Numerical models for evaluation thermal conductivity of coatings

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Abstract

This paper is dealing with simulation and model development for the evaluation of thermal conductivity of coatings by the Laser Quasistatic Thermography (LQT) method. The main principles of the measurement method are introduced and the process of thermal conductivity evaluation based on numerical simulation is presented. The evaluation requires special procedure to simulate thermal process induced by laser pulse in coating on some substrate. The thickness of the coating is manifold less than the thickness of the substrate and total sample surface. In numerical system Cosmos/M there are created two suitable models: “Shell-Clink-Solid” model and model based on physical similarity. In this paper there are also described characteristics of both models and their comparison with classical axisymmetric and volume models.

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1. Introduction

Thermal conductivity is one of fundamental thermo-physical properties of material. It is the intrinsic property of a material which relates its ability to conduct heat. It is also important in the case of coatings, where it can influence the resultant coatings properties and practical applicability. Measurement of thermal conductivity of coatings is therefore an important technical problem. Moreover it cannot be mostly measured by standard measurement methods for bulk materials as the Axial Steady-State method [1], the HotWire method [2] or the Transient Plane Source method [3].

The Laser Quasistatic Thermography (LQT) [4, 5] is a non-contact one-sided method for coatings thermal conductivity investigation. This method uses a continual diode laser (wavelength 810 nm, max. output 40W) as the heat source and an infrared camera for surface temperature measurement (fig. 1a)). The thermal conductivity of the coating is evaluated based on differences of surface temperature evolution on the measured and reference (substrate without coating) samples during the laser heating.

Sufficient sample (substrate) dimensions compared to the laser spot radius and its high thermal conductivity results in achieving equilibrium between the laser heating and heat removal to the substrate volume, i.e. a quasi-stationary state is achieved. Then the surface temperature during the heating of the sample with and without the coating differs. The thermal conductivity of the coating is determined based on the measurement of this difference.

The time dependence of sample surface heating is measured by infrared camera system ThermaCAM SC2000. For the evaluation of sample heating the numerical system Cosmos/M

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based on finite element method is used. Thermal conductivity is determined from iterative
process of solving inverse problem, that temperature difference obtained from numerical calcu-
lations matches to the temperature difference provided by the experiment.

Considering measurement of coatings with thickness from 1 to several micrometers the
usage of classical models is problematic for reasons of large differences of coating and total
sample thicknesses. With the view of this a requirement to create new models, which are able to
simulate processes in coatings, has arisen. In numerical system Cosmos/M [6] there are created
two suitable models: “Shell-Clink-Solid” model and model based on physical similarity.

![Fig. 1. Measurement of thermal conductivity of coatings by LQT method using heating by laser pulse and measuring of thermal response by infrared camera, a) experimental setup, b) experimental scheme](image)

2. The models of heating the sample with coating

The models were created in numerical system Cosom/M produced by Solidworks company.
The goal was to create model of sample with coatings for evaluation of thermal effect of laser
and further to use it for the evaluation of thermal conductivity of coating measured by LQT
method. Geometric model presents axisymmetric cylindrical sample, thickness \( d_{sub} = 10 \text{ mm} \)
and radius \( r_{sub} = 25 \text{ mm} \), with coating, thickness \( d_{coat} = 1 \mu\text{m} \). The laser takes effect on
the coating surface in axis of symmetry (fig. 1b)). For evaluation of thermal conductivity it is
necessarily to determine temperature evolution both on surface and on coating-sample.

Using of axisymmetric model or volume model, number of elements is too large, hence the
models are ill-calculated. Shell type elements can be used to simulate heat transfer problems,
however they are not usable concerning the LQT method, because they do not provide two
different temperatures on the coating surfaces. For that reason there was proposed a 3D model
Shell-Clink-Solid based on combination of three types of elements and a 2D axisymmetric
model based on the theory of similarity used to increase coating thickness.

2.1. Model Shell-Clink-Solid

This model uses Shell elements for the simulation of coating, however these elements are not
placed on Solid elements representing the sample volume, but they are connected with them
by Clinks. The Clink is a one dimensional element to model the heat flow due to convection
(fig. 2). This combination of elements makes possible the simulation of heat propagation in
radial direction along the surface and also in axial direction throughout the coating-substrate
interface.

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Shell elements can simulate heat transfer along surface, whereas Clink elements simulate heat transfer into sample. An important property of Clink elements is the area of the convection surface. The first computation found, that the area of the convection for one Clink element is not a fraction of total area divided by number of Clink elements, because final temperature field is asymmetrical as is shown in fig. 3. This is caused by the state, that the heat transferred by the Shell elements can diffuse into the sample only throughout the Clink elements, but each Clink element is contiguous to different number of Shell elements thereby different size of surface area.

In the second computation there was the area of convection derived from the number of Shell elements adjacent to each Clink element. This solution does not bring good results as well.

In the last step, the area of convection takes into consideration the real area of each Shell element. It is assumed that heat is uniformly carried off from each element throughout all adjacent Clink elements (fig. 4a). Application of this correction leads to proper setting of the area of convection for the computations.

The area of convection is a sum of all Shell elements conducive to the given Clink element divide by 3 (for triangle elements) (fig. 4b)). The area of convection is set up in real constants.
For the each Clink element it is needed to define new real constants. Determination of element area and conversion to the area of convection take place outside the computational system Cosmos/M. From the Cosmos/M there were exported the list of nodes with coordinates and the list of elements, which contain numbers of nodes constituting given element. Back to the Cosmos/M there is imported the list of Clink elements with size of the area of convention. Final symmetric temperature field is shown in fig. 5.

The main restriction of the model is different area of convection by Clink elements, because Cosmos/M allows to define only 5000 real constants. The larger models need to assign one set of real constants to several Clink elements.

2.2. Model with increasing thickness of coating by the theory of similarity

This model is based on classic two dimensional axisymmetric model with Plane2d elements. On the basis of dimensional analysis and the theory of similarity [7] in this model the thickness of coating is increased (fig. 6) accompanied with a modification of its material properties. Material properties are modified with a view to conserve similarity criterion, in this case it is the Fourier number. This procedure makes it possible to use larger elements and therefore to decrease their number with respect to maintain the aspect ratio of the elements.
 Lets introduce a scale factor $\mu$ and the coatings thickness $L_y$ in model is increased by this scale factor. In $x$ direction the proportion is kept unmodified. Thus

$$L_{yM} = L_y \cdot \mu,$$

$$L_{xM} = L_x,$$

where $L$ is the original length and $L_M$ is transformed length in the model. By scratching the volume of coating has increased. As its mass is constant, the density must be modified with the scale factor

$$\rho_M = \rho \cdot \mu^{-1}.$$

By the theory of similarity it must be satisfied

$$F_{oxM} = F_{ox},$$

$$F_{oyM} = F_{oy},$$

where $Fo$ is dimensionless Fourier number defined as

$$Fo = \lambda \tau (\rho c)^{-1} L^{-2}.$$  

It represents dimensionless time of the heat propagation. The thermal capacity and time are independent to length dimension, hence after substitution the following expressions for thermal conductivity are given

$$\lambda_{yM} = \lambda_y \cdot \mu,$$

$$\lambda_{xM} = \lambda_x \cdot \mu^{-1}.$$
All the boundary conditions on the face with changed geometry must be modified according to previous expressions. In this case it concerns only the convection heat transfer to surroundings by lateral side. It is expressed by dimensionless Biot number

\[
Bi = \frac{\alpha L \lambda^{-1}}{1}
\]

(9)

\[
Bi_M = Bi
\]

(10)

which affects the convection coefficient \( \alpha \)

\[
\alpha_x M = \alpha_x \cdot \mu^{-1}.
\]

(11)

3. Results of comparison

Both models were compared with the volume model and the axisymmetric model without increasing the thickness of the coating. Parameters of models (tab. 1) were chosen suitably, in order to be able to construct the models and compare their results.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( R_{\text{sample}} ) (m)</td>
<td>0.025</td>
<td>sample semidiameter</td>
</tr>
<tr>
<td>( R_{\text{spot}} ) (m)</td>
<td>0.01</td>
<td>semidiameter of laser beam</td>
</tr>
<tr>
<td>( d_{\text{sub}} ) (m)</td>
<td>0.01</td>
<td>substrate thickness</td>
</tr>
<tr>
<td>( d_{\text{coat}} ) (m)</td>
<td>0.001</td>
<td>coating thickness</td>
</tr>
<tr>
<td>( P_{\text{laser}} ) (W)</td>
<td>21</td>
<td>laser power</td>
</tr>
<tr>
<td>( T_0 ) (°C)</td>
<td>20</td>
<td>initial temperature</td>
</tr>
<tr>
<td>( \alpha ) (W m(^{-2}) K(^{-1}))</td>
<td>10</td>
<td>heat transfer coefficient</td>
</tr>
<tr>
<td>( t ) (s)</td>
<td>5</td>
<td>laser pulse width</td>
</tr>
<tr>
<td>( \Delta t ) (s)</td>
<td>0.5</td>
<td>time step</td>
</tr>
</tbody>
</table>

In the model with increasing thickness of the coating scale factor \( \mu = 10 \) was chosen. In tab. 2 there are referred material properties of the sample (Cu) and the coatings, which were used in computations.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Substrate (Cu)</th>
<th>Coating</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda ) (W m(^{-1}) K(^{-1}))</td>
<td>350</td>
<td>10</td>
</tr>
<tr>
<td>( c_p ) (J kg(^{-1}) K(^{-1}))</td>
<td>385</td>
<td>750</td>
</tr>
<tr>
<td>( \rho ) (kg m(^{-3}))</td>
<td>8 920</td>
<td>4 000</td>
</tr>
</tbody>
</table>

Temperatures in three places of sample are compared. They are located on the axes of rotation: on surface of coating, on coating-substrate interface and on bottom side of the sample. Final temperatures provided by all models are in tab. 3.
Table 3. Temperature (°C) in selected locations of sample in time 5 s

<table>
<thead>
<tr>
<th>Location</th>
<th>Volume model</th>
<th>Shell-Clink-Solid model</th>
<th>Axisymmetric model</th>
<th>Model with increasing thickness of coating</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coating surface</td>
<td>29.26</td>
<td>29.14</td>
<td>29.25</td>
<td>29.25</td>
</tr>
<tr>
<td>Coating – substrate interface</td>
<td>22.63</td>
<td>22.57</td>
<td>22.62</td>
<td>22.62</td>
</tr>
<tr>
<td>Bottom side of sample</td>
<td>21.77</td>
<td>21.72</td>
<td>21.77</td>
<td>21.77</td>
</tr>
</tbody>
</table>

The model with increasing the coating thickness give the results equal with the classic axisymmetric model and it agrees with the results of the volume model. The results of the Shell-Clink-Solid model differ about 1.3%. From this results one can conclude, that both models are equivalent.

When the coating thickness is 1 µm and only one row of elements on coating is considered, the number of elements in volume model is more than $10^{14}$, in axisymmetric model is about 2 billion elements. In “Shell-Clink-Solid” model the number of elements is up to 100 thousands and in the model with increasing the coating thickness only 2 thousands.

Evaluation of coatings thermal conductivity in LQT method requires to perform mostly several iterations. With respect to this the speed of simulation is important, which depends largely on the number of elements. Hence as the best model there is evaluated the model with increasing the coating thickness based on the theory of physical similarity. Moreover this model provides the results equal with the standard models in terms of the process simulation accuracy.

4. Conclusion

In this contribution there are shown new methods for computational solution of coating — substrate heat transfer problems, that has not been previously published. There arise especially specific requirements of the LQT method for the measurement of coating thermal properties. It concerns the option to use the connection of Shell-Clink-Solid elements in the COSMOS/M FEM system and to use the theory of physical similarity in order to modify the problem geometry. Such solutions enable to evaluate the temperature difference on the coating.

Two different models have been proposed to simulate thermal process in the coating-substrate material structure, where the coating thickness is much smaller than the thickness of substrate. Both created models fulfil all requirements and give accurately results. The models allow to considerably decrease the number of elements necessary to simulate the given problem and rapidly accelerate the computation. For the evaluation of thermal conductivity of coatings in the LQT method it is better to use the model based on the theory of similarity, because it is simpler, the computation is quicker and the results are slightly more accurate.

Acknowledgements

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References