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Numerical Analysis of a DMA Epoxy-Carbon Composite Study

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Abstract. The results of numerical simulations performed for Dynamic Mechanical Analysis (DMA) measurements of thermal and mechanical (or thermomechanical) properties performed on a model composite structure are presented herein. The simulated elastic response of an epoxy-carbon fibre composite specimen was analysed for a case by which the model specimen was subjected to three-point bending with a free support. The epoxy-carbon fibre composite studied as explained herein exhibited extreme differences between the elastic properties of the epoxy resin matrix and the carbon fibre reinforcement. In addition, the carbon fibre reinforcement was both internally and structurally anisotropic. The numerical simulations were performed to demonstrate a qualitative dependence of the DMA measurement results on a certain structure of the investigated specimen and to determine if the DMA results could be qualified as effective or apparent. A macro-mechanical model of the specimen was developed and the numerical calculations were performed by applying a COMSOL/M FEM (Finite Element Method) modelling software. The carbon fibre reinforcement was modelled with an orthotropic composite structure of planar laminar inclusions or as a disperse composite with circular inclusions. While modelling different characteristic dimensions of inclusions were taken into account. Representative material properties were assumed from the results of the appropriate experimental investigations and form certain literature reference data. The effect of the composite layer configuration and their characteristic dimensions on the evaluated model elastic modulus value was also studied. The numerical modelling results are in a qualitative agreement with the results of the DMA investigations performed on real composite. They also proved the effectiveness of the developed numerical simulation methodology in modelling of micro- and macromechanical phenomena occurring during the DMA study.

Keywords: composite material, DMA, numerical simulation, COMSOL

1. BACKGROUND

DMA (Dynamic Mechanical Analysis [1, 2], a.k.a. dynamic thermal mechanical analysis, dynamic thermomechanical analysis) is currently among the most popular tools used to determine viscoelastic properties of materials. DMA has proven itself especially well in the determination of the viscoelastic properties of heterogeneous composites. DMA comprises testing with application of oscillating force and observation of a test specimen oscillating response. The oscillating response is, essentially, the displacement of the test specimen. By analysing the response, it is possible to determine the elastic modulus, E' (the so-called 'storage modulus'), and the loss modulus, E'', which are, respectively, the real component and the imaginary component of a generalized complex Young's modulus determined with DMA. The real component complies with the strain phase. The imaginary component is offset by $\pi/2$. The real component of Young's modulus is zero for perfectly viscous bodies. The imaginary component of Young's modulus is zero for perfectly resilient bodies [3]. Composites which feature viscoelastic characteristics have both moduli not equal to zero, whereas E'' < E'.

One of the most practical methods of determining the properties of glass (or graphite) fibre reinforced composite materials is to test their flat specimens with the edges freely supported and the oscillating variable force input applied along the centreline of the specimen (see [1]). This method has been developed for testing the properties of homogeneous viscoelastic materials. It is highly sensitive to changes in the dimensions and geometry of the specimens. It is then necessary to determine the reliability of experimental results obtained with the method. For heterogeneous materials, it is problematic to determine the modulus of elasticity, E', and the relation of the calculated value with Young's modulus values determined with other test methods, e.g. tensile tests.

The problem here is to qualify the calculated values of E' either as effective properties or apparent properties, as the case may be.

The concept of 'effective properties' is a category of parameters which can homogenised; note that macroscopic test results do not facilitate be a determination of whether the tested structure is heterogeneous or not. 'Apparent properties' are the calculated material parameters of heterogeneous structures that can be characterised as substitutive homogeneous materials. The potential contributors to apparent properties include physical phenomena which exceed the confines of the theoretical description of the primary phenomenon. For the DMA discussed herein, it may include adhesion at the matrix/fibre interface. Macroscopic test results usually facilitate the effective ones among the properties being determined. Mathematical modelling is applied for testing the sensitivity of methods, i.e. to determine its metrological preconditions and to qualify the values determined with the method as effective or apparent ones. Unfortunately, given the sheer complexity of the theoretical description, analytical modelling is largely restricted and poorly effective for the purposes contemplated in the previous sentence.

Numerical modelling suffers from less problematic restrictions in the same context. The primary challenge in numerical simulations run with commercial software products is the missing facilities to model the properties of viscoelastic materials. It is however possible to run calculations and determine the displacement within test specimens in response to an input of mechanical loads. A facility for those calculations is provided in the environment of COMSOL Multiphysics software [4, 5, 6]. The results of numerical simulations can provide inputs for an analysis of method sensitivity regarding the determination of the modulus of elasticity. It is also feasible to do a qualitative determination of how the layout of graphite fibres in an epoxy resin matrix composite and the geometrical features of test specimens of the material affect the calculated viscoelastic effective or apparent properties.

This paper describes operations involving an application of numerical modelling in testing the metrological preconditions of DMA-based measurements carried out on specimens of a carbon (or graphite) fibre reinforced epoxy matrix composite. All tests were limited to an analysis of the elastic response of the specimens, which condensed the problem at hand to a statistical problem of a loaded beam. The development of the methodology of numerical simulations and the verification of efficiency of modelling for the numerical simulations aside, the numerical simulations were performed to demonstrate a qualitative dependence of the DMA measurement results on a certain structure of the investigated specimen and to determine if the DMA results could be qualified as effective or apparent. Positive results would enable expansion of the scope of future theoretical and numerical analysis.

2. FORMULATION OF THE COMPUTATIONAL PROBLEM

The authors assumed that a module of COMSOL Multiphysics would be used to run numerical calculations to produce the response of a test specimen to a mechanical load input. The numerical simulations were limited to a DMA test with a three-point support of the specimen by which the test specimen was placed on two supports with the contact points of the supports on the specimen's surface prevented from moving along the axis *Oy* (Fig. 1). The surface of the test specimen opposite to the side contacting the supports was loaded with a force sufficient to cause the test specimen material to bend.



Fig. 1. Diagram of loading the test specimen (a beam) with a force input applied in between the supports

A problem of static bending loads was formulated for a test specimen with a constant rectangular cross-section, a height of h and a width of b (in the direction perpendicular to plane Oxy). The spacing of the supports under the test specimen was l. An analytical solution of the problem provided a dependence by which the beam bend, f, could be determined: [7]

$$f = \frac{l^3}{48} \frac{P}{E J_a} \tag{1}$$

with: E – Young's modulus; J_a – moment of inertia of the cross-section relative to the horizontal neutral line; P – pressure input applied to the middle of the beam (the test specimen).

For the rectangular cross-section, the moment of inertia was:

$$J_a = \frac{h^3 b}{12} \tag{2}$$

Substitution of (2) in (1) provided this:

$$f = \frac{l^3}{4bh^3} \frac{P}{E}$$
(3)

A transformation of the foregoing dependence allowed a determination of E:

$$E = \frac{l^3}{4bh^3} \frac{P}{f} \tag{4}$$

3. THE NUMERICAL MODEL

The test specimen had a two-dimensional numerical model developed for the numerical simulation. However, the applied software suite adopted the model as a three-dimensional structure with a specific declared dimension of b along the axis Oz (Fig. 1, see the perpendicular to the plane of view). The authors assumed b = 10 mm, according to the data from standard specimens.

The inner structure of the composite material was modelled by applying rectangular or round inclusions representing the modelled fibres. The areas declared for the numerical calculations were divided into finite triangular elements (Fig. 2). The numerical calculations were run for three different types of the specimen models.



Fig. 2. Diagram of the three-layer laminate specimen breakdown into finite triangular elements

For each type, the fibre content was the same and 50% by volume. Three basic types of the test specimens were investigated:

a) a multi-layer laminate with thin layers of the modelled rowing and the carbon fibres aligned along the axis *Ox*. Here, for the sake of retaining symmetry, an 11-layer fibre reinforcement was adopted with the first and last layer on the exterior of the test sample, and with all 11 layers alternating with 10 layers of the matrix (Fig. 3(a));



Fig. 3. Models of the specimen internal structure types

- b) a three-layer laminate constructed with the same principle as above (Fig. 3(b));
- c) a sample with regular, dispersed circular inclusions which provided a rough model of the rowing carbon fibres aligned with the axis O_z , i.e. in perpendicular to the side surface of the specimen model (and essentially being the rowing cross-section, Fig. 3(c)).

Only one half of the test specimen was numerically modelled for the numerical calculations by applying the symmetry of load (a flip around the axis Oy). Hence, Figures 3(a), (b) and (c) show only one half of the test specimen subject to loading. In each version of the numerical calculations, the support point was at the coordinates (-25.0 mm; 0.0 mm) with an analogical (not shown) support point at the coordinates (0.025 m; 0 m). A force input of 10 N was applied to the point at the coordinates (0 m; 0.002 m). However, given the applied flip of the test specimen around the axis Oy, the applied force input was double the value. Thus, the actual force input studied in this paper was 20 N. The characteristic dimension of the specimen models are shown in Table 1.

Characteristic dimensions of the specimen models					
Support spacing, <i>l</i> , mm	Height, <i>h</i> , mm	Width, <i>b</i> , mm			
50	2	10			

For the numerical modelling, it was assumed that the carbon fibre reinforcement could be flat inclusions of a homogeneous anisotropic material. The material properties of the resin and the carbon fibres from the reference literature data [2, 6, 8, 9, 10] were used to determine the representative material properties of the modelled composite structures. The list of model data is shown in Tables 2-4. The purpose of the numerical simulations was first to determine qualitative results; specific physical parameter values for the resin and the graphite were irrelevant. Of importance was to retain a disproportion between the properties of the matrix and the properties of the fibres, to represent the anisotropy of the fibres, and to reproduce a generally proper internal structure of the test specimens which (given their constant geometrical features) was the primary contributor to the variations in the calculated values of E'.

Note that a numerical simulation check was run for each of the test specimen models with an assumption that the matrix and the fibres featured the physical characteristics of the resin. The checks were intended to verify whether the modulus of elasticity calculated from dependence (4) in the parametric identification procedure complied with Young's modulus value assumed when building the numerical model. Further numerical simulations were run on the laminate specimens in two different configurations:

- zgz where the outer layer was the resin;
- *gzg* where the outer layer was the carbon fibre rowing.

Multi-layer laminate / Three-layer laminate – graphite fibres							
Young's modulus, GPa			Poisson's ratio			Modulus Gxv. GPa	Density ρ , kg/m ³
E_{x}	$E_{\rm y}$	$E_{\rm z}$	ry, yz rz				
385	6.3	6.3	0.20	0.20	0.20	7.7	1940

 Table 2. Selected material properties of the graphite fibres in the multi-layer laminate and the three-layer laminate

Table 3. Selected material properties of the graphite fibres in the rowing model

Rowing model – graphite fibres							
Young's modulus, GPa		Poisson's ratio		tio	Modulus G GPa	Density $a_k g/m^3$	
E_{x}	E_{y}	$E_{ m z}$	Vxy, Vyz, Vxz			Oxy, OI a	p, kg/m
6.3	6.3	385	0.20	0.20	0.20	7.7	1940

Table 4. Selected material properties of the resin in all three specimen types

Multi-layer laminate / Three-layer laminate / Rowing model					
Young's modulus, <i>E</i> , GPa	Poisson's ratio	Density ρ , kg/m ³			
3	0.49	1200			

4. NUMERICAL SIMULATION AND CALCULATION RESULTS

The result of the numerical calculations was the determination of the modelled beam bend, f, at the point of force input in each of the analysed cases. Figure 4 shows examples of the calculations for the three-layer laminate model. For the determined bends, dependence (4) was applied to calculate the values of E', as was the case in the processing of the results of recording the specimen's response in the DMA tests (see [1]). Table 5 and Figs. 5–8 show the calculation results for the different versions of this study.

As already said, the mesh was built with triangular elements (Fig. 2). Test calculations were also run to analyse the sensitivity of the numerical model to the numerical mesh number. The calculations were run for nominal and dense versions of the numerical mesh. The nominal mesh had 308 elements, while the dense numerical mesh had 19,712 elements. The maximum deflection values were, respectively: $f_1 = 2.617$ mm for the nominal numerical mesh and $f_2 = 2.619$ mm for the dense numerical mesh.

	Case no.	Configuration	Bend, <i>f</i> , m	Modulus of elasticity, Pa
Multi-layer laminate	1	gzg	4.864 · 10 ⁻⁵	$1.61 \cdot 10^{11}$
	2	zgz	5.270 · 10 ⁻⁵	$1.48 \cdot 10^{11}$
	3	Resin	2.621 · 10 ⁻³	$2.98 \cdot 10^{9}$
Three-layer laminate	4	gzg	3.417 · 10 ⁻⁵	$2.29 \cdot 10^{11}$
	5	zgz	$1.600 \cdot 10^{-4}$	$4.88 \cdot 10^{10}$
	6	Resin	$2.619 \cdot 10^{-3}$	$2.98 \cdot 10^{9}$
Rowing cross-section model	7	Resin	$2.620 \cdot 10^{-3}$	$2.98 \cdot 10^{9}$
	8	Fibres	1.029 · 10 ⁻³	$7.59 \cdot 10^{9}$

Table 5. Specimen bend values and the modulus of elasticity value for different models and configurations







Fig. 5. Calculated values of the modulus of elasticity for the multi-layer laminate specimen models



Fig. 6. Calculated values of the modulus of elasticity for the three-layer laminate specimen models



Fig. 7. Calculated values of the modulus of elasticity for the rowing cross-section model in the transverse configuration



Fig. 8. Calculated values of the modulus of elasticity for all specimen models, all configurations studied (the numbering is applied from Table 5)

A conclusion was valid that given that the difference between both values was below 0.1%, the density of the mesh elements of the specimen model had no significant impact on the results of the numerical simulation. Similar results were produced for other numerical calculation versions.

5. ANALYSIS OF RESULTS

The analysis of the results listed in Table 5 and shown in Figures 4-7validated a conclusion that the values of the identified modulus of elasticity, E', for the specimens made from the resin only generally complied with the values declared for the model in COMSOL. It was reasonable to conclude that all other results of the numerical simulations were reliable. Among the analysed specimen types, the rowing cross-section model featured the lowest modulus of elasticity, equal to 7.59 GPa. Conversely, the highest modulus of elasticity, equal to 229 GPa, was produced for the three-layer laminate model with the gzg configuration. Significant differences were found when the results were compared between the multi-layer laminate models and the three-layer laminate models. The three-layer laminate models had higher absolute and relative differences between the calculated modulus of elasticity (180.2 GPa, respectively, which provided a higher to lower value ratio of 4.7/1) than the multi-layer laminate models (13 GPa, respectively, and 1.08/1). For the threelayer laminate models, a major contributor was the orientation of the layers: the gzg configuration specimen was 4.7 times more rigid than the zgz configuration specimen. This was an effect of the transfer of stress within the specimens.

The stresses would become smaller as they approached the plane of symmetry of the specimen. The plane of symmetry was perpendicular to plane Oxz and crossed the centre of the test specimen. When a more rigid material was located in the outer layers, the entire test specimen became more rigid. These conclusions seem obvious from a strength analysis perspective. However, the tests completed, as discussed herein, helped visualise the problem of homogenising the properties of heterogeneous composite structures. The multilayer laminate did not reveal differences as big as above. Given the assumed number of 11 layers of inclusions, which meant that the transverse dimension of an inclusion was approximately 20 times less than the transverse dimension of the whole structure, the difference between the calculated values of stiffness was 8% between the two cases. The calculated values of the modulus of elasticity, E', for the modelled multi-layer structure were between the limit values (229 GPa to 48.8 GPa) achieved for the three-layer model.

6. CONCLUSION

The general conclusion of the tests discussed here should focus on the effectiveness of the developed method of numerical analysis.

The results provided by the author pointed to a qualitative agreement with the results of testing real-life composite structures [12]. The results also proved the effectiveness of the method of DMA modelling for structurally homogeneous and heterogeneous specimens both on macrostructural and microstructural levels. The macrostructural heterogeneousness were represented by the three-layer laminate models. Here, the dimension of the inclusions was comparable to the characteristic dimension of the investigated specimen. The multi-layer laminate models could be generally qualified as microstructural models. The dimension of the inclusions was small enough that, provided a uniform distribution of the inclusions, an 8-percent difference resulted in the calculated values of the modulus of elasticity between two special cases, zgz and g_{zg} (Table 5). This condition permitted characterisation of the structure with volumetric composition fractions (with the structure homogenised, see [11]). An important practical conclusion was the proof of a strong directional dependence of the modulus of elasticity, E', determined in these tests. The bend, or deflection, or the response of the modelled system configuration to the inputs depended highly on the orientation of fibres in the modelled specimens, as shown in the lengthwise and transverse configuration tests done on the models. This was confirmed by the differences in the modelling results between the laminates and the transverse rowing cross-section model (Table 5). The natural course of further research would be operations related to threedimensional modelling with consideration of the large-scale nature of modelled composite structures. Application of other calculation models in COMSOL/M, or the addition of proprietary subroutines, could facilitate the viscous component, represented by the loss modulus, E", in the models.

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Analiza numeryczna metodyki badań DMA kompozytu epoksydowo-węglowego

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Streszczenie. W pracy przedstawiono wyniki numerycznych badań symulacyjnych właściwości cieplnomechanicznych (termomechanicznych) pomiaru strukturv kompozytowej. Uwagę skupiono na symulacji sprężystej odpowiedzi próbki kompozytu epoksydowo-węglowego poddanego analizie termomechanicznej DMA (Dynamic Mechanical Analysis) w trybie zginania z trójpunktowym swobodnym podparciem. Kompozyt epoksydowo-weglowy jako obiekt analizy charakteryzuje się bardzo dużą dysproporcja właściwości spreżystych materiału osnowy i wypełnienia. Dodatkowo cechy anizotropii wykazuje już sam materiał wypełnienia w postaci włókien weglowych. Celem wykonanych badań numerycznych było jakościowe określenie wpływu struktury na wyniki badań DMA i określenie możliwości zaklasyfikowania uzyskiwanych wyników jako właściwości efektywnych bądź pozornych. Do opracowania modelu makromechanicznego badanej próbki i przeprowadzenia obliczeń wykorzystano program modelowania MES COMSOL. Wypełnienie włóknami weglowymi modelowano za pomocą ortotropowych wtrąceń warstwowych lub kołowych o różnych wymiarach charakterystycznych. Reprezentatywne dane materiałowe przyjęto na podstawie wyników badań własnych i danych literaturowych. Zbadany został wpływ rozmieszczenia poszczególnych warstw oraz ich wymiaru charakterystycznego na określany z modelowej zależności moduł sprężystości E'. Slowa kluczowe: materiał kompozytowy, DMA, symulacja numeryczna, COMSOL