SELECTION OF MATERIAL MODEL OF CHOSEN PHOTOCURABLE RESIN FOR APPLICATION IN FINITE ELEMENT ANALYSES

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Received 30 November 2020, accepted 14 December 2020, available online 14 December 2020.

Key words: additive manufacturing, photocurable material, Finite Element Method, constitutive models.

Abstract

In the paper, a literature study of a modelling methods of a photocurable materials developed by additive techniques is presented. The main aim was to assess which material model is appropriate for such kinds of matter. The Finite Element Method and the LS Dyna software was assumed as a possible environment for the investigations. The material models that can be apply for photopolymers analysing were described as well as examples of such materials. The conclusions is that the material model selection must be based on the observation of the material behaviour and the possible loading conditions (e.g. strain rate).

Introduction

The stereolitography (SLA) is one of the additive manufacturing techniques. The main idea of this method is a printing with the use of a photocurable resin, e.g. epoxy or acrylic one. During the crosslinking process the resin is exposed to a ultraviolet (UV) light of a specific wavelength. This physico-chemical process is known as a photopolymerization (Dizon et al. 2018). In practice the SLA
is carried out on 3D printers. Such printer working method is presented schematically in Figure 1. The model for the printing is created in a CAD software (Fig. 1a), transformed to STL format (Fig. 1b), divided into slices (Fig. 1c) and printed. The printer is built of a moving platform (1 in Fig. 1d) placed in a tank (2 in Fig. 1d) filled with a liquid polymer (3 in Fig. 1d). The light from an UV laser (4 in Fig. 1d) cures a designed cross-sectional pattern of the sample (5 in Fig. 1d) on the surface of the liquid polymer through a mirror (6 in Fig. 1d). In the next step the platform moves and the curing cycle repeats. The part is built layer by layer of a designed thickness $\Delta z$ (Fig. 1e), until the object is fully formed (VAEZI et al. 2013).

![Fig. 1. SLA printing scheme: a – CAD model, b – STL model, c – division into slices, d – printer setup (1 – moving platform, 2 – resin tank, 3 – liquid polymer, 4 – UV laser, 5 – printed object, 6 – mirror), e – printed model; z – layer thickness](image)

The SLA printed objects can have very complicated shapes, what can be the basis of using it for developing real constructions elements such as energy absorbers or connectors. This idea is also the purpose of designing such elements using finite element method (FEM).

In FEM, a very important problem is to choose and to verify a proper constitutive model for the analyzed material.

In this paper the possible models found in software libraries were reviewed as well as the approaches to such modelling found in the literature. Finally, the numerical analyses of tensile test of a selected SLA resin using different material models was shown.
Numerical aproach to polymers modelling – review

Some approaches to numerical modeling of polymers can be found in literature, as well as in calculation software libraries. In the work described in the paper the LS Dyna computer code was used, so the material constitutive models implemented in this software were reviewed and shown below.

The easiest way to model elasto-plastic material, but without considering the chemical changes in polymer chain structure, is to apply the linear plasticity model (in LS Dyna it is *MAT_PIECEWISE_LINEAR_PLASTICITY – MAT_24, HALLQUIST 2007). The material description is based on Young’s modulus, Poisson’s ratio, yield stress, hardening modulus, ultimate plastic strain, and time step size for element deletion. Also an arbitrary stress versus strain curve and arbitrary strain rate dependency can be defined. In this model deviatoric stresses are determined due to the yield function as:

\[ \frac{1}{2} s_{ij}s_{ij} - \frac{\sigma_y^2}{3} \leq 0 \]  

(3)

The yield stress is calculated as:

\[ \sigma_y = \beta \left( \sigma_0 + f_h(\varepsilon_{eff}^p) \right) \]  

(4)

where:

- \( \beta \) – the strain rate effect parameter,
- \( f_h(\varepsilon_{eff}^p) \) – the hardening function,
- \( \varepsilon_{eff}^p \) – the effective plastic strain.

The other model that can be found in LS Dyna is MAT_168 (*MAT_POLYMER), available since version 971 (HALLQUIST 2007). This model is based on the assessment that the polymer has two resistances to the deformation: an inter – molecular one, related to the relative moment between molecules (A), and the other one evolving anisotropic, which is connected to the molecules chains straightening (B). This model was is based on the study showed in BOYCE et al. (2000). It can be schematically presented as the mechanical setup built of two springs and a damper (Fig. 2). A resistance of the spring A is described on the base of the Neo-Hookean law. On the base of this scheme the deformation gradient tensor is the same for A and B resistance:

\[ F = F_A = F_B \]  

(5)

and Cauchy stress tensor is a sum of A and B resistances ones:

\[ \sigma = \sigma_A + \sigma_B \]  

(6)
In LS Dyna also the following material models for polymers are available:
- *MAT_081 (MAT_PLASTICITY_WITH_DAMAGE),
- *MAT_089 (*MAT_PLASTICITY_POLYMER),
- *MAT_101 (*MAT_GEPLASTIC_SRATE_2000A),
- *MAT_112 (*MAT_FINITE_ELASTIC_STRAIN_PLASTICITY),
- *MAT_141 (*MAT_RATE_SENSITIVE_POLYMER),
- *MAT_187 (*MAT_SAMP-1).

MAT_081 (HALLQUIST 2007) is the elasto-visco-plastic material description, where stress-strain curve or strain rate dependency can be defined. Damage is considered before rupture occurs. In this model the constitutive properties for the damaged material are obtained from the undamaged material properties. The amount of damage evolved is represented by the constant, $\omega$, which varies from 0 (no damage) to 1 (complete rupture). For the uniaxial loading, the nominal stress, $\sigma_{\text{nominal}}$, in the damaged material is given as:

$$\sigma_{\text{nominal}} = \frac{P}{A}$$

(7)

where:

$P$ – the applied load and $A$ is the surface area.

The true stress is given by:

$$\sigma_{\text{true}} = \frac{P}{A - A_{\text{loss}}}$$

(8)

where:

$A_{\text{loss}}$ – the void area.
The damage variable is defined as:

\[ \omega = \frac{A_{\text{loss}}}{A} \]  

(9)

In this model damage is defined in terms of plastic strain after the failure strain is exceeded:

\[ \omega = \frac{\varepsilon_{\text{eff}}^p - \varepsilon_{\text{failure}}^p}{\varepsilon_{\text{rupture}}^p - \varepsilon_{\text{failure}}^p} \quad \text{if} \quad \varepsilon_{\text{failure}}^p \leq \varepsilon_{\text{eff}}^p \leq \varepsilon_{\text{rupture}}^p \]  

(10)

MAT_089 (HALLQUIST 2007) describes the elasto-plastic material, for which also stress-strain or strain rate curve can be considered. This model can be applied when the elastic and plastic responses are not clear, as e.g. in metals. Also polymers brittle behavior in high strain rates can be considered. This model is only applicable for 2D elements. MAT_89 is similar to MAT_24 expect the following points:

– loadcurve lookup for yield stress is based on the equivalent uniaxial strain, not the plastic strain;
– elastic stiffness is initial equal to Young modulus but will be increased according to the slope of the stress-strain curve;
– the failure strain depends on the strain rate.

The strain used for failure and damage calculation, \( \varepsilon_{pm} \), is based on an approximation of the greatest value of maximum principal strain encountered during the analysis:

\[ \varepsilon_{pm} = \max_{i,sn}\left( \varepsilon_H^i + \varepsilon_{VM}^i \right) \]  

(11)

where:

\( n \) – a current time step index,
\( \max(...) \) – the maximum value attained by the argument during the calculation and:

\[ \varepsilon_H = \frac{\varepsilon_x + \varepsilon_y + \varepsilon_z}{3} \]  

(12)

where:

\( \varepsilon_x, \varepsilon_y, \varepsilon_z \) – the cumulative strains in the local x, y, and z direction, respectively,

\[ \varepsilon_{VM} = \sqrt{\frac{2}{3} \text{tr}\left( \varepsilon'^T \varepsilon' \right)} \]  

(13)

where:

\( \varepsilon' \) – a deviatoric strain tensor.

MAT_101 (HALLQUIST 2007) is dedicated for thermoplastics. It was developed by General Electric Company to model commercial materials subjected to
high strain rate loading. In this model yield stress is a function of strain rate. This model is described by the constitutive equation:

$$\dot{\varepsilon}_p = \dot{\varepsilon}_0 \exp(A\{\sigma - S(\varepsilon_p)\}) \times \exp(-paA)$$  \hspace{1cm} (14)

where:
- $\dot{\varepsilon}_0$ and $A$ – rate dependent stress parameters,
- $S(\varepsilon_p)$ – internal resistance (strain hardening),
- $a$ – a pressure dependence parameter.

MAT_112 is almost similar to MAT_89, but the elastic response of the model uses a finite strain formulation so that large elastic strains can develop before yielding occurs.

Finally, MAT_141 is a model for isotropic ductile polymers modelling with consideration of strain rate effects. The constitutive equation for the model is as follows:

$$\varepsilon_{ij} = D_0 \exp \left[ -\frac{1}{2} \left( \frac{Z_0^2}{3K_2} \right) \left( s_{ij} - \Omega_{ij} \right) \right]$$  \hspace{1cm} (15)

where:
- $D_0$ – the maximum inelastic strain rate,
- $Z_0$ – the isotropic initial hardness of the material,
- $\Omega_{ij}$ – the internal stress,
- $s_{ij}$ – the deviatoric stress component,
- $K_2$ – defined as:

$$K_2 = \frac{1}{2} (s_{ij} - \Omega_{ij})(s_{ij} - \Omega_{ij})$$  \hspace{1cm} (16)

and represents the second invariant of the overstress tensor. The elastic components of the strain are added to the inelastic strain to obtain the total strain. The internal stress variable rate is defined as:

$$\dot{\Omega}_{ij} = \frac{2}{3} q \Omega_m \dot{\varepsilon}_{ij} - q \dot{\varepsilon}_e \dot{\varepsilon}_e$$  \hspace{1cm} (17)

where:
- $q$ – a material constant,
- $\Omega_m$ – a material constant that represents the maximum value of the internal stress,
- $\dot{\varepsilon}_e$ – the effective inelastic strain.

MAT_187 is a semi-analytical model dedicated for polymeric materials. In this model an isotropic smooth yield surface is implemented for non-reinforced plastics description. Three yield curves are here used and the yield surface has a quadratic shape. When less than three curves are defined the model calculates the remaining curves as follows (HALLQUIST 2007):
where:

\( \sigma_t, \sigma_s, \sigma_c \) – stress values obtained from tensile, shear and compression tests, respectively,

\( \sigma_{vM} \) – von Mises stress,

\( p \) – pressure.

The interesting approaches to the modelling of the photocurable polymers can be found in the literature. The scientists use the micro-macro modelling as well as the global one. For example the approach with consideration the micro and macro structure of a printed material using FEM (finite element method) can be found in Rodriguez et al. (2003). The authors applied the elasticity approach to assess the stiffness of ABS material printed with Fused Deposition Modelling (FDM) additive technique. The asymptotic theory of homogenization was applied to predict unidirectional FD-acrylonitrile butadiene styrene material behavior.

In Ajoku et al. (2006) the Nylon printed in SLS (Selective Laser Sintering) technique was modeled using FEM, but the positively validated results were achieved only for the elastic range of the stress. The researched material showed a 7% porosity and voids were placed in the 2D geometric model used for the FE analyses. The authors postulated that the applied geometry is too idealistic to reflect the material behavior in the nonelastic stress rate.

In Zarbakhsh et al. (2015) the sub-modeling approach and FEM were proposed to analyze the mechanical characteristics of 3D-printed parts, whereas the details of 3D printing patterns were included in sub-model.
FEM is not the only method used in modeling the printed materials behavior. In Sugavaneswaran and Arumaikkannu (2015) the rule of mixture and analytical approach were applied to estimate the elastic properties of the additively manufactured composite parts. The analytical method was validated with the use of the experimental results. The experimental and analytical methods have quite good agreement; hence methodology proposed can be used for estimating the elastic properties of additively manufactured multi material structures.

Another approach was presented in Wu (2018), where the evolution of the mechanical properties of the photopolymer during the photocuring process was investigated using theoretical modeling and experimentation. The chemical reaction kinetics was modeled using the first order reaction differential equations.

### Chosen photocurable resins description

As it was mentioned the solid sample is developed in the 3D printer using UV light. At the molecular level this process starts from the short chains of photocurable resin, which have active groups in their ends. The resin also includes photoinitiators which exposed to UV light break into two molecules and two radicals. Those radicals are transferred to polymer chains active groups. The chains begin to form longer chains and the liquid resin becomes a solid material. The process was schematically presented in Figure 3 (The Ultimate Guide... 2020).

![Scheme of photopolymerization process](image)

Fig. 3. Scheme of photopolymerization process: a – liquid resin short chains and photoinitiator under UV light, b – photoinitiator brakes into two molecules and two radicals, c – radicals react with polymer chains active groups, d – short chains react to create long structure; 1 – photoinitiator, 2 – short chains, 3 – active group, 4 – radical, 5 – long chain  
Source: based on The Ultimate Guide... (2020).
Currently there are many photocurable resins for the engineering, dental or even jewelry applications. For example the Formlabs company offers the following engineering resins (Materials Data Sheet... 2018):

- Grey Pro Resin for high precision printings characterized with moderate elongation, and low creep;
- Tough Resin which handles compression, stretching, bending, and impacts without breaking;
- Rigid 10K - highly glass-filled resin;
- Durable resin highly pliable, impact resistant, and lubricious material.

The mechanical properties of those resins were given in Table 1.

### Table 1

|                        | Grey Pro resin | Tough resin | Rigid 10K resin | Durable resin |
|------------------------|---------------|-------------|----------------|---------------|
| Ultimate tensile strength [MPa] | 61            | 33          | 55             | 28            |
| Tensile modulus [GPa]   | 2.6           | 15          | 10             | 10            |
| Elongation [%]          | 13            | 51          | 1              | 55            |

Source: based on Materials Data Sheet... (2018).

### Summary and conclusions

The models described above were grouped in Table 2 according to their application (type of material, strain rate effect, elements type etc.).

### Table 2

| Material model | Application (material type) | Strain rate effect | Failure effect | Damage | Element type | Remarks |
|----------------|-----------------------------|--------------------|----------------|--------|--------------|---------|
| 1              | 2                           | 3                  | 4              | 5      | 6            | 7       |
| MAT_24         | elasto-plastic materials, metals, plastics, polymers | yes               | yes            | no     | 2d, 2d       | the most universal model, based on the true stress – true strain curve |
| MAT_081        | elasto-visco-plastic materials considering damage, metals, plastics, polymers | yes               | yes            | yes    | 2d, 3d       | model based on the true stress – true strain curve |
| MAT_089        | plastics, polymers          | yes               | no             | no     | 2d           | for materials with plastic and elastic sections not clearly separated |
On the base of presented review it can be assumed that the model selection should be preceded by at least basic material tests (uniaxial compression and/or tensile test). Then, the analysis of the library of models available in the software should be carried out for the most appropriate reflection of the material properties (e.g. brittleness, thermoplasticity, viscoelasticity, etc., see Tab. 1). Finally the conditions, in which the material will be tested (e.g. strain rate) must be considered. In order to determine the material parameters for the selected model, the necessary experimental tests should be performed. It should also be remembered that each material model must undergo a validation process.

Acknowledgements

The article was written as part of the implementation of the university research grant No. 22-754, MUT, 2020, Warsaw, Poland.
Selection of material model of chosen photocurable resin...

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