

Wafer Bifurcation as a Spontaneous Symmetry Breaking

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Abstract

A connection between the phenomenon of wafer bifurcation and that of spontaneous symmetry breaking (SSB) has been established. Indeed, by developing an analytical approximation of the elastic energy of a wafer coated with a thin layer (e.g. a metal), it is shown as the elastic potential energy, interpreted as a quantity contributing to the thermodynamic free energy, can be investigated within the framework of the Landau theory of the second order phase transitions. The elastic energy of a bifurcated wafer is a complex function of the stress and the curvatures in the two perpendicular directions. In this work, it is shown as a translation of the coordinate system of the curvatures allows to gain a potential which has a “Mexican hat” shape. This is a distinctive trait of the phenomenon of spontaneous symmetry breaking (SSB). Moreover, it is shown as the values of the coordinates at the minimum of the SSB potential agrees with those provided by the theory. Bifurcation is hence a phenomenon that can also be interpreted as a spontaneous symmetry breaking where the rotational symmetry of a disc shaped wafer is broken. It occurs because of a lowering of the wafer energy in the SSB broken symmetry configuration.

Keywords: Bifurcation, Wafer, Spontaneous Symmetry Breaking, Finite Element Analysis (FEA), Simulations.

Introduction

Wafer bifurcation [1] [2] [3] [4] [5] [6] occurs when the mismatch strain overcomes a specific and system dependent critical value. The result is an asymmetric warpage increase [7] [8]. For example, in a semiconductor wafer (considered as a symmetric disc) it determines a transition from a high symmetric configuration, namely a symmetric paraboloid (usually referred as the spherical case) to a lower symmetry, specifically an elliptic paraboloid (usually referred as the cylindrical case). In the work [9] we have investigated the phenomenon of bifurcation. In particular, an analytical model of the dependence of the bifurcation energy of the substrate on the residual stress has been developed for a metalized wafer and validated by exploiting Finite Element Analysis (FEA) methods. Some results are hereafter summarized. In Fig. 1, the normalized curvature versus normalized mismatch strain of a wafer, including the linear and nonlinear (large deformation) regimes and the case of the bifurcation regime [2]. Below the bifurcation point, the behavior is approximated by the Freund's equation [8] [10], whereas the behavior determined by the Stoney's theory is described by the line of slope 1. In the bifurcation regime, the average curvatures of a bifurcated wafer lie on the line from the origin to the bifurcation point. In Fig. 2 the distribution of the directional deformation, along z in an 8" silicon wafer, 500 μm thick metalized with a 4.5 μm Al layer, simulated with ANSYS 2021 R1 [11], is reported from ref [9].

In this work we want to evidence a link that exists between the elastic energy of a wafer and the phenomenon of the spontaneous symmetry breaking (SSB). SSB [12] is a mechanism which manifests in several fields of physics, ranging from second order phase transitions to particle physics mass diversification. It occurs when a configuration is energetically favored at the expenses of a loss of symmetry of the whole system.

SSB mechanism in the elastic energy of a bifurcated wafer

The configuration that a metalized wafer assumes, at thermal equilibrium, is related to the minimum of the elastic potential energy V accumulated in the substrate. This energy, which solves the role of a thermodynamic free energy, depends on the residual stress σ and the curvature κ . As reported in [9], by reasoning on the linear regime, the non-linear approximation in the spherical case, and the extension to the bifurcation case, we can write the elastic energy of a bifurcated wafer as:

$$V(\sigma, \kappa, \kappa_{\perp}) = -\frac{4}{3} h_f h_s \pi R^2 \left[\sigma \frac{\kappa + \kappa_{\perp}}{2} - \frac{1}{24} \frac{E_s}{1 - \nu_s^2} \frac{h_s^2}{h_f} (\kappa^2 + 2\nu_s \kappa \kappa_{\perp} + \kappa_{\perp}^2) - \frac{E_s}{24} \frac{1}{h_f} \frac{R^4}{16} \kappa^2 \kappa_{\perp}^2 \right] \quad (1),$$

where κ and κ_{\perp} are the principal curvatures of the bifurcated wafer, h_s the substrate and h_f the film thicknesses, R the radius of the wafer, E_s the Young's module and the ν_s Poisson's coefficient of the substrate. This equation can be modified further. Indeed, by rescaling the curvatures as $K = \frac{\kappa}{\kappa_{bif}}$ and $K_{\perp} = \frac{\kappa_{\perp}}{\kappa_{bif}}$ with respect to the curvature κ_{bif} , which marks the onset

of the bifurcation, and by defining a new energy scale as $F_0 = -\frac{4}{3} h_f h_s \pi R^2 \frac{1}{24} \frac{E_s}{1 - \nu_s^2} \frac{h_s^2}{h_f} \kappa_{bif}^2$, as

well by writing a new factor \mathcal{H} as $\mathcal{H} = \frac{24(1 - \nu_s^2) h_f}{E_s} \frac{1}{h_s^2 \kappa_{bif}}$, the elastic energy of a bifurcated wafer can be simplified as:

$$V(\sigma, K, K_{\perp}) = F_0 \left[\sigma \mathcal{H} \frac{K + K_{\perp}}{2} - (K^2 + 2\nu_s K K_{\perp} + K_{\perp}^2) - (1 - \nu_s) K^2 K_{\perp}^2 \right] \quad (2)$$

In fig.3 the 3D plot of $V(\sigma, K, K_{\perp})/F_0$ as a function of K and K_{\perp} , rescaled by a factor of 0.15, has been reported for the case of $\sigma \mathcal{H} = 25$, $\nu_s = 0.27$. The green humped curve is determined by the intersection of the surface with the plane of equation $K + K_{\perp} = 5.2$.

Now, to make evident the mechanism of SSB, we can consider, in eq. 2, a further change of variables, namely, the translation of the coordinates K and K_{\perp} :

$$\begin{cases} K' = K - \frac{\sigma}{\sigma_{bif}} \\ K'_{\perp} = K_{\perp} - \frac{\sigma}{\sigma_{bif}} \end{cases} \quad (3)$$

and the evaluation of the elastic energy along the plane of equation $\frac{K + K_{\perp}}{2} = \frac{\sigma}{\sigma_{bif}}$.

In this case, being $K'_{\perp} = -K'$, eq. 2 becomes:

$$V(\sigma, K') = F_0 \left[\sigma \mathcal{H} \frac{\sigma}{\sigma_{bif}} - 2(1 + \nu_s) \frac{\sigma^2}{\sigma_{bif}^2} - 2(1 - \nu_s) K'^2 - (1 - \nu_s) \left(-K'^2 + \frac{\sigma^2}{\sigma_{bif}^2} \right)^2 \right] \quad (4)$$

By focusing on the terms depending on K' , eq. 4 can be rescaled in a dimensionless potential F :

$$F = \frac{1}{1 - \nu_s} \left[\sigma \mathcal{H} \frac{\sigma}{\sigma_{bif}} - 2(1 + \nu_s) \frac{\sigma^2}{\sigma_{bif}^2} \right] - \frac{V(\sigma, K')}{F_0(1 - \nu_s)} - \frac{\sigma^4}{\sigma_{bif}^4} = 2K'^2 + \left(-K'^2 + \frac{\sigma^2}{\sigma_{bif}^2} \right)^2 - \frac{\sigma^4}{\sigma_{bif}^4} \quad (5)$$

This potential grasps in its essence the physics of the SSB, which occurs during the bifurcation of a wafer. Indeed, the potential F depends on the even power of K' , namely K'^2 and K'^4 . It

has two minima of equal energy, symmetrical positioned at $K' = \pm \sqrt{\sigma^2 / \sigma_{bif}^2 - 1}$, which correspond to the principal curvatures of the bifurcated wafer.

In Fig.4, we report the plot of the potential F as a function of K' for several values of $\frac{\sigma}{\sigma_{bif}} \geq 1$.

It describes the mechanism of the SSB. Indeed, it is evident how the potential F is consistent with the description of a “Mexican-hat” shaped potential, usually invoked in the description of the SSB phenomenon and the thermodynamical second order phase transitions [12]. Moreover, the minima of the potential have values which go lower and lower in energy and step away from the origin as $\frac{\sigma}{\sigma_{bif}}$ increases.

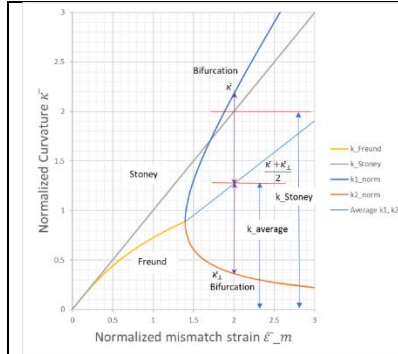


Fig. 1. Normalized curvature versus normalized mismatch strain of a wafer, including the linear and nonlinear (large deformation) regimes and the case of the bifurcation regime. Below the bifurcation point, the behavior is approximated by the Freund's equation [10], whereas the behavior determined by Stoney's theory is described by the line of slope 1. In the bifurcation regime, the average curvatures of a bifurcated wafer lie on the line from the origin to the bifurcation point.

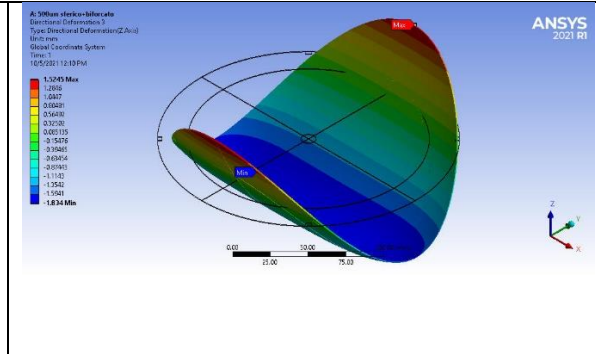


Fig 2. Simulation of a bifurcated wafer, obtained with ANSYS 2021 R1, for the case of a nominal temperature of 420 °C. in terms of the distribution of the directional deformation, along z in an 8" silicon wafer, 500 μm thick metalized with a 4.5 μm Al layer. To obtain the bifurcation two slight forces of 0.0775 N and 0.0096 N were applied along the x and y directions, respectively. (Magnification= 30x) [9] [11].

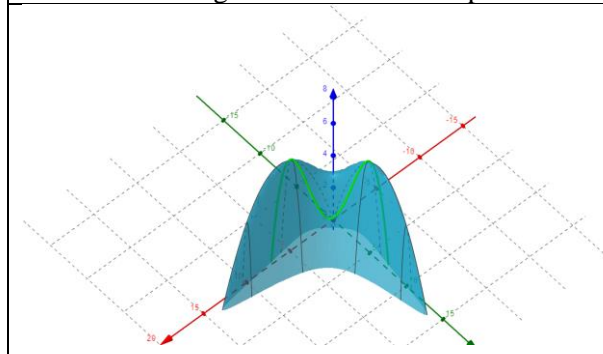


Fig.3. 3D graph of the function $0.15 \left[\sigma \mathcal{H} \frac{K+K_{\perp}}{2} - (K^2 + 2v_s K K_{\perp} + K_{\perp}^2) - (1 - v_s) K^2 K_{\perp}^2 \right]$, where $\sigma \mathcal{H} = 25$, and $v_s = 0.27$. The green humped curve is the intersection of the surface with the plane of equation $K + K_{\perp} = 5.2$. The graph was obtained with GeoGebra [13].

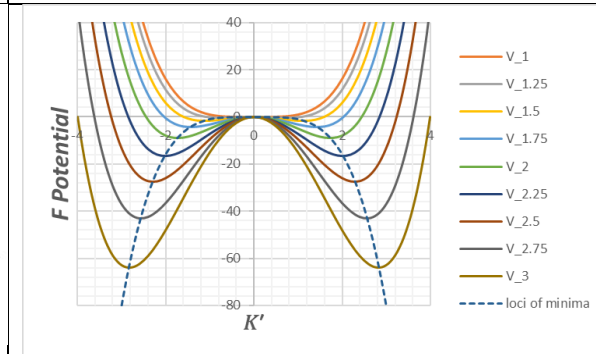


Fig. 4. Rescaled potential F of the elastic energy of a bifurcated wafer, plotted as a function of the rescaled curvature K' , for different values of the ratio $\frac{\sigma}{\sigma_{bif}}$. The dotted curve reports the minima values of the potential at the bifurcation point, for each value of $\frac{\sigma}{\sigma_{bif}}$. The potential shows the SSB mechanism occurring in a bifurcated wafer.

Conclusion

In conclusion, we demonstrated as wafer bifurcation can be described in terms of a spontaneous symmetry breaking mechanism, which involves the elastic energy of the wafer. The SSB mechanism occurs because of a lowering of the energy of the bifurcated wafer, but at the

expenses of a loss of symmetry of the system, namely the cylindric symmetry. These findings may result in a further understanding and control of the phenomenon of bifurcation.

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