Model of layers bonding during LOM-process

Anna Knyazeva[1], Nahum Travitzky[2]

[1] Tomsk Polytechnic University, 634050 Tomsk, Russia
Institute of Strength Physics and Material Science, 634055, Tomsk, Russia
[2] Department of Materials Science, Institute of Glass and Ceramics, University of Erlangen-Nuremberg, 91058 Erlangen, Germany

Email: anna-knyazeva@mail.ru

Abstract. The model of LOM-process with chemical reaction in intermediate layer is suggested in this paper. Maximal stress in contact zone and half-thickness of contact area are given from contact problem of mechanics. It was shown that this problem is similar to the problem of different material conjugation using synthesis in solid phase. Dimensionless variables and dimensionless criteria are identical for these processes. The qualitative examples of temperature field evolution for self-sustaining mode are demonstrated.

1. Introduction

Today additive manufacturing is a well-known technology for making real three dimensional objects from different materials, which may be subjected to various applications. Several AM techniques such as Stereo lithography (SLA) and its derivatives, Fused Deposition Modeling (FDM), Selective Laser Sintering or Melting (SLS/SLM), Laminated Object Manufacturing (LOM and similar sheet stacking processes), 3D-Printing (3DP) were applied for the manufacturing of structures with complex geometry [1-3]. Laminated object manufacturing (LOM) is one of categories of the sheet lamination processes in which material sheets are either cut by using laser or combined by using ultrasound. LOM-technique can be further classified based on the bonding mechanism between the sheets such as adhesive bonding, thermal bonding, and clamping [2] and includes several stages. For example, the LOM process of LZSA (LiO_2–ZrO_2–SiO_2–Al_2O_3) laminates included [4] three basic stages: tape casting of LZSA slurries, lamination by LOM machine accompanied by intermediate layers formation, and sintering accompanied by shrinkage.

   LOM-technique is characterized by some advantages in comparison with other methods [2-3]: the variety of used organic and inorganic materials including multi-materials and multi-colors; high fabrication speed; low warping and internal stresses; no support structures are needed. Using this method it is possible to create the multilayered structures with different composition and properties of layers. To improve the layer joining, special materials can be used between layers. In this case the process can be accompanied by chemical reactions between components. It has been used to develop composite synthesis with the help of combustion during lamination or post-processing [5]. Today this possibility has the limitations connecting with bad controllability [6]. Note the chemical reactions can proceed during laser cut when detail is formed based on CAD-model.

   There are numerous theoretical papers devoted to the description of mechanical and thermal properties of LOM-composites, for example [7-9]. However the physical and chemical processes accompanying the intermediate layers formation during LOM stages are modeled scarce. Appearing here problems need a special investigations. In this paper the mathematical model of different

materials conjugation (with different thermal physical properties) is studied numerically. It is assumed that chemical reaction starts in intermediate layer. Substance flow is not taken into account in a first approximation.

2. Mathematical problem formulation

Schematically the LOM-process is presented in fig.1a,b and post-processing accompanied by the chemical reactions in Fig.1c. The roll with temperature T_s moves along the surface of above layer A. the contact area between roll and A-layer depends on roll-diameter 2R and applied pressure P.
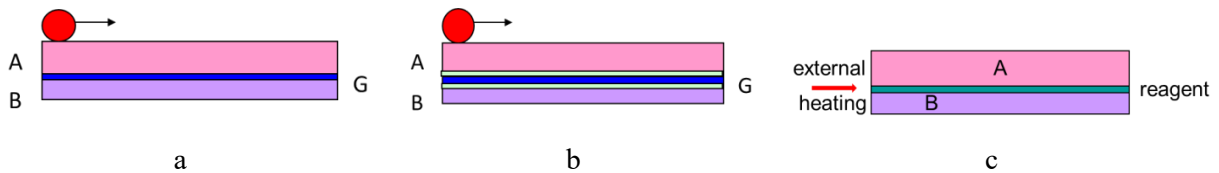

Fig.1 schematic presentation of some stages of LOM-process: a) process without intermediate layers formation; b) process with intermediate layers formation; c) post-processing with external heating

Maximal stress in contact zone can be evaluated by formula

$$\sigma_{max} = \left[\frac{P}{2R(\alpha_1 + \alpha_2)}\right]^{1/2} \tag{1}$$

and half-thickness of contact area – by formula

$$s = 0.798\left[2PR(\alpha_1 + \alpha_2)\right]^{1/2} \tag{2}$$

where

$$\alpha_k = \frac{1 - v_k^2}{E_k}, \tag{3}$$

v_k, E_k are the Poisson coefficients and elastic modulus for contacting materials, R – is roll radius. Elastic modulus of layered composite is

$$\frac{H}{E} = \frac{H_A}{E_A} + \frac{H_B}{E_B} + \frac{H_G}{E_G}. \tag{4}$$

Linear velocity of roll V is given.

Temperature field follows from conjugate thermal conductivity problem solution that includes equations

$$c_k \rho_k \frac{\partial T_k}{\partial t} = \lambda_k \left[\frac{\partial^2 T_k}{\partial x^2} + \frac{\partial^2 T_k}{\partial y^2}\right] + W_k, \tag{5}$$

where $k=A, G, B$, c_k, ρ_k, λ_k are the heat capacities, densities and thermal conductivity coefficients of layers A, B, G; t is the time; x, y are the spatial coordinates; $W_A = W_B = 0$;

$$W_G = Qz_0 \varphi(a) exp\left(-\frac{E}{RT_G}\right), \tag{6}$$

E, z_0, Q are the activation energy, pre-exponential factor, heat release for total chemical reaction in layer G; R is universal gas constant; a is conversion level following from the equation

$$\frac{\partial a}{\partial t} = z_0 \varphi(a) exp\left(-\frac{E}{RT_G}\right),$$ (7)

$\varphi(a)$ is some kinetic function representing the reaction mechanism in the micro scale level.

The conditions of ideal thermal contact are correct in the interfaces, where temperatures of layers and heat fluxes are equal; the adiabaticity condition takes a place in low surface; heat exchange is given in lateral surfaces or adiabaticity condition also. For $y = H = H_A + H_B + H_G$ we have

$$T = T_S, \ \text{if} \ Vt + x_0 - s \le x \le Vt + x_0 + s,$$ (8)

and $\partial T / \partial y = 0$ outside this interval.

At the initial time moment, we write:

$$T = T_0, \ a = 0.$$

In this problem it is necessary to calculate the temperature field and study the possible conversion modes in layer G varying the properties, thicknesses of layers and heating conditions.

The post-processing (Fig 1. c) is characterized by similar (the moving heat source instead roll) or other heating condition. The mathematical problem formulation is the same with other boundary conditions including constant temperature T_S on the left surface during given time interval.

3. Dimensionless variables

To investigate the model qualitatively it is convenient to go to dimensionless variables:

$$\theta_k = \frac{T_S - T_k}{RT_S^2} E, \xi = \frac{x}{H_G}, \eta = \frac{y}{H_G}, \tau = \frac{t}{t_a}$$ (9)

where t_a is adiabatic time or time during which the chemical reaction will complete in adiabatical conditions with given temperature [10],

$$t_a = \frac{c_G \rho_G R T_S^2}{z_0 E Q} exp\left(\frac{E}{RT_S}\right),$$ (10)

In new variables, the problem takes the form:

$$K_{CB} \frac{\partial \theta_B}{\partial \tau} = \frac{K_{\lambda B}}{\delta}\left[\frac{\partial^2 \theta_B}{\partial \xi^2} + \frac{\partial^2 \theta_B}{\partial \eta^2}\right], \ 0 < \eta < \Delta_B;$$ (11)

$$\frac{\partial \theta}{\partial \tau} = \frac{1}{\delta}\left[\frac{\partial^2 \theta}{\partial \xi^2} + \frac{\partial^2 \theta}{\partial \eta^2}\right] + \varphi(a)F(\theta), \ \Delta_B < \eta < 1 + \Delta_B;$$ (12)

$$\frac{\partial a}{\partial \tau} = \gamma \varphi(a)F(\theta) = \gamma \varphi(a) exp\left(\frac{\theta}{1 + \beta\theta}\right),$$ (13)

$$K_{CA} \frac{\partial \theta_A}{\partial \tau} = K_{\lambda A}\left[\frac{\partial^2 \theta_A}{\partial \xi^2} + \frac{\partial^2 \theta_A}{\partial \eta^2}\right], \ 1 + \Delta_B < \eta < 1 + \Delta_B + \Delta_A;$$ (14)

$$\eta = 0 : \partial \theta_B / \partial \eta = 0;$$ (15)

$$\eta = \Delta_B : K_{\lambda B}\frac{\partial \theta_B}{\partial \eta} = \frac{\partial \theta}{\partial \eta}; \ \theta_B = \theta;$$ (16)

$$\eta = \Delta_B + 1: \frac{\partial \theta}{\partial \eta} = K_{\lambda A}\frac{\partial \theta_A}{\partial \eta}; \; \theta = \theta_A; \tag{17}$$

$$\eta = 1 + \Delta_B + \Delta_A:$$

$$\xi_0 + \omega\tau - \xi_A < \xi < \xi_0 + \omega\tau + \xi_A: \theta = 0; \tag{18}$$

$$\xi \le \xi_0 + \omega\tau - \xi_A \text{ and } \xi \ge \xi_0 + \omega\tau + \xi_A: \partial\theta_A/\partial\eta = 0;$$

$$\xi = 0, L: \partial\theta_k/\partial\xi = 0; \tag{19}$$

$$\tau = 0: \theta_B = -\theta_0; \theta_A = -\theta_0; \theta = -\theta_0; a = 0. \tag{20}$$

This problem includes dimensionless parameters

$$\beta = \frac{RT_S}{E}; \; \gamma = \frac{c_G\rho_G RT_S^2}{EQ}; \; \theta_0 = \frac{T_S - T_0}{RT_S^2}E; \; \delta = \frac{H_G^2 c_G\rho_G}{\lambda_G t_a},$$

typical for combustion theory [10], geometrical parameters

$$\Delta_A = \frac{H_A}{H_G}; \; \Delta_B = \frac{H_B}{H_G}$$

and parameters characterizing the heating rate

$$\xi_0 = \frac{x_0}{H_G}; \; \omega = \frac{Vt_a}{H_G}; \; \xi_A = \frac{s}{H_G}.$$

Until the substances do not heated to temperature T_S, the temperature $\theta_k < 0$. If $\omega < 1$, roll runs during the time t_a the distance less then layer G thickness; if $\delta > 1$, the layer with thickness H_G does not have a time for the heating; and etc.

For situation presented in the Fig.1 c, the conditions change

$$\eta = 1 + \Delta_B + \Delta_A: \partial\theta_A/\partial\eta = 0;$$

$$\xi = 0: \theta = 0, \; \tau < \tau_0 \text{ and } \partial\theta_k/\partial\xi = 0 \text{ for } \tau \ge \tau_0.$$

The both problems are solved numerically.

4. Example of calculation

The calculations show that various regimes of reaction propagation between materials A and B are possible depending on the heating conditions. When the heat in the heated zone is enough for self-sustaining mode, the reaction front propagates along the layer G. When materials are given, to stabilize the reaction front, one can vary the sizes of layers. On the Fig. 2,a the sizes of A and B layers are identical. The no symmetrical reaction front appears because the thermal conductivity of layer B is high. In the Fig 2,b, the upper layer has the same thickness as the reagent. In this case the ignition point is earlier that connects with the fact that the top layer stores more heat and thereby it facilitates to the reaction acceleration. The reaction front stays not symmetrical

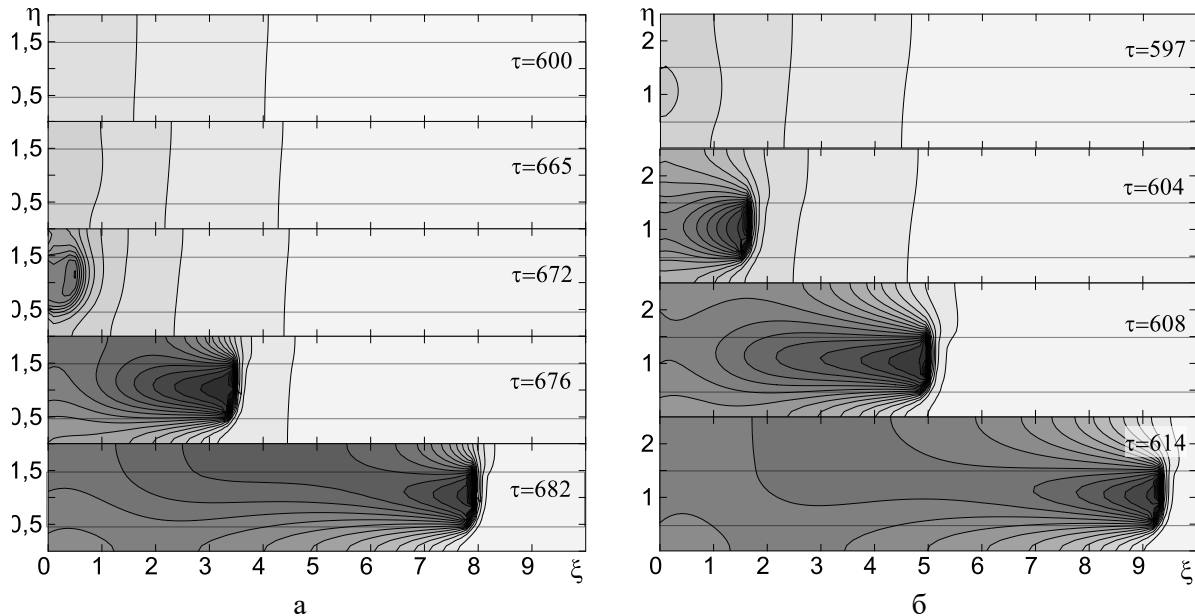Note that similar problems were investigated in [11, 12].

Fig. 2 Temperature field evolution with time for various sizes of the layers.
Parameters: $\theta_0 = 10$; $\beta = 0.03$; $\gamma = 0.03$; $Fr = 20$; $K_{\lambda A} = 4$; $K_{\lambda B} = K_{cA} = K_{cB} = 1$.

5. Conclusion

So, the problem on reaction propagation between inert layers during LOM-process was formulated. It was shown that this problem is typical combustion problem appearing during materials conjugation using chemical reacting connecting materials. The reaction front is non-symmetrical due to the different properties of conjugated layers and due to different thicknesses of the same layers. Reaction front can be stable because stored heat in conjugated materials can facilitate the reaction propagation.

6. Acknowledgments

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