that the neutral plane of the wafer has the form:

$$\hat{u}_3^{(0)} = a\hat{x}_1^2 + a\hat{x}_2^2. \tag{42}$$

From Eq. (42) we obtain:

$$\hat{\varepsilon}_{11} = \hat{\varepsilon}_{22} = -2a\hat{x}_3, \quad \hat{\varepsilon}_{12} = 0. \tag{43}$$

From the free surface of the wafer with the moments being constant, we have:

$$\hat{\sigma}_{13} = \hat{\sigma}_{23} = \hat{\sigma}_{33} = 0. \tag{44}$$

Combining Eqs. (43), (44) with Eq. (41) yields all stresses and strains:

$$\begin{pmatrix} \hat{\sigma}_{11} \\ \hat{\sigma}_{22} \\ \hat{\sigma}_{33} \\ \hat{\sigma}_{23} \\ \hat{\sigma}_{13} \\ \hat{\sigma}_{12} \end{pmatrix} = -2a\hat{x}_3 \begin{pmatrix} \frac{6}{4s_{11} + 8s_{12} + s_{44}} \\ \frac{6}{4s_{11} + 8s_{12} + s_{44}} \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{45}$$

$$\begin{pmatrix} \hat{\varepsilon}_{11} \\ \hat{\varepsilon}_{22} \\ \hat{\varepsilon}_{33} \\ \hat{\varepsilon}_{23} \\ \hat{\varepsilon}_{13} \\ \hat{\varepsilon}_{12} \end{pmatrix} = -2a\hat{x}_3 \begin{pmatrix} 1 \\ 1 \\ \frac{4s_{11} + 8s_{12} - 2s_{44}}{4s_{11} + 8s_{12} + s_{44}} \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{46}$$

Just as in the case of the Si(001) wafer, the stress in the silicon wafer is an equiaxed biaxial stress, as would be expected from a plane stress in the film. Not a priori expected, however, is the fact that the strain in the silicon is rotationally symmetric (Eq. (46)). This, again, is a consequence of the symmetry and orientation of the silicon crystal.

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Now, working through the formulas as for Si(001), we find:

$$\sigma_f t_f = \left(\frac{6}{4s_{11} + 8s_{12} + s_{44}}\right)\frac{h^2}{6R}. \tag{5}$$

This is the Stoney equation for Si(111) wafers. The numerical value of $6/(4s_{11}+8s_{12}+s_{44})=2.291(1)\times10^{11}$ Nm^{-2}, based on the stiffness constants reported in Refs. [24] and [25].

In this section, we derived an analytical solution for Si(111) wafers. It should be emphasized however, that this was only possible due to the very special structure of the constitutive equation as shown in Eq. (41). In the solution the only non-zero stress components are σ_{11} and σ_{22}. Eq. (41) demonstrates that the effect of σ_{11} and σ_{22} on components ε_{11} and ε_{22} exhibits symmetry, that is the 11 and 22 components of the matrix are identical.

5. Experimental results

In order to discuss the validity of the Stoney equation for the deformation of silicon wafers we need to look at radial symmetry and at the shape of the radial deformation. Is the shape purely quadratic, see Eqs. (13a) and (13b), or does the deformed shape contain higher order terms?

From previous work [29], we know that the deformation of 100 mm diameter Si(001) wafers due to a film under stress is not completely radially uniform. We now present two series of measurements of the direction dependent curvature for three film thicknesses, one series on 100 mm diameter Si(001) and one series on 100 mm diameter Si(111) wafers. Moreover, we used a sample reported on previously [29] to check the radial shape of the deformation in order to confirm the validity of the assumed deformation mode in Eqs. (13a) and (13b).

We deposited two series of W films on Si(001) and Si(111) wafers for 30 min, 1 hour and 2 hours in an AJA magnetron sputter deposition system. The target diameter was 5.1 cm and target power was 148 W, resulting in a target voltage of approximately 400 V. The target to substrate distance was 11 cm. The argon pressure was kept at 0.20 Pa. The substrate was rotated at 10 rpm in order to obtain an in-plane isotropic film. The resulting growth rate was 3 nm/min. The thicknesses of the films deposited on Si(001) wafers were 89, 178 , and 355 nm. The thicknesses on Si(111) were 88, 179, and 358 nm. The thicknesses were determined from weighing the wafers before and after deposition and assuming bulk film density. The curvature of the wafers was measured before and after deposition by reflecting two parallel laser beams, 40 mm apart, off the wafer and recording the distance between the two beams on a distant screen [30]. The plane through the laser beams intersects the plane of the wafer at a 90 degrees angle. We record the curvature as a function of the angle α between this intersection line and the optical flat (see Fig. 4). We start with the intersection line parallel to the flat, α=0°, and measured at 15° intervals from 0° to 360°. At angles greater than 180°, the two laser beams are interchanged, yielding an internal check on the accuracy of the measurement. The angle dependent curvature of all six samples can be fitted with:

$$1/R_{f/s} - 1/R_s = C_1 + C_2 \sin\left(4\pi\left(\frac{\alpha - C_3}{360}\right)\right), \tag{47}$$

with $1/R_{f/s}$ the curvature of the film/substrate sample and $1/R_s$ the curvature of the substrate prior to deposition of the film. C_1 is the average curvature, C_2 the amplitude of the perturbation on the average curvature, and C_3 gives the phase of the perturbation with respect to the [1$\bar{1}$0] direction. In Fig. 5 an example of this angle dependent curvature is presented for a 358 nm-thick tungsten film on a Si(111) wafer. The angle dependent curvature is given for all six samples in Table 3.

In column 5 of Table 3, it can be seen that for Si(001) wafers the deviation from a radially symmetric deformation is largest, 4.7%, at small curvatures and decreases rapidly for larger curvatures. For Si (111) wafers, the deviation from radially symmetric deformation is of the order of 2–3% and independent of curvature.

In a previous publication [29], we reported on the deviation from cylindrical deformation symmetry of the shape of a Si(001) wafer covered with a 230 nm-thick W film. We now also report on the uniqueness of the curvature along line scans through the center of the wafer, obtained with a WYKO optical profiler. We made line scans through the center of the wafer in the stiff directions [$\bar{1}$10] and [110], and along the crystal axes [100] and [010]. The line scan in the [$\bar{1}$10] direction is shown in Fig. 6. After correcting for tilt, the curves were fitted to a quadratic expression. Fig. 7 shows the residuals of the quadratic fit to the data presented in Fig. 6. The residuals of the four fits are small compared to the deformation and do not contain a symmetric component. Thus the assumption of a quadratic deformation is justified.

In Fig. 8, the curvature C_1 as a function of thickness is presented for the Si(001) wafers (dots) and Si(111) wafers (squares). The lines are

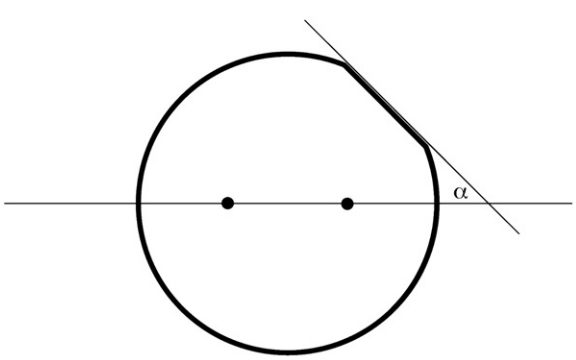

Fig. 4. Definition of the angle α between line through the laser spots and the flat of the wafer.

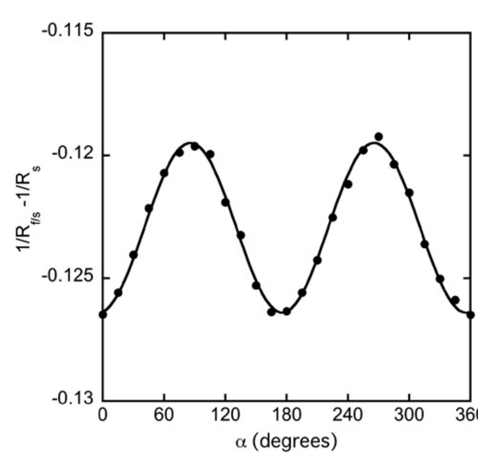

Fig. 5. Angle dependent curvature of a Si(111) wafer covered with a 358-nm-thick tungsten film. For the definition of α, see Fig. 4. The subscripts f/s and s refer to film/substrate and substrate, respectively.

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Table 3
Sample parameters, including Si substrate orientation and W film thickness for all six angle-dependent curvature measurements

Si wafer orientation	W film thickness (nm)	C_1 (m^{-1})	C_2 (m^{-1})	$\lvert C_2/C_1 \rvert$	C_3 (°)	Rc
001	89	−0.03909	0.001751	0.0479	11.7	0.982
001	178	−0.08138	0.000709	0.0087	42.8	0.857
001	355	−0.17057	0.000879	0.0051	51.6	0.823
111	88	−0.02905	0.000933	0.0321	47.7	0.949
111	179	−0.06327	0.001314	0.0208	64.2	0.991
111	358	−0.12294	0.003462	0.0282	40.7	0.997

C_1 and C_2 are fitting parameters, with units of m^{-1}, in Eq. (47). The ratio $|C_2/C_1|$ represents relative size of the deviation from a cylindrical deformation. C_3 is a fitting parameter with units of degrees. It signifies the orientation of the deviation with respect to the [011] direction. R_c is the linear correlation coefficient, a measure for the quality of the fit.

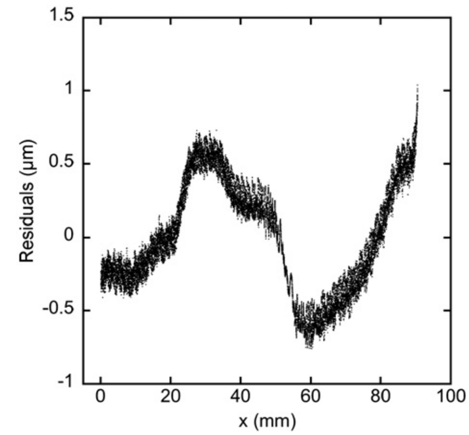

Fig. 7. Residuals of the quadratic fit to the shape of the Si(001) wafer, depicted in Fig. 6.

linear fits through the origin. It can be seen that the magnitude of the curvature increases linearly with film thickness. This is interpreted as a thickness-independent stress in the film. It can also seen that for the same W film thickness, the Si(001) wafers exhibit more curvature than the Si(111) wafers. In principle the ratio of the slopes of the two straight lines yields the ratio of the biaxial moduli of the substrates. However, not all wafers have exactly the same thickness and on average the (111) wafers are a few percent thicker than the (001) wafers; therefore, we calculated the ratio of the biaxial moduli, M_{111}/M_{001}, per pair of measurements. We corrected the measured curvature of the Si(001) wafers by the thickness ratio of the W films on Si(001) and Si(111). The result for the three film thicknesses is: $M_{111}/M_{001}=1.30\pm0.05$

6. Discussion

The first point to be discussed is the amazing result that (001) and (111) silicon single crystal substrates, with an elastic anisotropy of 30% [21,22], deform radially symmetric, within a few percent under the action of a film in plane stress. This is due to the form of the strain tensors given in Eqs. (24) and (46). The tensors are a result of the symmetry in the constitutive equations, Eqs. (12) and (41). It is because of this symmetry that it is possible to define a biaxial modulus M_{hkl} for Si(001) and Si(111) wafers, see Eqs. (4) and (6). For silicon wafers with a less symmetric orientation, e.g. Si(011) wafers, a film in plane stress does not induce a rotationally symmetric strain in the silicon, and the resulting deformation will not be rotationally symmetric [2].

The biaxial modulus of Si(001) is $M_{001}=1.803(1)$ GPa. The biaxial modulus of Si(111) is $M_{111}=2.291(1)$ GPa. The ratio of these moduli is 1.27. In the section on experimental results, we determined the curvature of Si(001)- and Si(111)-wafers due to the same force per unit width. The ratio of these curvatures is 1.30±0.05 agreeing with the ratio of the biaxial moduli within the experimental accuracy.

From Figs. 6 and 7, it is clear that the shape of the deformed wafer is indeed quadratic, as assumed in Eqs. (13a) and (13b). The 230 nm thick W film induces a force per unit width of 0.77 GPa µm, leading to a curvature of −0.093 m^{-1}. According to finite elements calculations a force per unit width up to 1.9 GPa µm will yield a quadratic deformation [16].

An unresolved point remains the deviation from a radially symmetric curvature. This deviation is on the order of a few percent. For Si(001), the relative deviation ($|C_2/C_1|$) decreases with increasing curvature; for Si(111) wafers, the relative deviation seems constant. Also, the orientation of this deviation, C_3, is not understood. At present, we assume that the deviation from a radially symmetric deformation is due to the non perfect radial symmetry of the problem, caused by the flat of the Si-wafer.

7. Conclusions

Forms of the Stoney equation for Si (001) and (111) wafers have been derived, Eqs. (3) and (5), respectively. These forms remove the problem of having to assign values for E and ν to an elastically anisotropic material and should therefore be used instead of Eq. (2) in wafer curvature measurements for describing film stress on Si (001) and Si(111) wafers. The validity of Eqs. (3) and (5) is demonstrated by the fact that the measured ratio in curvature

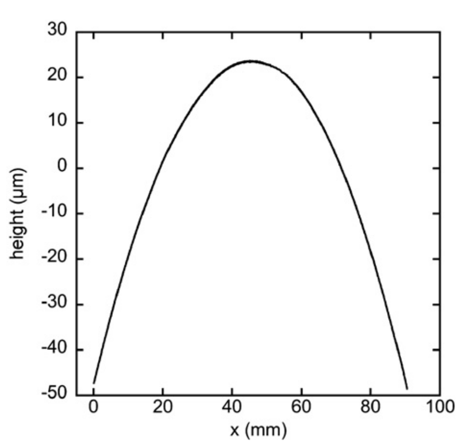

Fig. 6. Shape of a Si(001) wafer covered with a 230-nm-thick tungsten film, measured in the [$\bar{1}$10] direction.

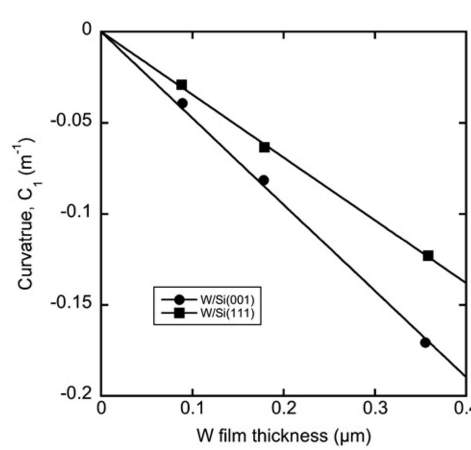

Fig. 8. Curvature, C_1, as function of tungsten film thickness for all samples from Table 3. Dots depict the Si(001) wafer data, squares represent Si(111) wafer data.

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between Si(001) and Si(111) substrates covered by identical films is equal to the calculated ratio of biaxial moduli of Si(001) and Si(111) wafers.

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Appendix A. Reduction of the Stoney Equation for Si(001) and Si(111) substrates to the "isotropic" Stoney Equation

The anisotropy ratio AR for a cubic material indicates the degree of departure from elastic isotropy [27]. This ratio is defined as:

$$\mathrm{AR} = \frac{2c_{44}}{c_{11}-c_{12}}, \quad \text{or } \mathrm{AR} = \frac{2(s_{11}-s_{12})}{s_{44}}. \tag{A1}$$

For silicon, the anisotropy ratio is 1.57. For elastically isotropic crystals, AR = 1, and E and ν have a well defined meaning independent of direction:

$$E = \frac{1}{s_{11}}, \quad \text{and } \nu = -\frac{s_{12}}{s_{11}}. \tag{A2}$$

Substitution of Eq. (A2) in Eq. (3) yields Eq. (2). To arrive at Eq. (2) starting from Eq. (5) one has also to use the relation AR = 1.

Appendix B. Clamped substrate

The stress in the film, σ_f in Eq. (3), is the value for the curved state of the substrate. A typical deposition procedure is to deposit the film on a clamped substrate, which is allowed to bend after the deposition. In this Appendix it is demonstrated that by this bending only a very small fraction of the stress in the film is relieved. If the film is deposited on a clamped substrate in a stressed state, σ_i, then the relation between those two stresses is:

$$\sigma_i = \sigma_f + \Delta\sigma_f \tag{B1}$$

with

$$\Delta\sigma_f = \frac{2hE_f}{3R(1-\nu_f)}. \tag{B2}$$

Combining Eqs. (B2) and (3) we see the magnitude of the correction:

$$\frac{\Delta\sigma_f}{\sigma_f} = 4\frac{E_f(s_{11}+s_{12})}{(1-\nu_f)}\frac{t_f}{h} \tag{B3}$$

Since the thickness of the film is typically a few orders of magnitude smaller than the thickness of the substrate, and the stiffness of the film is never an order of magnitude larger than the stiffness of the substrate, the correction is typically less than 1%.

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