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A comparative study on the 3D printing process of semi-crystalline and amorphous polymers using simulation

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Abstract

Polymers have been widely used in the field of fused deposition modelling (FDM). The part integrity of the final printed part is affected by parameters such as processing conditions and the material properties of the polymer. Build-up of residual stresses are the main cause of shrinkage and warpage (i.e., part distortion) in the FDM parts. Among the thermoplastic polymers, semi-crystalline polymers are more prone to part distortion due to crystallisation. Therefore, it is important to understand and predict part distortion in FDM of polymers to achieve good quality prints with desirable mechanical properties. Several studies have investigated the resulting part distortion in FDM parts through empirical, analytical, and numerical approaches. In most cases, the simulation results are not quantitatively validated, mainly because the temperature dependent properties of the polymers and the crystallinity of semi-crystalline polymers are often overlooked. In this study, the thermal-mechanical properties of the polymer of study such as specific heat capacity, thermal conductivity and density and the crystallisation kinetics are invoked as a function of temperature. Furthermore, an amorphous polymer was also simulated with consideration of its respective material properties. Both the semi-crystalline and the amorphous polymer models were simulated under various layer thickness (0.1 and 0.5mm), in order to investigate the effect of layer thickness on the induced thermal stress and resulting warpage. Based on the simulation results, for 0.1mm layer thickness, the amorphous polymer model exhibited a warpage drop of 77%. And for 0.5mm, the warpage noted was found to decrease by 63%, on comparison with the warpage noted from semi-crystalline polymer model. These warpage values from the simulated models were then measured against the 3D scan results of the printed samples for quantitative validation. An excellent agreement was observed between the experimental and the simulated samples.

Keywords: *Fused Deposition Modelling (FDM); Finite Element Analysis (FEA); Polymers; Layer thickness; Warpage*

1. Introduction

Fused Deposition Modelling (FDM) is one of the additive manufacturing (AM) techniques that has been gaining attention due to its ability to print thermoplastic polymers. FDM is also known for the simple printing technique, economic capital investments and potential to print complicated geometries [1]. However, printing thermoplastics through FDM can lead to various part distortions such as delamination, warpage, and shrinkage [2]. Due to the layer-by-layer deposition process, the induced thermal stresses inside the melted polymer are trapped and leads to continuous increase in accumulation of internal residual stress affecting the structural integrity of the printed part. Simulation has been employed as a tool to study and understand the effects of various printing conditions on part distortion by researchers in the past few years. Although many have successfully demonstrated the significance of printing conditions such as raster orientation, raster pattern, layer thickness, nozzle speed, extrusion temperature, the data available in literature is still not clear on their relationship to warpage and shrinkage. This paper aims to investigate the influence of layer thickness parameter on semi-crystalline and amorphous polymer models through quantitative validation.

2. Problem description

In this present study, polypropylene (PP) was selected to simulate semi-crystalline model and ABS P400 for amorphous model investigation. For the printing, modified Ultimaker 2 was used with processing conditions: nozzle diameter 0.8mm, bed temperature 100°C, line (90°/90°) raster pattern, infill 100%, nozzle speed 30mm/s, ambient temperature 25°C and nozzle temperature 210°C with layer thickness 0.5mm and 0.1mm. Due to the complexity of the physics involved, sample dimensions of 50*50*2mm and 50*50*0.4mm (each four layers) were printed and simulated, respectively.

2.1. Modelling

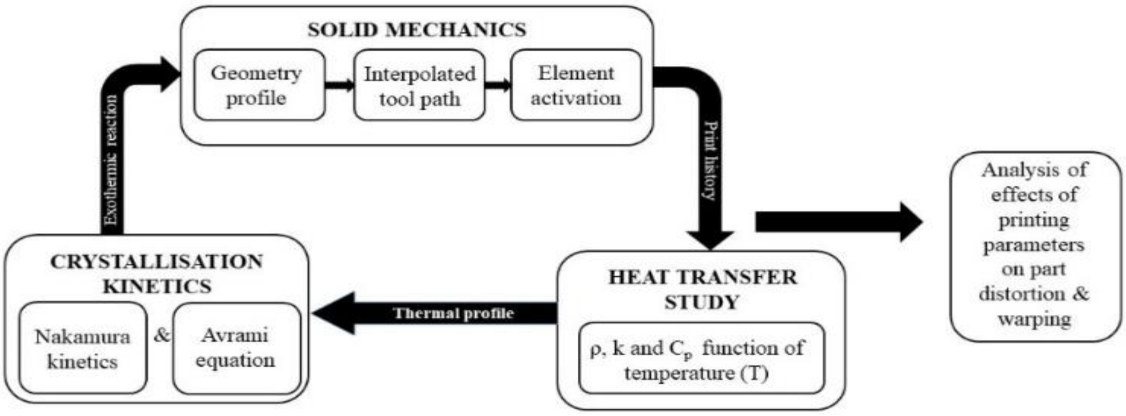


Figure 1. Process simulation plan for semi-crystalline polymer

The schematic representation of the physics incorporated in this study for semi-crystalline polymer simulation is presented in Figure 1. In solid mechanics, the in-house developed tool path is integrated with the element activation method where the meshed elements of the model are activated with respect to the FDM material deposition process. To investigate post processing warpage, spring foundation boundary condition is defined between the bottom layer of the simulated model and the print bed [2]. For simplification, print bed was assumed to have a fixed temperature throughout the printing process. Generalised Maxwell model and shift factor were considered for assigning viscoelastic properties of the semi-crystalline polymer to the model. Since semi-crystalline polymers are highly temperature dependent, the thermo-mechanical material properties (ρ density, C_p specific heat capacity and, λ thermal conductivity) of the polymer are interpolated as function of the temperature gradient of the model [3].

For crystallisation kinetics, crystalline physics developed by Levy [4] was modified using Nakamura crystallisation kinetics with the values provided from Koscher as follows [5]:

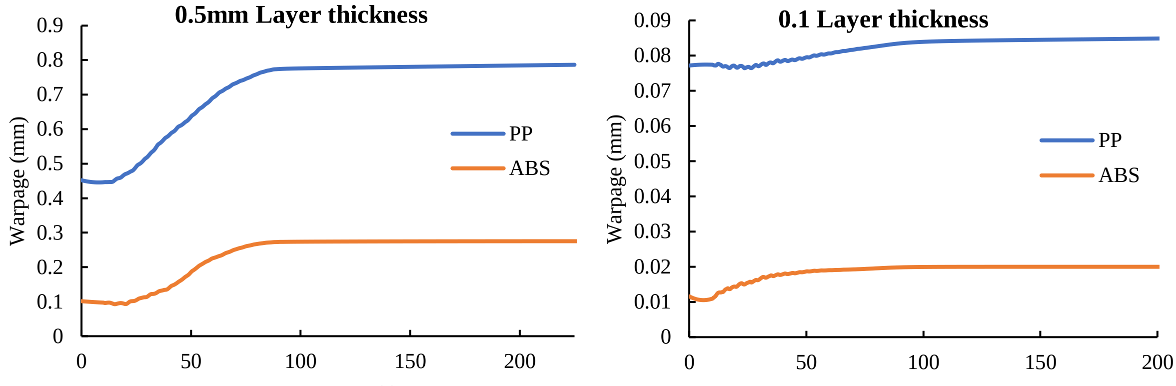
$$K(T) = (\frac{4}{3}\pi N_0(T))^{\frac{1}{3}} G_0 * exp\left(-\frac{U^*}{R(T-T_\infty)}\right) ex\,p\left(-\frac{K_g}{T(T_f-T)}\right) \quad (1)$$

Thus, the semi-crystalline model was simulated with respect to crystallisation and temperature through this approach.

For amorphous polymer (ABS P400), the material properties were considered from the study performed Armillotta et al. [6]. The amorphous model was simulated with boundary conditions similar to semi-crystalline polymer model except the crystallisation kinetics. Effects of gravity on the melt was considered in both amorphous and semi-crystalline polymer models.

3. Numerical results

In this study, a specific element was selected from the top layer, infill region of the samples and referred to as element m throughout the study for reference. Here for warpage investigation, an element was selected specifically from the top layer mainly because, due to the usage of bonding/adhesive agents to promote bonding between the first deposited layer and the print bed in the experimentally printed part, there were discrepancies found between the simulated and the measured warpage data. Figure 2(a) and (b), depicts the warpage trend predicted by the simulation from element m, after it was being deposited and allowed to cool till the sample reaches the room temperature.



(a) (b)

Figure 2. Warpage measured from element m from simulated semi-crystalline and amorphous polymer models are plotted against their overall printing time. The graphs presented here are plotted for sample printed at (a) 0.5mm and (b) 0.1 mm layer thickness.

In both Figure 2(a) and (b), during the initial stages of printing, the warpage trend from both PP and ABS appears flat, representing that the deposited melt settling down followed by gradual warping upon cooling. Among Figure 2(a) and (b), due to the larger layer thickness in Figure 2(a), it can be clearly seen that PP during its cooling phase exhibits warping which appears to be significantly higher than ABS. Even though the warpage curve from ABS model resembles the trend from PP, the warpage behaviour observed here is drastically smaller and cools at a much faster rate. This is mainly because, when the semi-crystalline polymer (PP) is cooled, due to crystallisation of the polymer molecules, extensive change in the volume occurs [7]. Once the sample reaches the room temperature, it can be seen from the graphs that the warpage trend becomes flat.

Furthermore, on comparison between Figure 2(a) and (b), it is evident that decreasing layer thickness has contributed to significant decrease in warpage in both semi-crystalline and amorphous models. It has been shown in the literature that decreasing layer thickness predominantly leads to decrease in warpage of the FDM printed samples [8]. Increasing layer thickness of a sample inadvertently leads to increase in accumulation of thermal stress within the layer. Additionally, increase in layer thickness also reduces the reheating that occurs in FDM while new layers are deposited on a previously deposited layer. During the deposition process, the thermal gradient from the newly deposited layer reheats the subsequent layer and releases the accumulated stress to a certain extent. Whereas, due to the poor thermal conductivity property of semi-crystalline polymers, increasing layer thickness considerably reduces the reheating effect as the layer deposition progresses. Hence, samples with 0.1mm layer thickness exhibit warpage significantly lower than samples with 0.5mm layer thickness.

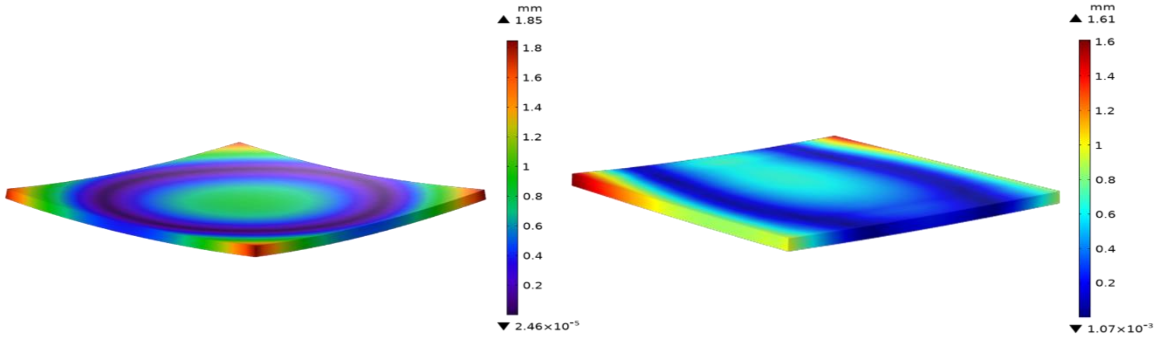


Figure 3. Warpage comparison between simulated semi-crystalline model (left) and amorphous model (right)

Figure 3 shows the graphical representation of the warpage predicted by the simulation in semi-crystalline and amorphous models. It can be seen that the semi-crystalline model exhibits warpage in all four corners while the amorphous model is only affected by geometrical instability in some corners.

Table 1. Experimental validation of simulated semi-crystalline model.

Samples	Predicted warpage (FEA) (mm)	Measured warpage (3D scan) (mm)	Deviation (%)
PP – 0.5mm layer thickness	0.786	0.796	-1.26
PP – 0.1mm layer thickness	0.085	0.093	-8.6

Table 1, shows the validation of the predicted warpage results by the simulated samples through the measured 3D scan values. Due to time constraint and lack of resources, only semi-crystalline polymer model was validated. However, the ability of the developed model to predict warpage can still be validated through the semi-crystalline model due to the authenticity of the incorporated crystalline physics.

4. Conclusion

In the presented study, a comparative study on the transient 3D models of amorphous and semi-crystalline polymer was performed. Through the semi-crystalline model, it has been demonstrated that considering the crystallisation kinetics, viscoelastic property, and accounting material properties as function of temperature leads to a quantitative validation with less than 8% deviation. Also, influence of layer thickness on amorphous and semi-crystalline polymer has been investigated through the developed models. In both cases ABS polymer model has exhibited significantly low warpage compared to PP. For layer thickness 0.1mm, 77% drop in warpage and for 0.5mm layer thickness, 63% decrease in warpage. On the other hand, by decreasing layer thickness from 0.5mm to 0.1mm, ABS alone showed a significant drop of 27% in warpage while PP showed a significant drop of 89%. Therefore, from the study, it can be concluded that even though semi-crystalline polymers warps at an order of magnitude higher than amorphous polymer, decreasing layer thickness reflects in considerable decrease in warpage in both polymer models.

References

[1] M. Rinaldi, T. Ghidini, F. Cecchini, A. Brandao, and F. Nanni, ‘Additive layer manufacturing of poly (ether ether ketone) via FDM’, *Compos. Part B Eng.*, vol. 145, no. March, pp. 162–172, 2018, doi: 10.1016/j.compositesb.2018.03.029.

[2] B. Courter, V. Savane, J. Bi, S. Dev, and C. J. Hansen, ‘Finite Element Simulation of the Fused Deposition Modelling Process Modelling Process’, no. June, 2017.

[3] R. Le Goff, G. Poutot, D. Delaunay, R. Fulchiron, and E. Koscher, ‘Study and modeling of heat transfer during the solidification of semi-crystalline polymers’, *Int. J. Heat Mass Transf.*, vol. 48, no. 25–26, pp. 5417–5430, 2005, doi: 10.1016/j.ijheatmasstransfer.2005.06.015.

[4] A. Levy, ‘A Novel Physics Node for Nakamura Crystallization Kinetics’, *Int. J. Numer. Methods Eng.*, no. November, 2016, doi: 10.1002/nme.

[5] E. Koscher and R. Fulchiron, ‘Influence of shear on polypropylene crystallization: Morphology development and kinetics’, *Polymer (Guildf).*, vol. 43, no. 25, pp. 6931–6942, 2002, doi: 10.1016/S0032-3861(02)00628-6.

[6] A. Armillotta, M. Bellotti, and M. Cavallaro, ‘Warpage of FDM parts: Experimental tests and analytic model’, *Robot. Comput. Integr. Manuf.*, vol. 50, no. August, pp. 140–152, 2018, doi: 10.1016/j.rcim.2017.09.007.

[7] M. Spoerk, C. Holzer, and J. Gonzalez-Gutierrez, ‘Material extrusion-based additive manufacturing of polypropylene: A review on how to improve dimensional inaccuracy and warpage’, *Journal of Applied Polymer Science*. 2019.

[8] H. Yang and S. Zhang, ‘Numerical simulation of temperature field and stress field in fused deposition modeling’, *J. Mech. Sci. Technol.*, vol. 32, no. 7, pp. 3337–3344, 2018, doi: 10.1007/s12206-018-0636-4.