Modeling the Thermally Induced Curvature of Multilayer Coatings with COMSOL Multiphysics^{TM}

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Abstract: Within this paper the so called "birth and death" method is demonstrated in use with *COMSOL Multiphysics^{TM}*. With this method the free and reactionless (*death*) movement of a solid structure on deformed geometries and the activation of this solid structure at later simulation steps (*birth*) is possible. For demonstrating the benefit, this method was applied to simulate the thermal induced bending of multilayer coatings. The "birth and death" method is more accurate than standard bulk approaches because it is possible to calculate the influence of layer deposition on deformed substrates.

Keywords: Birth and Death Method, Multilayer Coatings, Layer Deposition

1. Introduction

Coatings are commonly used in a wide range of applications and industrial products to enhance the mechanical and chemical resistivity of surfaces or providing optical functionalities as an example. Multilayer coatings can be used for highly reflective optical coatings [1] or as mechanically deformed plates in surface micromachined systems [2] and are commonly used in microsystem technology.

According to the coating technology and process temperature these thin layers deform the substrate because of intrinsic stresses which include thermal and non-thermal parts. For a good quality of optical microsystems like reflective micromirrors a high surface flatness is needed. So a very exact calculation of the curvature in multilayered coatings is essential for understanding the curvature generation depending on process parameters.

In contrast to single coatings the calculation of the stress induced curvature in multilayer coatings is more complex. Analytical calculations [3] are valid for a low magnitude of deformation and do not respect that the layers are deposited on deformed substrates. To consider nonlinear deformations and respect the layer deposition on deformed substrates finite element analysis (FEA) has to be utilized.

Stressless layers deposited on already deformed multilayers have to be simulated with the so called "birth and death" method. This method is predefined in other commercial FEA-programs and causes the free and reactionless (*death*) entrainment of layers deposited later on. The free and reactionless movement of layer-elements can be switched into a mechanically active status (*birth*) at the simulation step where the layer should be deposited.

In this paper an adaptation of the "birth and death" method to *COMSOL Multiphysics^{TM}* is presented. For better comprehension we first introduce the problem with an example case. Secondly the implementation of the "birth and death" method in *COMSOL Multiphysics^{TM}* is explained. The thermal induced curvature of the exemplary multilayer coating calculated with the "birth and death" method is compared with the predefined method in the reference FEA-software in section 4.

2. Problem Description

An exemplary process flow for the deposition of two layers onto a 20 µm thin silicon plate is shown in Figure 1 and was taken from [4]. The length of the silicon plate is 500 µm. Layer deposition in microsystem technology occurs normally on thicker (typically: 400 µm to 675 µm) and laterally larger (typically in the cm-range) substrates. Due to the geometric aspect ratio of the deposited layer thickness to the substrate thickness this value was chosen to avoid extreme fine meshing and computing power respectively. Furthermore the thin substrate enhances the effect of the layer deposition on bended substrates and emphasizes the benefit of the "birth and death" method.

At the first process step the silicon plate is heated up to 900°C where the thermal grow of 1 µm silicon oxide (SiO_2) occurs. Afterwards the two layers are cooled to room temperature. The stack bends due to different coefficients of thermal expansions α. Since the process temperature of the next layer is 400°C, the change in curvature K_1 while cooling down form 900°C to 400°C is from interest. Thereby the curvature is the reciprocal value of the radius of curvature of a spherically deformed plate. The deposition of 1 µm aluminum (Al, third step) occurs on the curved surface. If no non-thermal stress results from the deposition process, the aluminum layer is relaxed at this process step. At the final process step the three layered stack is cooled down to room temperature and the resulting curvature K_2 can be measured. Furthermore it is assumed that no creep or relaxation behavior occurs during cooling the aluminum layer.

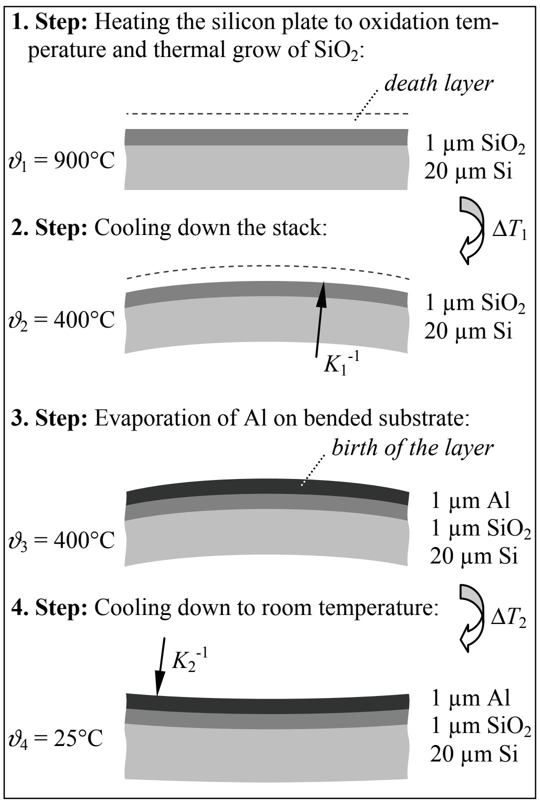

Figure 1: Exemplary process flow: schematic cross-sections of the layer deposition at different process steps

For correct modeling of thermally induced curvature in multilayered coatings with finite element analysis three features are required:

- free and stressless movement of layers deposited later in the process (aluminum layer at step 2 in Figure 1),
- activation of the subsequent layers (step 3 in Figure 1) and
- additional simulation steps to simulate forward (step 4 in Figure 1).

3. Applying the Birth and Death Method to *COMSOL Multiphysics*^{TM}

The free and reactionless movement of *death* layer elements is done by applying a very low YOUNG's modulus E as a subdomain setting. For the exemplary process flow a YOUNG's modulus of 10^{-12} Pa was used. This low YOUNG's modulus ensures that death elements do not influence the bending stiffness of the underneath stack at the first simulation step. Moreover no mechanical stress but strain will result in the death elements. The strain in the death elements is generated from the deformed layers underneath. Activation of the elements is realized by switching the YOUNG's modulus back to the physical material value.

Three layered example

The successive simulations of the thermally induced deformations are realized by multiple application modes. For the exemplary simulation of the change in curvature, caused by the changes in temperatures ΔT_1 and ΔT_2 (Figure 1), two plane stress application modes are used (2D structural mechanics from the MEMS module). All layers are active in their domains and all application modes share the same geometry, mesh and boundary conditions as shown in Figure 2.

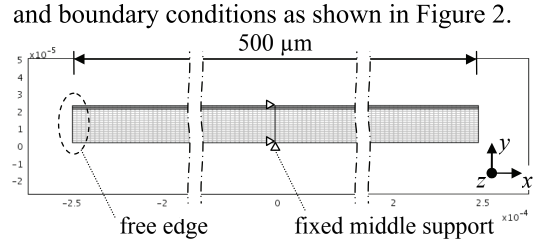

Figure 2: Mechanical constrains and mapped mesh used for the simulation of the three lay model

At the first *plane strain* application mode (*smps*), the thermal contraction of silicon oxide on silicon is included for the temperature decrease from `Tempref` = 900°C to `Temp` = 400°C. For the *death* aluminum layer (E = 10^{-12} Pa) no thermal expansion is applied by deactivating the thermal expansion (`Temp` = `Tempref`).

The second *plane strain* application mode (*smps2*) is used for simulating the thermal contraction of all layers by applying the change in temperature ΔT_1 = -875K for the silicon and silicon oxide layers and ΔT_2 = -375K for the aluminum layer. The YOUNG's modulus of aluminum is adjusted to 70 GPa. To respect the aluminum deposition on the deformed substrate, initial stress values σ_{xi}, σ_{yi} and σ_{zi} are applied by coupling them to the resulting strain from the first plane stress application mode (`ex_smps`, `ey_smps` and `ez_smps`) and multiplying them with the YOUNG's modulus of aluminum.

The relevant properties and coupling parameters of the exemplary process flow shown in Figure 1 are summarized in Table 1. The used material properties are shown in Table 2.

Table 1: Relevant properties and coupling parameters for the application modes used in the presented model

parameter	application modes			sub-domain
	smps	smps2	…	
Material *E* / Pa `Temp`	… 10^{-12} Pa `Tempref`	… 10^{-12} Pa `Tempref`	…	…

Material
E / Pa
σ_{xi} / Pa
σ_{yi} / Pa
σ_{zi} / Pa
`Temp`
`Tempref`
	-
	10^{-12}
	-
	-
	-
	400 °C
	400 °C
		Al
		$70\cdot10^{9}$
		`-ex_smps`·70e9
		`-ey_smps`·70e9
		`-ez_smps`·70e9
		25 °C
		400 °C
			…	3

Material
`Temp`
`Tempref`
	SiO_2
	400 °C
	900 °C
		SiO_2
		25 °C
		900 °C
			…	2

Material
`Temp`
`Tempref`
	Si
	400 °C
	900 °C
		Si
		25 °C
		900 °C
			…	1

	example from Figure 1			

Table 2: Applied material properties for the model case shown in Figure 1

parameter	**layer / subdomain**		
	1	**2**	**2**
material	Si	SiO_2	Al
thickness / µm	20	1	1
YOUNG's modulus: *E* / GPa	169	73	70
POISSON ratio: ν	0	0	0
CTE: α / 10^{-6} K^{-1}	3.8	0.5	23
coating temperature / °C	-	900	400

General approach of "birth and death" in *COMSOL Multiphysics*™

To expand the presented model of thermally induced curvatures for a three layered stack to an arbitrary multilayered model the following features have to be taken into account:

- For n deposited layers, $n-1$ application modes which deal with the same geometry, mesh and mechanical clamping have to be set up.
- Each application mode addresses one process step where only the thermally expansion of the lower and actual deposited layers to the current process temperature is applied. The layers above refer the *death* option while applying a very low YOUNG's modulus.
- Every layer in each application mode keeps its reference temperature.
- For the currently deposited layer the physical value of YOUNG's modulus is used. This acts as a *birth* of the layer. To incorporate the layer deposition on a deformed substrate the strain coming from the *death* layer at the previous step (application mode) has to be multiplied with the YOUNG's modulus and inserted as initial stress.

Due to the very low sheer strain resulting in thin bended plates the coupling of the initial sheer stress σ_{xyi} can be neglected. The disregard of sheer deformation agrees with the assumption of the KIRCHHOFFs plate theory which is valid for the bending of thin plates. If thick plates or other solid structures are simulated, the coupling of sheer stress have to be included. For isotropic materials the initial sheer stress coupling can be realized by multiplying the strain of the *death* elements with the sheer modulus *G*:

$$G = \frac{E}{2 + 2\cdot\nu}\,. \qquad (1)$$

Additional non-thermal stresses, for example coming from the deposition process like lattice mismatch between material intersections or stress on grain boundaries in polycrystalline materials, can be linearly superposed with the coupled initial stress values.

4. Results

Both application modes in the three layered example were solved simultaneously. Due to the coupling of both application modes this increases the number of degrees of freedoms by the factor of two. Because of the unidirectional coupling a stepwise solving of each application mode can be performed to reduce the number of degrees of freedom, the computing time and memory consumption.

In Figure 3 the y - displacement v and total deformation profile after thermal oxidation and aluminum deposition is shown using linearly calculated and linear LAGRANGE elements. For the correct determination of the surface deformation profile the x - displacement u has to be kept in mind as can be seen in the 40 times scaled deformed shape plot.

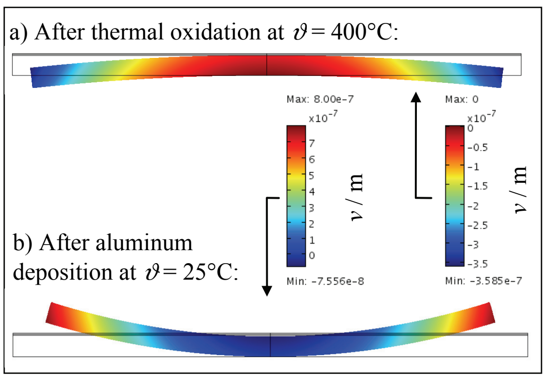

Figure 3: Stack deformation after a) thermal oxidation and b) aluminum deposition

Verifying the presented model

To verify the accuracy of the presented "birth and death" method a reference model was adapted from [4]. This reference FEA uses a predefined "birth and death" method of the commercial software *ANSYS*^{TM}. To ensure a valid comparison of the model from [4], the presented model was verified according to:

- an identical mapped mesh with equal numbers of mesh points as shown in Figure 2 and equal amount of degrees of freedom respectively,
- equal mechanical constrains,
- linear element functions and
- identical material properties as shown in Table 2.

The large deformation option was switched on at each application mode in the *COMSOL Multiphysics*^{TM} model. Because the reference FEA can only use the "birth and death" method with activated large deformation and nonlinear solving the equation system using the NEWTON-RAPHSON algorithm.

The top surface y - displacement v depending on the lateral displaced x - position after the deposition of the thermal silicon oxide on silicon is shown in Figure 4 and after coating the aluminum layer is shown in Figure 5.

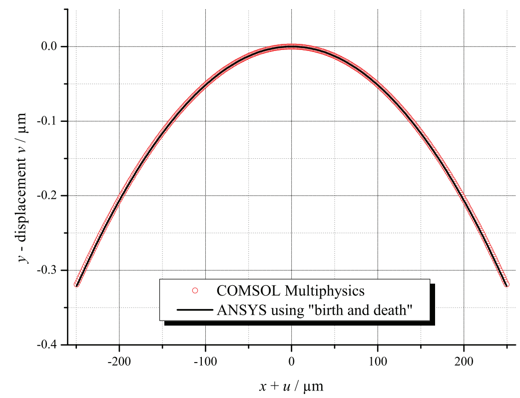

Figure 4: Comparison of the nonlinear solved surface deformation after deposition of layer 2 at 400°C

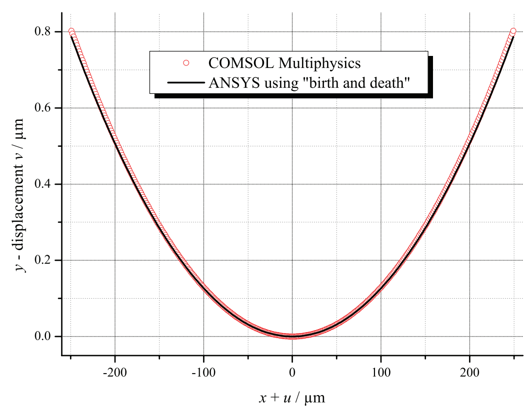

Figure 5: Comparison of the nonlinear calculation of surface deformation after deposition of layer 3 at 25°C

The resulting surface deformations are consistent for the *ANSYS*^{TM} and *COMSOL Multiphysics*^{TM} models. For a correct determining the deviation between both models, a circular function is fitted into each curve and the curvatures of the spherical deformed plates are calculated. A comparison of the resulting curvatures is given in Table 3.

To illustrate the benefit of the "birth and death" method, the calculated curvature of the thermally induce deformation of the free layered coating without the "birth and death" option was done within both FEA tools. In this models all layers are simulated at once by applying the thermal contraction of ΔT_1 = -875K for the silicon and silicon oxide layers and ΔT_2 = -375K for the aluminum layer. The resulting curvatures are also given in Table 3.

Table 3: Comparison of the resulting curvatures solved by different methods and FEM-tools

Method	**curvature K / m^{-1}**	
after deposition of:	**layer 2**	**layer 3**
COMSOL with "birth and death":		
linear	-10.23	25.78
large deformation	-10.25	**25.87**
COMSOL without "birth and death":		
linear	-	15.32
large deformation	-	15.37
ANSYS with "birth and death":		
large deformation	-10.32	**25.34**
ANSYS without "birth and death":		
large deformation	-	14.95

Using the predefined "birth and death" method in *ANSYS*^{TM} as reference, the relative deviation of the solved curvatures is calculated and presented in Table 4.

Table 4: Relative deviation of the resulting curvatures with *ANSYS*^{TM} "birth and death" method as reference

Method	**relative deviation / %**	
after deposition of:	**layer 2**	**layer 3**
COMSOL with "birth and death":		
linear	-0.9	1.7
large deformation	-0.7	**2.1**
COMSOL without "birth and death":		
linear	-	-39.6
large deformation	-	-39.4
ANSYS with "birth and death": reference		
large deformation	0.0	**0.0**
ANSYS without "birth and death":		
large deformation	-	-41.0

As can be seen in Table 4 the self defined "birth and death" method which was applied to *COMSOL Multiphysics*^{TM} in section 3 produces a relative deviation of two percent. In contrast to the 40 percent deviation of modeling without "birth and death" this is a remarkably good result. The deviation between modeling with and without "birth and death" method is very high for the presented case. However it strongly depends on:

- the ratio between substrate (first layer) thickness and the thicknesses of the deposited layers,
- the bending stiffness of the deposited layers by means of the YOUNG's modulus and layer thicknesses,
- the total number of deposited layers and
- the magnitude of intrinsic stress or the magnitude of deformation respectively.

Due to these numerous influences no general gain in accuracy can be derived for the "birth and death" method. The effect of the "birth and death" method on simulation results of a specific process flow has to be evaluated individually.

5. Conclusions

In this paper the so called "birth and death" method was successfully applied to *COMSOL Multiphysics*^{TM}. With this method the correct calculation of the thermally induced curvature of multilayered coating processes was possible. The comparison with a predefined method coming from reference FEA software shows a deviation of only two percent for the given model case which is much lower than the deviation of simulating without "birth and death" method.

Due to the benefit of this method and the extensive realization for high numbers of deposited layers the general implementation of the "birth and death" method in future versions of *COMSOL Multiphysics*^{TM} seams to be desirable.

8. References

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