

# Deformation in Silicon Wafers: Influence of Material Symmetry and Boundary Conditions

Edeltraud Gehrig

Hochschule RheinMain University of Applied Sciences, Wiesbaden Rüsselsheim, Kurt-Schumacher-Ring 18, 65197 Wiesbaden, Germany

**Abstract**—The spatial displacement of a silicon wafer in a mounting is studied using finite elements including stress-strain relations, frequency analysis and gravity load. Simulations of various mounting configurations visualize the dependence of deformations and eigenmodes on boundary conditions such as positioning of four fixation points at the rim, the orientation of the wafer in the geometry and of the relative orientation of the crystallographic axis of this orthotropic material with respect to the wafer plane.

**Keywords**— Material, simulation, eigenmode, wafer.

## I. INTRODUCTION

Silicon wafers are known for their relevance in a large variety of applications such as integrated circuits or solar cells and have been in the focus of various theoretical investigations [1-4]. The handling and storage of Silicon wafers requires suitable holding devices realized e.g. by a number of fixation points along the rim of the wafer. The mounting conditions can significantly stress the material leading to unwanted deformations and mechanical oscillations [5] that strongly depend on the orientation of the wafer within the mounting. Inspired by this observation we here analyze the dependence of the wafer deformation and of the eigenmodes belonging to the ten lowest eigenfrequencies on the mounting geometry. We focus, in particular on the influence of the spatial positions of fixation points along the rim under the influence of gravitational load for different orientations of the crystal lattice relative to the geometry.

## II. THEORETICAL DESCRIPTION

We start from Hooke's law [6] assuming a linear response of a deformable continuum to tension

$\mathbf{t} = \mathbf{C}\boldsymbol{\varepsilon}$  or, in index notation,  $t_{ij} = C_{ijkl}\varepsilon_{kl}$  where  $\mathbf{t}$  is Cauchy' stress tensor and  $\boldsymbol{\varepsilon}$  the total strain tensor, which can be expressed in terms of the displacement gradient as [7-9]

$\varepsilon_{i,j} = \frac{1}{2}(u_{i,j} + u_{j,i})$  where,  $i$  is chosen as notation for the spatial derivatives.

The elasticity tensor can be represented by a 6x6 matrix which for the orthotropic material Silicon reads [7-9]

$$C = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} \quad (1)$$

with  $C_{11} = C_{1111}, C_{12} = C_{1122} = C_{2211}$  where we have used the Voigt notation [7.8] for the elastic stiffness of the material with  $C_{11} = 165,7 \cdot 10^9$  Pa,  $C_{12} = 63,9 \cdot 10^9$  Pa, and  $C_{44} = 79,6 \cdot 10^9$  Pa

The wafer is located in a 4-point mounting with variable boundaries. We vary the angle  $\alpha$  within a pair of mounting points and the angle  $\beta$  describing the rotation of the Silicon wafer within the wafer mounting (see Fig.1). Due to the anisotropic elastic properties of the material, the orientation within the mounting has, as we will see in the following, an additional influence on eigenforms.

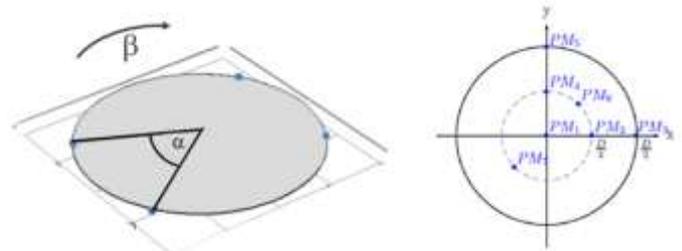


Fig. 1. Wafer geometry and angles used in the simulations.

We here refer to [100] and [111] wafer where the brackets refer to the Miller indices [6] of a particular plane. Generally, our model allows the simulation of any orientation of the material system relative to the geometry of a mounting by rotating the local material coordinate system with respect to the global geometry parameters.

We perform our calculations on the basis of finite elements using the software COMSOL Multiphysics®.

Solving

$$\rho\omega^2\mathbf{u} - \nabla\mathbf{t} = \mathbf{F}_v \quad (2)$$

with the volume force (due to the wafer's weight)  $\mathbf{F}_v$ , angular frequency  $\omega$  (with  $\omega = 2\pi f$ ), the density of silicon  $\rho$  and the displacement vector  $\mathbf{u}$  allows a study of eigenfrequencies  $f_i$  and eigenmodes and the calculation of stationary displacements.

## III. SIMULATION OF THE DEFORMATION

The equilibrium displacements are summarized in Fig. 2 and Fig. 3 in dependence of  $\alpha$  for the situations with maximum changes, i.e.  $\beta=0^\circ$  and  $\beta=45^\circ$ . The displacements at seven reading points are additionally shown in table I for the [100] wafer and in table II for the [111] wafer, respectively.

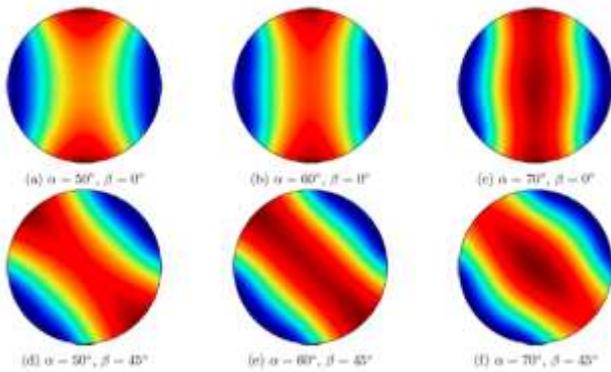


Fig. 2. Deformation in equilibrium ([100] wafer).

TABLE I. Displacement ( $10^{-3}m$ ) in the reading points  $PM_i$ ([100] wafer).

$\beta$	0 deg			45 deg		
$\alpha$	50 deg	60 deg	70 deg	50 deg	60 deg	70 deg
$PM_1$	0.2789	0.2285	0.1868	0.3287	0.2520	0.1790
$PM_2$	0.3269	0.2805	0.2414	0.2944	0.2434	0.1994
$PM_3$	0.3585	0.2923	0.2328	0.2346	0.1948	0.1638
$PM_4$	0.4596	0.3511	0.2460	0.2803	0.2417	0.2114
$PM_5$	0.2789	0.2285	0.1868	0.2346	0.1948	0.1638
$PM_6$	0.2066	0.1751	0.1536	0.1788	0.1543	0.1395
$PM_7$	0.0572	0.0495	0.0256	0.0397	0.0310	0.0104

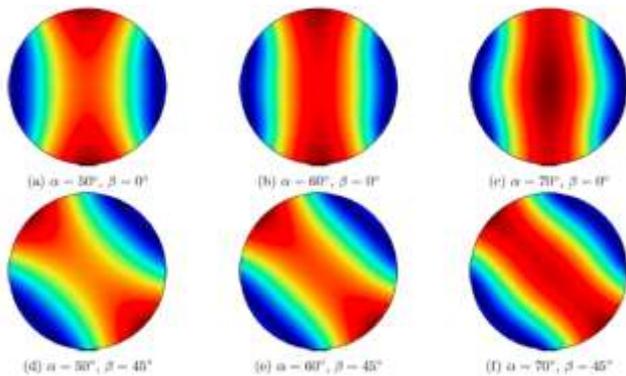


Fig. 3. Deformation in equilibrium ([111] wafer).

TABLE II. Displacement ( $10^{-3}m$ ) in the reading points  $PM_i$ ([111] wafer).

$\beta$	0 deg			45 deg		
$\alpha$	50 deg	60 deg	70 deg	50 deg	60 deg	70 deg
$PM_1$	0.2148	0.1791	0.1494	0.4519	0.3480	0.2482
$PM_2$	0.2555	0.2206	0.1912	0.3574	0.2884	0.2270
$PM_3$	0.2731	0.2262	0.1836	0.2791	0.2244	0.1793
$PM_4$	0.3206	0.2482	0.1772	0.3275	0.2743	0.2297
$PM_5$	0.2148	0.1792	0.1495	0.2791	0.2245	0.1793
$PM_6$	0.1624	0.1401	0.1252	0.2070	0.1697	0.1430
$PM_7$	0.0386	0.0307	0.0115	0.0585	0.0531	0.0330

A comparison of the average displacement in the central point  $PM_1$  shows that the [111] wafer reacts much more critical to changes in the angle  $\beta$  although the average deformation within the mounting looks rather uniform in all cases. Indeed, this sensitivity leads to characteristic

oscillations as observed in experiments [5]. This behavior is a direct consequence of the orientation of the crystal structure within the plane of the mounting leading to different frequency contributions as will be discussed in the next section.

#### IV. SIMULATION OF THE ROTATION SENSITIVITY OF THE EIGENMODES

In the following, we will look at the dynamic behavior of the device in its mounting. Generally, one has a superposition of various eigenfrequencies that determine the elongation at a specific time step and the eigenmodes. The shift of the frequencies in dependence on geometry has been discussed in [10]. Here we focus on the eigenmodes that strongly affect the displacement and tension of a wafer in a given geometry. The number of these modes and their influence in the overall dynamics thereby depends on the initial conditions, e.g. excitation via external vibrations in the environment or simply the influence of gravitational load.

In the following we refer to a typical configuration with an angle  $\alpha=60^\circ$  between the fixation points and rotate a [111] wafer with a diameter of 450 mm and a thickness of 0,925 mm in the plane of the mounting configuration (rotation angle  $\beta$ ). Due to the [111] orientation (i.e. the material system is rotated with respect to the mounting plane) and the large diameter this system is expected to show a significant dependence on rotation angle under the influence of gravitational load.

We calculate the eigenmodes belonging to the first ten eigenfrequencies  $f_1 \dots f_{10}$  of the device and investigate their dependence on rotation angle.

Fig.4 summarizes the eigenmodes calculated for the wafer for  $\alpha = 60^\circ$  and  $\beta = 0^\circ$ . In order to visualize the dependence on  $\beta$  we refer to mode  $f_4$  and  $f_7$  which showed a quite distinct change in deformation.

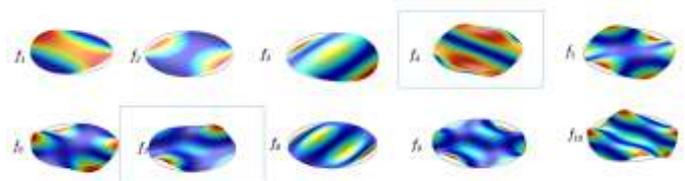


Fig. 4. Eigenforms belonging to the ten lowest frequencies

Figs. 5 and 6 visualize the dependence of the eigenmodes belonging to  $f_4$  and  $f_7$  on rotation angle  $\beta$ . The repetitions in the pattern directly reflect the crystal symmetry of the device.

The simulations reveal a dependence of the eigenmodes of the [111] wafer on mounting geometry. As a consequence, a wafer in a mounting may show a quite unstable behavior and show characteristic oscillations due to a high sensitivity to the exact positioning in the mounting. This is a direct consequence of the relative orientation of the crystal axis in the mounting leading to a corresponding dependence of the elastic properties via a rotation of the elasticity tensor (eq. (1)).

V. CONCLUSION

Simulations of Silicon wafer oscillations demonstrate deformations and oscillations that depend on boundary conditions realized by a wafer mounting. Taking into account, in particular, the orthotropic material properties and the arbitrary orientation of the wafer within the mounting the model allows a prediction of experimentally observed behavior as well as an optimization of a system. Our results demonstrate that the mode shapes can be controlled by suitable positioning and orientation of the wafer in the mounting. In particular, a deliberately chosen mounting configuration may stabilize the system and allow the suppressing of oscillations.

REFERENCES

- [1] F. Ebrahimi and L. Kalwani, "Fracture anisotropy in silicon single crystal," *Materials Science and Engineering A*, vol. 268, pp. 116-126, 1999.
- [2] J. Chen, I. De Wolf, "Study of fagme and stress induced by backgrounding in Si Wafers," *Semiconductor Science and Technology*, vol. 18, issue 4, pp. 261—268, 2003
- [3] P.-O. Logerais, O. Riou, F. Delaleux, J.-F. Durastanti, A. Bouteville, "Improvement of temperature homogeneity of a silicon wafer heated in a rapid thermal system (RTP: Rapid Thermal Process) by a filtering window," *Applied Thermal Engineering*, vol. 77, pp. 76-89, 2015.
- [4] G. Ionascu, A. Sandu, E. Manea, L. Bogatu, "Aspect regarding the elastic properties of Silicon and its influence of the behavior of micro-mechanical components," *International Research Journal of Engineering and Technology*, vol. 3, issue 1, pp. 16-20, 2016.
- [5] H. Wenz, Private Communication, Rudolph Technologies Germany GmbH.
- [6] P. Hofmann, *Solid State Physics*, Wiley, 2008.
- [7] A. J. M. Spencer, *Continuum Mechanics*, Courier Corporation, 2004.
- [8] J. N. Reddy, *An Introduction to Continuum Mechanics*, Cambridge University Press, 2007.
- [9] H. Altenbach, *Advanced Materials Modelling for Structures*, Springer, 2005.
- [10] E. Gehrig, *Proceedings of the 2015 COMSOL Conference*, Grenoble, 2015.

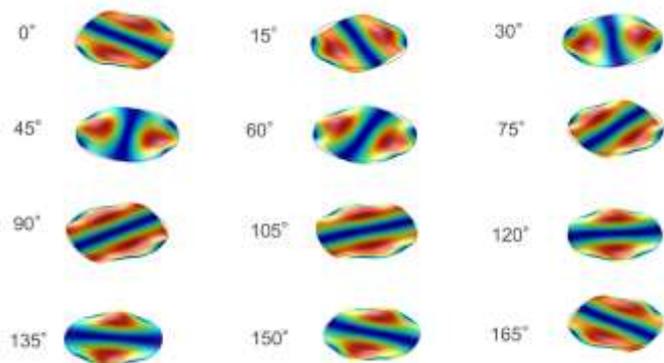


Fig. 5. Dependence of  $f_4$  on rotation angle  $\beta$ .

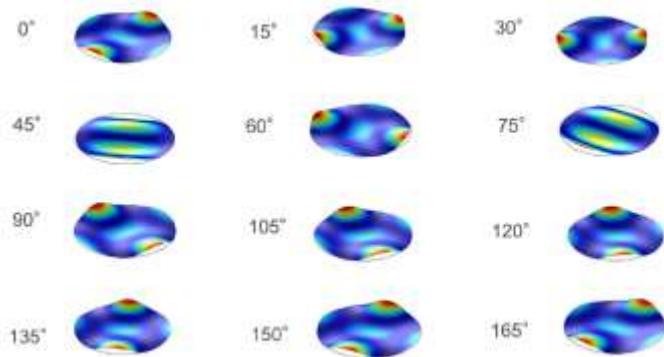


Fig. 6. Dependence of  $f_7$  on rotation angle  $\beta$ .

As an example Fig. 7 shows the temporal behavior of a [111] wafer close to the angular position where the mode pattern changes under the influence gravitational load. The directional dependence of the elasticity properties entering the equations in combination with the changes in the displacement lead to characteristic oscillations revealing the switching between neighbouring modes even though the temporal average of the induced tension appears uniform.

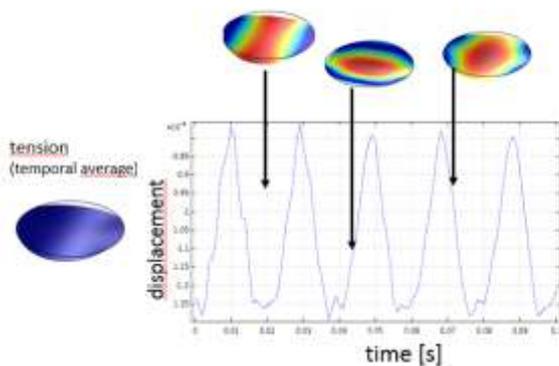


Fig. 7. Temporal behavior under gravitational load close to  $\beta=45^\circ$ .

Our simulation show that the symmetry of a given material strongly affect both eigenforms and stability of a device. The simulations thus allow for a given situation the prediction of experimental observations and an optimization of boundary conditions.