Part Quality Prediction Tools for Fused Deposition Processing

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Abstract

Fused Deposition process fabricates requested part geometries by sequentially depositing discrete curvilinear beads of material next to and on top of each other. The part integrity depends strongly on the bonding quality at the bead interfaces. Since diffusion bonding of thermoplastic components in the material system is thermally driven, temperature history of interfaces determine the bonding quality. Detailed thermal analysis of deposition region and layer building simulation for a model geometry have been performed to investigate local and global material behavior during processing. A simple transport property prediction model has also been developed for the determination of thermal transport properties of the particle loaded systems used in Fused Deposition. Based on the information obtained from thermal models, a computationally efficient part building model has been developed to predict bonding quality in the whole part. The model is driven by the same command file, *sml* file, that drives the Fused Deposition hardware; and hence is capable of replicating the building process. The model has been tested for a model geometry, spur gear, and three dimensional bonding quality distribution has been predicted for the part.

1. Introduction

Fused Deposition process has been available for a number of thermoplastic materials [1]. Recent research efforts have been directed towards production of ceramic and metallic green bodies with Fused Deposition technologies [2]. These green bodies then undergo binder burnout and sintering operations, which result in fully dense functional parts. Employment of particle filled material systems required hardware and software modifications for Fused Deposition, besides the ongoing development effort for fused deposition of neat thermoplastic materials [3].

As part of the ongoing development effort for fused deposition of particle filled systems, process analysis tools are being developed [4,5,6]. These tools will be instrumental in achieving relative materials selection and processing freedom in significantly large subsets of engineering materials space. The tools will also be utilized for manufacturability assessment, and part quality prediction purposes.

Present paper outlines the progress that has been made in the process analysis of road cooling and diffusion bonding phase of Fused Deposition. Next section describes a simple computational model, which is capable of predicting effective transport properties of particle loaded heterogeneous systems. Section three presents a detailed local model for thermal analysis of deposition region. Section four presents the semi-global heat transfer model for layer building, where the production of a whole layer is simulated. Section five outlines the heuristic part building model developed, which is capable of extracting geometrical information and process scenario out of the FD command file. Finally, conclusions are given in section six.

2. Thermal Conductivity Prediction

A simple numerical experiment has been devised to predict the thermal conductivity of particle loaded thermoplastic binder systems. A finite element model, which is capable of solving two-dimensional steady-state heat conduction equation on heterogeneous material systems, has been developed. A rectangular geometry has been chosen as the experiment geometry, Figure 1. Top and bottom sides of the rectangle are insulated, left boundary is kept at a constant temperature and constant heat flux boundary conditions are prescribed at the right boundary. A skin layer is generated along constant temperature and heat flux boundaries. Random pattern generators are utilized to generate random compositions for the specified particle volume percent.



Figure 1. Sample Microstructure and Geometry

The heat transfer problem is solved, and average temperature is obtained for the constant heat flux boundary. Analytical solution for one-dimensional conduction problem is utilized to calculate the effective thermal conductivity of the part. The solution for a sample materials system is presented in Figure 2. Thermal conductivity prediction for %56 has been validated with Modulated Differential Scanning Calorimetry for RU960, and the results are given in Table I.



Figure 2. Dependence of Effective Thermal Conductivity on Particle Volume Fraction

Thermal Conductivities [W/(m*K)]	
Binder	Particle
0.1	20
Predicted Ke	Measured Ke
1.2 (+- 0.2)	1.17

Table I. Validation of Thermal Conductivity Model for RU960

It has been observed from simulations, that the effective material thermal conductivity is sensitive binder thermal conductivity. The dependence of k_eff on k_p, is weak especially for higher k_p to k_b ratios. Hence, a stainless steel particle loaded material system has more or less the same thermal conductivity of silicon nitride loaded material if particle volume fractions.

3. Detailed Thermal Analysis of Deposition Region

Current Fused Deposition hardware has been designed for thermoplastic material production. The liquefier temperature is set just above the viscosity drop temperature. Deposited material cools fast, forming a seam with previously deposited material. If the frame of observation is fixed with the deposition, it can be observed that the seam length and depth changes dynamically. For material systems loaded with particles to high volume fractions, and have the same thermoplastic materials binder; liquefier temperatures need to be elevated significantly (50 - 80 C) to enable FD of these materials. The modified rheology of the particle loaded materials necessitates this overheating. Magnitude of seam length and depth are changed significantly too due to the availability of the extra thermal energy.

A two-dimensional quasi steady-state thermal model has been developed to investigate the effect of process parameters as well as size effects on temperature distribution. It has been assumed that the deposition process takes place on an adiabatic table, previously deposited roads have been quenched to ambient temperature, and deposition head thermal dynamics may be replaced by a constant effective liquefier temperature and the worktable translating at a constant speed. Lateral cooling in z-direction may be represented by a sink term in the governing equation.

The governing equation becomes steady state two dimensional advection-conuction equation with a convective cooling sink term. Constant ambient temperatures are specified at upstream boundary and no conduction boundary condition at the downstream boundary. Imperfect thermal contact is allowed between fresh road and substrate by defining a finite interface heat transfer coefficient, which makes the temperature field discontinuous across the interface. Constant effective liquefier temperature is assigned at deposition boundary, and convective cooling boundary conditions for the rest of the boundaries.

Finite volume method was used for discretization of governing equation as well as the boundary conditions. Upwinding methods have been utilized for the discretization of advective terms. Iterative solution schemes display relatively stable solution behavior due to the presence of sink terms in the governing equation.

Effects of process parameters on temperature distribution are described elsewhere [7]. Size dependence effects are depicted in this paper. Figure 3 shows the temperature distributions for three different number of roads in the substrate. RU960 material, with .508 mm road width and approximately 100 mm road length was simulated. Deposition speed was .5 "/s, ambient temperature was selected as 30 C, and effective liquefier temperature as 150 C. Empirical thermal properties have been used for RU960.



Figure 3. Temperature Distribution for Two and Ten Road Substrates



Figure 4. Size and Deposition Speed Dependence of Seam Length

Figure 4 shows the effect of deposition speed and substrate size on the seam length. The first two data points for each deposition speed curve have been interpolated from the available temperature data. The same figure also shows that the seam length becomes size independent for substrates which contain more than four roads. Hence the bonding enhancement per pass is greater for less populated road areas.

4. Layer Building Model

Although detailed information is produced through detailed local models, dynamic collective behavior of a roads that make up the part is also important. Previously developed [6] multi-road models have been extended to layer building model, incorporating perimeters/raster/grid style roads. For reasons of computational efficiency, the roads are idealized as one dimensional thermal entities, which are also capable of lateral thermal interactions with eachother when brought together. Mathematical form of equations are the same as [6], bookkeeping algorithms needed to be developed for inclusion of perimeter and raster style roads. The temperature evolution of a sample rectangular layer, with long raster scans is shown in Figure 5.



Figure 5. Temperature Evolution for Rectangular Layer Geometry

Temperature signatures shown in Figure 6, for long and short raster scans show different thermal paths the material points are experiencing. For long raster scans the material points that are at the center of the raster are visited twice as many times as the material points at raster ends; and the frequency of visits changes continuously along a raster line. For short raster lines on the other hand this effect becomes less pronounced, and the decoupling of material points occurs. Temperature measurements made with thermocouples, verified this behavior differences. Considering the geometrical complexity and arbitrariness of raster fills for real life parts, it is safe to hypothesize that different

material points in the layer may experience very different thermal histories during production.



Figure 6. Temperature Signatures for Long and Short Rasters

5. Part Building Model

Thermal layer building model would be computationally expensive, if it would have been used for the simulation of production of whole part. All the geometrical information, and most of the process parameter information for the production of a given part is contained in an ASCII command file, *sml* file, which is sent to FD hardware controller for part production. Interpreter codes have been developed to extract geometrical and process parameter information out of this file, enabling the digital replication of building process. This replication capability introduced the possibility of detecting **internal** build errors.

It is assumed that bonding quality of interfaces in the part, is a monotonically increasing function of time spent above the critical bonding temperature and temperature differential. hence a heuristic geometrical model has been devised for part building simulation. The model may be summarized as :

- 1. An effect zone, bonding cloud, is attached to the deposition head during the production.
- 2. The shape of the cloud is allowed to change during the production, depending on the instantaneous process parameters and production scenario. For the simulation presented in this paper an ellipsoidal shape was utilized.

- 3. Bonding potential is null outside the bonding cloud. The bonding potential is maximum at the deposition tip, and decays exponentially with increasing distance from the deposition dip.
- 4. At each time step during the simulation, the material points which have already been produced and fall into the bonding cloud are detected.
- 5. The bonding metric at these material points is incremented by an amount determined by the local bonding potential distribution, and time step.
- 6. Time stepping is continued till the end of part building.



Figure 7. Geometry of Spur Gear, Layers 23, 12 and 1 (top to bottom)

A 23 layer spur gear geometry has been chosen as the test case. Selective layers of the part are shown in Figure 7. Figure 8 shows the corresponding bonding metric distribution in the depicted layers. The most important finding was the existence of bonding metric gradients across the part. Generally speaking topmost layers tend to have lower magnitudes bonding metric distributions. The absence or low levels of reheating due to subsequent layer deposition for top layers produces lower vales for bonding metric. If on the other hand the spatial extent of bonding cloud was restricted to one interface, this gradient effect diminishes producing nearly uniform bonding metric distribution in z-direction. The bonding metric distribution in a given layer depends on the building style and how much time the deposition head spends at material points of interest.



Figure 8. Bonding Metric Distributionsfor Layers 23, 12 and 1

6. Conclusions and Ongoing Work

Road cooling and bonding phase of Fused Deposition process has great influence on final part quality. Since green part quality effects the downstream operations of binder burnout and sintering, process analysis tools have been developed to understand and control this phase. A microstructure dependent transport property prediction tool has been developed for particle loaded systems. This prediction tool may be used to assess the thermal suitability of future binder and particle systems. Detailed thermal analysis of deposition region has been performed, and the effects of process parameters as well as substrate size have been quantified. It has been observed that the extent of remelt zone can extend as well as two road widths for materials systems of interest. An unsteady layer building model has been developed and employed for dynamic thermal behavior of a model layer geometry. Predicted temperature signatures show a variety of different cooling behavior categories even in a single layer. Also, temperature measurements have been performed with thermocouples to investigate the temperature signature of material points in multi-layer parts. Significant behavior differences have been found for different build styles. Since thermal simulation of whole part building is computationally expensive, a command file (*sml*) driven heuristic part building model has been developed. The model is tested using a realistic part, namely 23 layer spur gear. Model predicted bonding quality gradient between layers (poor bonding for top layers), and also within a given layer.

Nonisothermal bonding behavior of particle loaded material systems employed in FD is being assessed, to calibrate and validate bonding quality distributions predicted by part building model. Local deposition model is being extended into three-dimensions. Layer building model is also being extended to include up to four layers.

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