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Applied and Computational Mechanics 2 (2008) 389–396

Applied and
Computational
Mechanics

Numerical models for evaluation thermal conductivity of coatings

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Received 31 August 2008; received in revised form 17 October 2008

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.

Keywords: computer modelling, coatings, thermal conductivity, laser quasistatic thermography method

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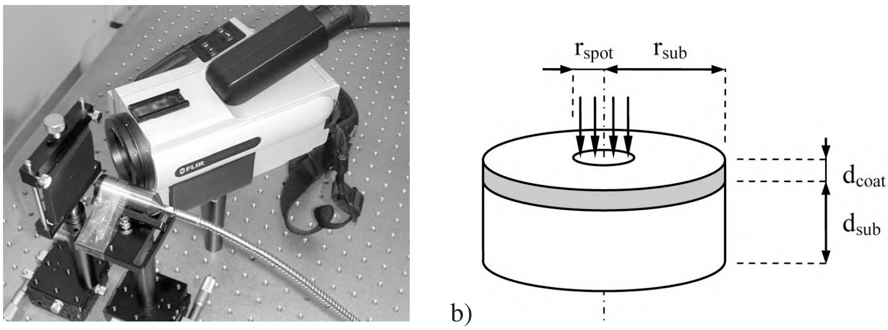
based on finite element method is used. Thermal conductivity is determined from iterative process of solving inverse problem, that temperature difference obtained from numerical calculations matches to the temperature difference provided by the experiment.

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.



a) b)

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

2. The models of heating the sample with coating

The models were created in numerical system Cosmos/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 $d_{sub} = 10$ mm and radius $r_{sub} = 25$ mm, with coating, thickness $d_{coat} = 1\,\mu$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.

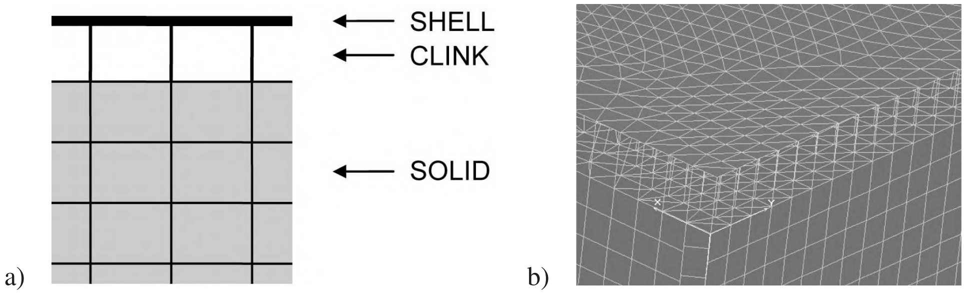


Fig. 2. a) scheme of model SHELL-CLINK-SOLID, b) mesh in system Cosmos/M

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.

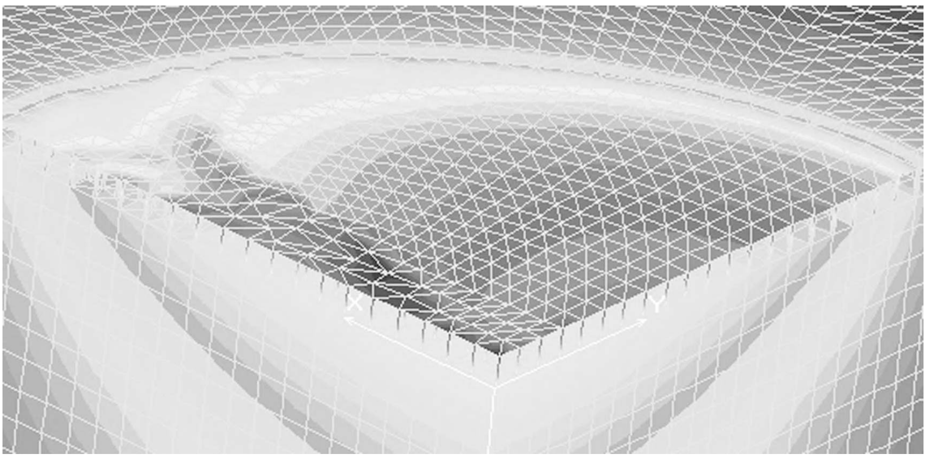


Fig. 3. Asymmetrical temperature field computed by Shell-Clink-Solid model without correct area of the convection for each Clink element

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.

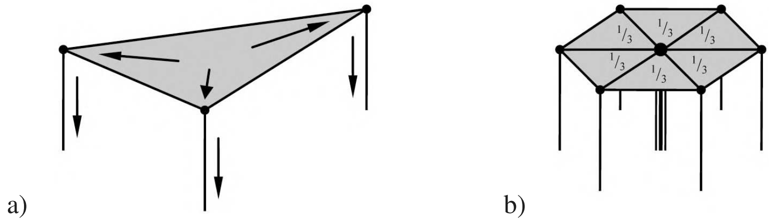


Fig. 4. a) heat propagation and removal from Shell element, b) area used for computation the area of convection for Clink element

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.

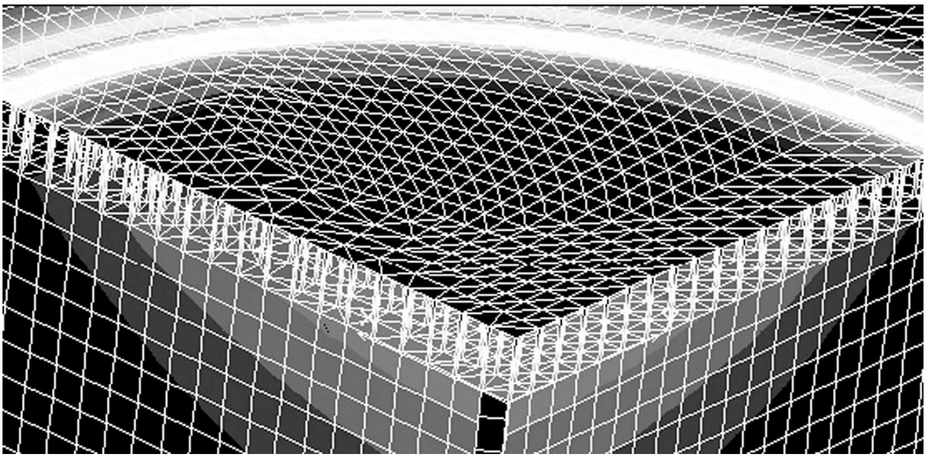


Fig. 5. Symmetrical temperature field computed by Shell-Clink-Solid model with correct area of the convection for each Clink element

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 μ and the coatings thickness L_y in model is increased by this scale factor. In x direction the proportion is kept unmodified. Thus

$$L_{y_M} = L_y \cdot \mu, \tag{1}$$
$$L_{x_M} = L_x \tag{2}$$

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

$$\rho_M = \rho \cdot \mu^{-1}. \tag{3}$$

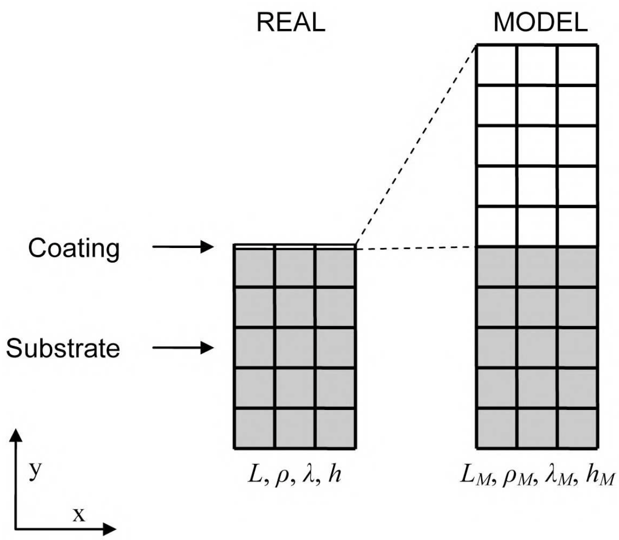


Fig. 6. Scheme of model with increasing coating thickness

By the theory of similarity it must be satisfied

$$Fo_{x_M} = Fo_x, \tag{4}$$
$$Fo_{y_M} = Fo_y, \tag{5}$$

where Fo is dimensionless Fourier number defined as

$$Fo = \lambda\tau(\rho c)^{-1}L^{-2}. \tag{6}$$

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

$$\lambda_{y_M} = \lambda_y \cdot \mu, \tag{7}$$
$$\lambda_{x_M} = \lambda_x \cdot \mu^{-1}. \tag{8}$$

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

$$Bi = \alpha L \lambda^{-1} \tag{9}$$

$$Bi_M = Bi, \tag{10}$$

which affects the convection coefficient α

$$\alpha_{x_M} = \alpha_x \cdot \mu^{-1}. \tag{11}$$

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 1. Parameters of comparing models

Variable	Value	Description
R_{sample} (m)	0.025	sample semidiameter
R_{spot} (m)	0.01	semidiameter of laser beam
d_{sub} (m)	0.01	substrate thickness
d_{coat} (m)	0.001	coating thickness
P_{laser} (W)	21	laser power
T_0 ($^\circ$C)	20	initial temperature
α (W m^{-2} K^{-1})	10	heat transfer coefficient
t (s)	5	laser pulse width
Δt (s)	0.5	time step

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 2. Material properties of the substrate and the coating

	Substrate (Cu)	Coating
λ (W m^{-1} K^{-1})	350	10
c_p (J kg^{-1} K^{-1})	385	750
ρ (kg m^{-3})	8 920	4 000

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

Location	Volume model	Shell-Clink-Solid model	Axisymmetric model	Model with increasing thickness of coating
Coating surface	29.26	29.14	29.25	29.25
Coating – substrate interface	22.63	22.57	22.62	22.62
Bottom side of sample	21.77	21.72	21.77	21.77

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

This paper is based upon work sponsored by the Ministry of Education, Youth and Sports of Czech Republic under research project no. MSM4977751302.

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