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MODELING NOVEL MANUFACTURING PROCESSES

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ABSTRACT

This paper proposes a methodology for acquiring adaptable surrogate models of novel manufacturing processes using statistical methods, numerical simulation of the physical models, and experimentation. These surrogate models must contain different levels of abstraction, complexity, and accuracy to be useful from conceptual design through manufacturing process control. In addition, the proposed process modeling framework combines models of different subprocesses. This methodology is being developed in the context of the Shape Deposition fabrication process in which a part is built by successively depositing molten materials in thin layers. Creating each layer requires several manufacturing subprocesses such as microcasting, thermal spraying, shot peening, and machining. The governing physical equations of the microcasting thermal phenomena are simulated and numerical results are compared with experimental measurements.

INTRODUCTION

Changes in the structure of US manufacturing are placing new requirements on manufacturing processes and process models. The current trend is to integrate design, manufacturing, and other life cycle concerns in all phases of a product's development. Integration of manufacturing concerns into all aspects of a product's life-cycle requires manufacturing models with different levels of abstraction and detail that can serve activities from conceptual design through process control. For example, during design, models of the manufacturing process may be used to constrain the shape and configuration of a design or may be used to set process variables to control attributes, such as surface finish, to achieve the required functions in the finished product.

Distributed manufacturing requires remote network access to manufacturing capabilities (Finger *et al.*, 1994). Many novel solid freeform manufacturing processes have been developed in response to the need for rapid manufacturing processes that do not require setups and fixturing so that parts can be manufactured directly from CAD models. Because these novel manufacturing processes are currently under development, there are many open research issues. Better process models will lead to faster development of the processes and to quicker use and acceptance. Good models will also allow better identification of design spaces so that manufacturing constraints can be brought into the early phases of the design cycle.

In the Shape Deposition process, which is a solid freeform fabrication process being developed at Carnegie Mellon (Hartmann *et al.*, 1994), a part is built by successively depositing molten materials in thin layers. Each layer can contain several materials and creating each layer requires several manufacturing subprocesses. Figure 1 shows the basic operations in the Shape Deposition process. Currently, we are depositing zinc, steel, and copper. The manufacturing subprocesses include microcasting, thermal spraying, shot peening, and machining. We do not have good models for many of these subprocesses, and their use in combination to form a single multi-material layer is not well characterized. In addition, the process of creating a mechanical part or assembly from thin multi-material layers is not well understood.

The Shape Deposition process removes traditional manufacturing constraints thereby allowing new classes of products. It allows us to manufacture complex geometric structures with multiple materials, to fabricate assemblies in place, and to embed electronics in structures. Thus, electronic packaging becomes an integral part of the mechanical structure and electro-mechanical assemblies can be fabricated as a single structure.

To create composite structures and to integrate mechanical, electronic components, and sensors into assemblies, the thermal

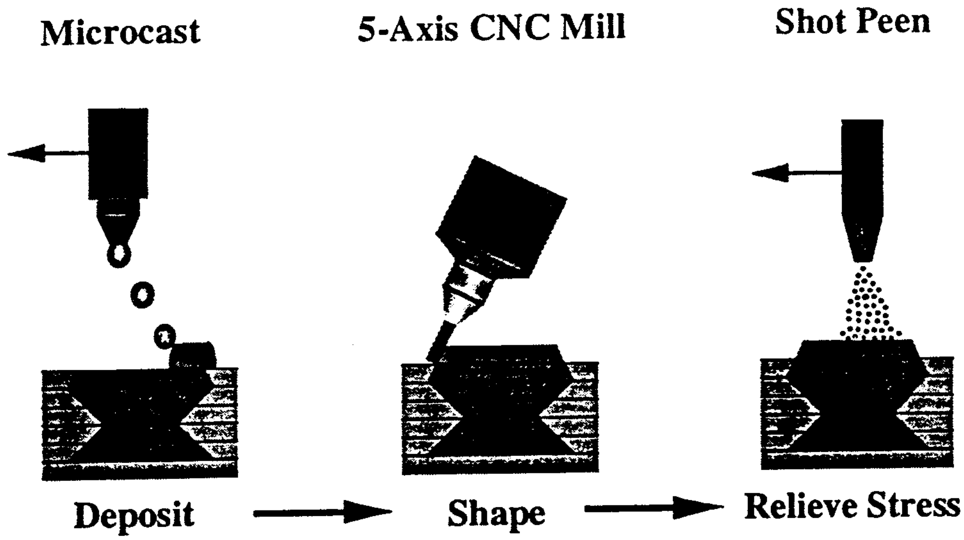


Figure 1: Creation of a Part using Shape Deposition

aspects of the Shape Deposition process must be understood, modelled, and controlled since they strongly affect the quality of the resulting artifacts. The mechanical strength of an artifact manufactured using Shape Deposition is determined by the strength within each layer and the strength of the bonds between layers. The bond strength can be improved greatly if the superheated, molten droplets partially remelt the previous layer upon impact. The bonding conditions and the rate of cooling affect the deposited microstructure and hence the ensuing thermal, electrical, and mechanical properties. The application of successive superheated depositions creates thermal stresses that must be controlled to avoid warping or delamination of the layers. When embedding electronic components within a layered structure, the temperature must be controlled during fabrication to protect the electronics within the growing structure. With a better understanding of the thermal phenomena, the process parameters can be selected to control the microstructure of the deposited material.

At Carnegie Mellon, we are also designing and manufacturing wearable computers (Siewiorek *et al.*, 1994). These portable, hands-off computers move with the user; they can track the user's motions in both time and space providing real-time information that can extend the user's knowledge and perception of the environment. Currently, the wearable computers are fabricated using traditional manufacturing processes for both the electronics and the mechanical structure. We plan to fabricate the next generation of wearable computers using Shape Deposition. Figure 2 shows an embedded electronic circuit manufactured using Shape Deposition.

Because the Shape Deposition process is under development, the manufacturing subprocesses are continually evolving and changing. Process models are needed to answer questions about the capabilities of the process as well as to control the process. We need a flexible, adaptable modeling framework in which

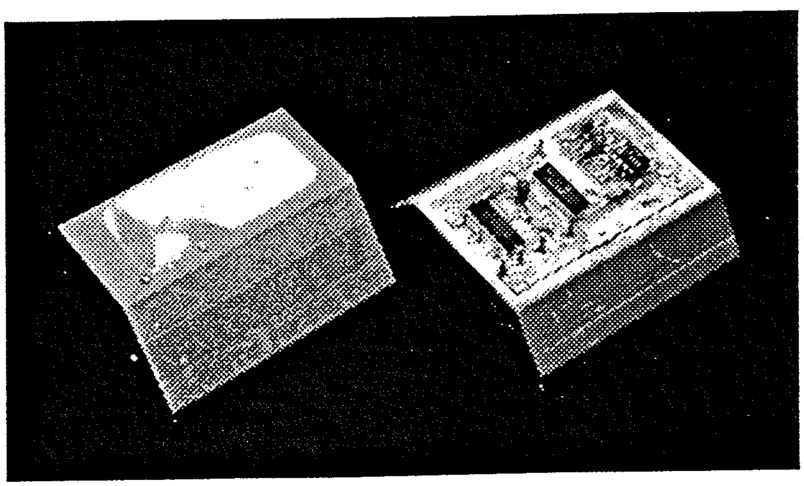


Figure 2: Shape Deposited Structure with Embedded Electronic Circuits

models for subprocesses can be updated and exchanged within a larger framework. The level of detail desired, the available resources, and the available knowledge about the phenomena involved dictate the type of model to be used. Accurate mathematical models require knowledge of the physics of the phenomena occurring in the process. Coarse models, based on approximations, can provide estimates of the general behavior of the process.

We are developing a methodology for acquiring robust process models of new manufacturing processes. We use statistical design of experiments to create coarse process models that identify important process variables and the relationships among them; that is, we design and run experiments on the Shape Deposition manufacturing system in order to characterize the process. For some subprocesses, such as microcasting, which are not well characterized, we must also develop models based on the underlying physics of the subprocesses guided by the statistical experiments. We perform Direct Numerical Simulation (DNS) of the governing equations obtained from fundamental principles and verify the results experimentally. For other subprocesses, such as machining, which are reasonably well understood, we use existing process models. In addition to modeling the individual subprocesses, we must model the interaction among all the subprocesses as they are used to create a layer within the part. And, we must model how the two-dimensional layers interact to create a three-dimensional artifact. If complete physical models of all the subprocesses and their interactions are concatenated, the resulting model is computationally intensive, even if feasible on supercomputers.

To create models that are responsive to differing requirements during the different stages of product design, we create surrogate models that capture the underlying phenomena within a given context. Surrogate models can accommodate previous knowledge, account for multidisciplinary issues, be easily constructed and validated, and offer *a posteriori* error estimates that permit guidance for subsequent adaptive improvement. The degree of confidence in the surrogate model can be quantified using Bayesian-validated model construction (Yesilyurt and Patera, 1994). Surrogate models are created and validated using statistical design of experiments to uncover the relationships between variables of interest within the space described by the numerical models. By running the DNS models as if each run were an experiment, surrogate models can be created using the same techniques as were used to create the initial statistical models. New data from experimental testing and numerical simulations can be incorporated easily into surrogate models. Surrogate models can be created with different levels of complexity so that inexpensive surrogate models can be used for the exploratory, early stages of a product, and expensive models for final analysis.

BACKGROUND AND RELATED WORK

Novel Manufacturing Processes

Shape deposition processes, also known as solid freeform fabrication, build parts by incremental material build-up of thin two and a half dimensional layers. A broad class of these processes build shapes from planar cross-sections, and the growing structure is supported by solid complementary shaped, sacrificial layers. The cross-sectional descriptions are generated by slicing three-dimensional computer representations into slices that may vary in thickness. Several alternative deposition materials and deposition processes are available for building products, including selective laser sintering (Deckard and Beaman, 1987), three-dimensional printing (Sachs, 1990), layered object manufacturing (Fagin, 1990), Cubital's Solider (Pomerantz, 1990), and ballistic particle manufacturing (Hauber, 1987; Masters, 1990). The principal advantage of the layered deposition approaches versus conventional CNC machining is the ease and speed with which one can go from design to part

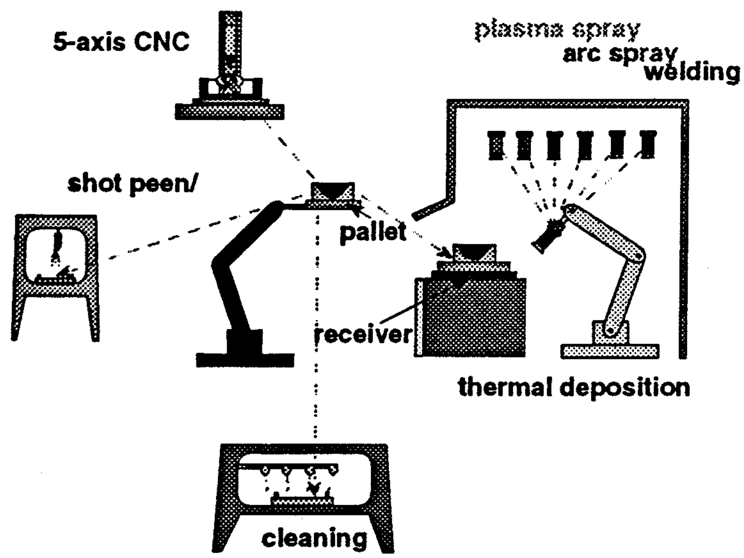


Figure 3: Shape Deposition Subprocesses to Form a Single Layer

fabrication without the need for part-specific tooling or fixturing and with minimal human intervention. The planning and execution effort for shape deposition is essentially independent of part complexity. Shape deposition technologies, however, cannot currently achieve the ultimate precision of CNC machining.

Shape Deposition manufacturing is a layered manufacturing process in which parts and assemblies are manufactured by successively depositing material in cross-sectional areas (Hartmann *et al.*, 1994). Starting from a geometric model, the part is discretized into thin layers based on geometric as well as material criteria. The part is built by a vertical concatenation of two and a half dimensional layers. Each layer undergoes a series of processes including material addition, stress relief, selective material removal, and surface preparation. The basic sequence of operations in the Shape Deposition process is shown in Figure 3. The Shape Deposition process allows encapsulation of prefabricated parts, such as computer chips and multi-chip components, by placing them in sockets and building the structure around them. Salient features of the process are its ability to handle complex geometries, to vary shape and material composition continuously with the part, to embed electronic components, and to make electronic packaging an integral part of the mechanical structure. One of the primary attributes of Shape Deposition from a design point of view is that it removes traditional manufacturing constraints thereby significantly increasing the space of possible products. It allows multi-material layers, allows assemblies to be fabricated in place, and allows electronics to be embedded in structures. Using a layered deposition process provides access to the interior of a part, as shown earlier in Figure 1.

The primary process for depositing material is referred to as weld-based spray or microcasting. The process is similar to conventional welding in which the deposition material is originally in the form of a wire. The wire is melted by a plasma gun in an inert atmosphere. The plasma gun moves over the substrate, depositing individual droplets of molten metal which free fall to the substrate surface at a rate of several droplets per second. The droplets merge to form a layer on the substrate, as illustrated in Figure 4. Traditional plasma spraying develops only mechanical bonding (El-Kaddah *et al.*, 1984; Pawlowski, 1981), while the continuous casting processes develops remelting bonding. The Shape Deposition microcasting process achieves a middle ground by forming free falling droplets that remelt the substrate — but, unlike continuous casting, the droplets are small enough (on the order of 1 mm diameter) for accurate near net-shape forming. The Shape Deposition process differs considerably from the traditional wire arc or plasma spray methods, where the deposition material is melted and propelled to the substrate generating a fine, high velocity mist. For all of the processes, droplet superheat temperatures are comparable, but microcasting droplets have a higher impact temperature because less heat is lost during flight due to the greater volume-to-surface ratio. For steel deposition, these temperatures are on the order of 2500°C. The high temperatures cause remelting of the substrate resulting in better metallurgical bonding between the successive deposition layers (Amon *et al.*, 1993a). In contrast, plasma and wire arc micron-sized droplets cool during flight to near solidification conditions. Of the three processes, only microcasting generates liquid droplet temperatures significantly above the melting point at impact. The material properties (thermal, electrical, and mechanical) are strongly affected by the bonding conditions, necessitating the ability to predict this remelting. The cooling rate also affects the resulting material properties.

The other subprocesses in the Shape Deposition process are shot peening, machining, and cleaning. Shot peening is used for stress release which is required due to the thermal residual stresses that result from the differential thermal contraction during material deposition. Even when the substrate is heated and both the sprayed material and the substrate are cooled

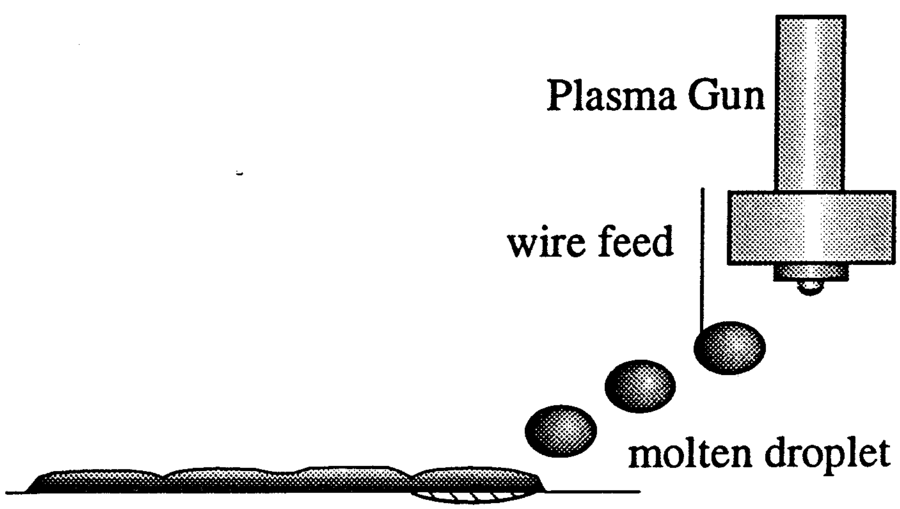


Figure 4: Material Deposition

together, a degree of differential thermal contraction is inevitable. In practice, large stresses are generated which cause spallation, distortion, and generation of cracks. During shot peening, metallic balls or shots under pressure strike the object. Varying the shot material, shot size, pressure, and length of time results in different process outputs. A high-precision, five-axis CNC machine removes excess material to shape the geometry of the layer and to make recesses for inserting prefabricated or electronic parts. The surface of each layer is prepared before depositing the next layer. Cleaning followed by grit blasting ensures better bonding between layers. Grit blasting, which consists of striking the cleaned surface with abrasive particles, increases the surface roughness. Grit blasting also removes the oxidized film on a welded layer. Not all operations need to be performed for each layer. Additional processes, like embedding prefabricated parts, can occur between repetitions of this loop.

When embedding electronic circuits within a structure, a balance is needed between keeping fabrication temperatures below manufacturing limits and improving the quality of the bonding between successive layers when the impinging liquid droplets have sufficient energy to slightly remelt the previously deposited layer. In addition, during operation of embedded electronic components the heat generated must be removed. Using Shape Deposition, heat spreaders can be designed and manufactured as an integral part of the structure, as shown in Figure 5. Vias and other mechanical components can be embedded in the same manner as electronic components.

Deposited material properties (mechanical, electrical, and thermal) vary depending on application parameters. Beyond remelting, the cooling rate of the deposited material also affects microstructure and, therefore, material properties. These properties can differ significantly from non-sprayed values for the same material. Predicting the temperatures that result from different application parameters allows us to model material properties. With better knowledge of the anticipated properties, modifications to the process and the system configuration can be proposed to maintain optimal operating temperatures for the device.

Statistical Models of Manufacturing Processes

For many new manufacturing processes, mathematical models based on physical principles have not been developed. In such cases, empirical models based on experimental data are widely used in industry. Statistical models obtained from input/output data provide a polynomial relationship between the process variables and the outputs of the process. If input/output data are not available in sufficient quantity, models are developed using a combination of regression techniques and a set of systematically designed experiments. The main advantage of statistical modeling is that any process can be modeled; however, the correctness of the model depends on the design of the experiments, the interpretation of the results, and the range of its application. Even though statistical models are not based on fundamental principles, they can provide insight and serve as the first step in developing more detailed models.

Most of the statistical models in the literature deal with modeling a single process, *e.g.*, (Gioia *et al.*, 1989), (Strojwas, 1990), (Donnelly, 1992), and (Hanrahan and Baltus, 1992). Other techniques such as neural nets and learning algorithms have been applied to modeling individual manufacturing processes. See for example, (Yerramareddy *et al.*, 1993), (Mahajan *et al.*, 1992), (Nadi *et al.*, 1991) and (Anderson *et al.*, 1990). None of these

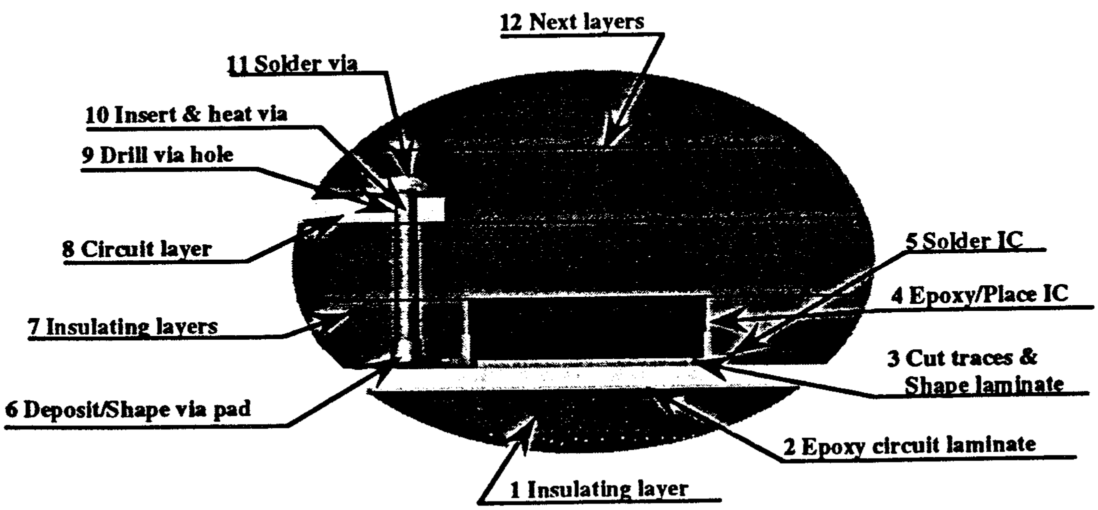


Figure 5: An Embedded Electronic Component and its Cooling Structure

models address the issue of multi-step processes, such as Shape Deposition, in which sequence subprocesses are repeated to create the artifact. We have begun to develop a method that can be used to create models of a manufacturing process which is repetition of a sequence of related subprocesses (Padmanabhan and Finger, 1994). Each subprocess is represented in terms of its input properties, control parameters, and output characteristics. A statistical model of each subprocess is developed using design of experiments (Box and Bisgaard, 1988; Taguchi, 1987). The intermediate outputs of the subprocesses form the input properties and control parameters of the model that combines the models of the subprocesses. Subprocess interactions are incorporated as crossed factors in the combined, comprehensive statistical model. The absence of a fundamental understanding of the overall process as well as the subprocesses, the lack of sufficient data, and the novelty of the process make statistical modeling most suitable for initial modeling of this process.

STATISTICAL MODELS OF SHAPE DEPOSITION

In the Shape Deposition process, the inter-layer effects are as important as the intra-layer effects, so we must model not only the sequence within a layer, but also the interactions between layers. The method presented here is based on the divide and conquer principle. The complex process is first divided into smaller subprocesses. The individual models are combined to form a model of the layer creation process. In addition to modeling the layer creation process, we must also model the process of concatenating layers. Some of the most interesting issues in both design and manufacture arise in the layer concatenation process. For design, features such as unsupportable overhangs arise from interactions between layers. For manufacturing, some of the most serious defects, such as delamination, occur between layers. When modeling the deposition of a layer, the output properties (temperature, surface roughness, etc.) of the previous layer affect the bonding between the two layers. The inter-layer effects are modeled by considering the output variables of the previous layer as input variables to the process of creating the current layer. Interactions between the properties of the previous layer and the control variables for the current layer make it possible to compensate for the properties of the previous layers.

For modeling purposes, the division into subprocesses must be conducive to studying the subprocess by itself. For example, for the material deposition process, layer thickness and stress development cannot be divided into two subprocesses even though separate models maybe be required to describe layer thickness and stress development. The division must also allow subprocesses to be combined with neighboring subprocesses. The combination of the subprocesses into a larger model requires that neighboring subprocesses have a common property or variable which forms a link between them. Ideally the output variable of a subprocess is the input variable or a control factor of the subsequent subprocess. Finally, each subprocess must possess output variables that are measurable and representative of the changes occurring in the subprocess.

The subprocesses are represented in terms of input properties, process or control variables, and output properties. The input properties are relevant attributes, such as geometry, required finish, and material. The control variables are the settings of the equipment, including the environmental controls, used in the subprocess. The output properties are measurable properties that are the result of the subprocess. The output properties can be modified input properties, such as surface finish in a machining process, or a new property, such as thermal stress. The outputs from the subprocesses are used to model the intra-layer process because the input and control variables of each subprocess control the corresponding output. We assume that the number of output variables in each subprocess will be less than the sum of the input and control variables. Hence the number of variables or factors involved in the model of the intra-layer process is reduced.

DIRECT NUMERICAL SIMULATION OF SHAPE DEPOSITION MICROCASTING

The Shape Deposition fabrication process combines several manufacturing subprocesses; most of the subprocesses are traditional, like machining and shot peening, but microcasting is non-traditional. Microcasting is the least well understood process and the most critical to the success of Shape Deposition. To understand the phenomena of microcasting requires detailed models of the underlying physical phenomena. Bonding between successive layers is a critical aspect of microcasting. Bonding can be achieved via mechanical interlocking of the sprayed droplets and the substrate material; however, improved bonding results when the molten droplets partially remelt the pre-solidified substrate.

The process variables, such as wire feed rate, laser or plasma power, droplet size, superheated droplet temperature, and substrate temperature, determine the remelting thickness, the induced thermal stresses, and the material microstructure. In addition, the thermal history (maximum temperatures, remelting, velocity of solidification front and cooling rates) as well as the oxidation of the deposited droplet affect the bonding between successive layers and the microstructure of the material. Direct numerical simulation of the governing physical equations that represent this process can provide the knowledge and data to create an accurate predictive tool of the microcasting process. Accurate models enable the thermal, mechanical, and electrical properties of the deposited material to be controlled and optimized. Therefore, the primary motivations for simulating the melting/solidification phenomena are to predict conditions that produce bonding through substrate remelting and to aid in the selection of process parameters that protect electronics and yield desirable material properties.

Thermal Issues in Shape Deposition Microcasting

The complex microcasting process involves many thermal properties of the materials such as conductivity, specific heat, phase change energy release, as well as parameters of the fabrication process such as application temperatures and droplet velocities which depend on wire feed rates and power selections. Standard non-dimensional heat transfer parameters such as Fourier and Biot numbers can be used to report analytical results; however, from a manufacturing point of view, only the droplet size and temperature can be controlled. Therefore, we investigate remelting only with respect to those parameters that can be altered during manufacturing and express the data in a format appropriate to the application process.

The properties of the materials created in thermal spray deposition processes are improved if remelting occurs; however, for the microcasting Shape Deposition process, which is a near-net shape process, the remelting extent must remain slight to maintain dimensional integrity. Accurate temperature modeling is important for other manufacturing considerations as well, including protection of support structures having lower melting temperatures than the sprayed material, control of application temperatures to protect embedded electronics, and control of thermal stresses that induce warping and delamination by successive layer depositions (Amon *et al.*, 1993b).

Another important issue in layered shape deposition processes is the thermal build-up of residual stresses as new layers are deposited onto existing layers. This build-up is due to the contraction that occurs in each new layer as it solidifies and cools. Residual thermal stresses can affect artifact performance and life due to warping, delamination, and stress cracking of layers. To control the build-up of thermal residual stresses, accurate prediction of the thermal response of the solidification of layers is necessary. Given accurate models, we can predict the residual thermal stresses in geometrically complex artifacts. More importantly, we can control the process to affect the distribution of residual stresses.

Residual stresses can also cause delaminations between layers by acting as a driving force in the propagation of interfacial cracks from the edges of the artifact. Delaminations can propagate through the entire length of the artifact. This problem is worse in layers of different materials because the large stress concentrations that exist at the bimaterial interface and the free edges due to elastic and thermal expansion coefficient mismatch. One approach to minimizing delaminations is to tailor the interface geometry to eliminate undesirable elastic stress singularities by intersecting materials tangentially at the free edge (Amon *et al.*, 1993b).

Physical Models of Thermal Phenomena in Microcasting

DNS (direct numerical simulation) of the governing physical equations allows us to predict the thermal history of a molten metal particle interacting with the substrate. The equations presented next can describe either of two systems: particles being melted on a substrate by a high-power laser and molten particles being dropped onto a substrate. This model allows us to investigate the conditions needed to achieve partial substrate remelting, to predict droplet solidification during the microcasting process, and to investigate the effect of operating conditions on the melting front migration rate and thickness, temperature distributions, and overall cooling rates. This knowledge is used together with knowledge obtained from experiments, statistics, analysis and heuristics to generate and validate the surrogate models. Application parameters such as power input, wire feed rate, and deposition rates may then be modified to optimize the deposited material microstructure.

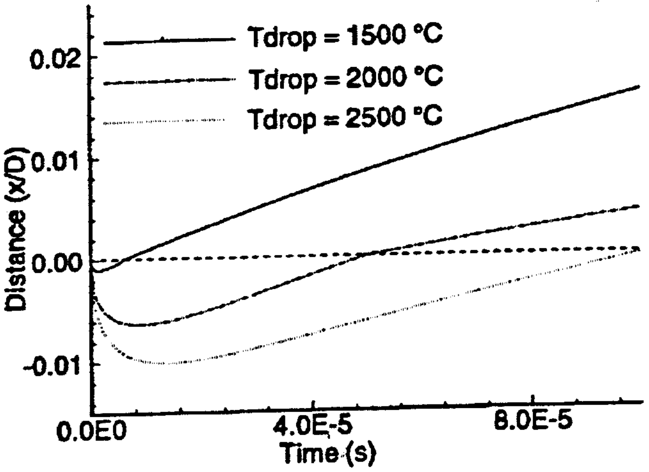
The Shape Deposition microcasting process, in which individual molten droplets free fall, impinge, and remelt a thin layer of the substrate before solidifying, is not covered by the physical models described in the literature (Gupta *et al.*, 1992; Gutierrez-Miravete *et al.*, 1989; Lawley *et al.*, 1990; Trapaga *et al.*, 1992). The solidification models in the literature do not address the physical processes of superheating, rapid deposition, conjugate heat transfer, and solidification that characterize the Shape Deposition process where remelting of the substrate is required. Moreover, thermal models of traditional spray processes do not predict the location of the melting front either within the deposition layer or within the substrate if initial remelting occurs.

The thermal history of the microcasting process affects the quality of the object generated. The thermal history influences the bonding between droplets and substrate, the thermal stresses that arise from the rapidly cooled droplets, and the microstructure and resulting material properties. Thermal history also affects the operating life of embedded electronic components. To gain an understanding of the thermal aspects of the process, an initial model that includes heat transfer and phase change, but excludes droplet dynamics, is formulated to track the melting front location during solidification. Numerical simulations provides insight into the likelihood of remelting, the remelt sensitivity to droplet and substrate conditions, and the prediction of droplet and surface temperatures and cooling rates.

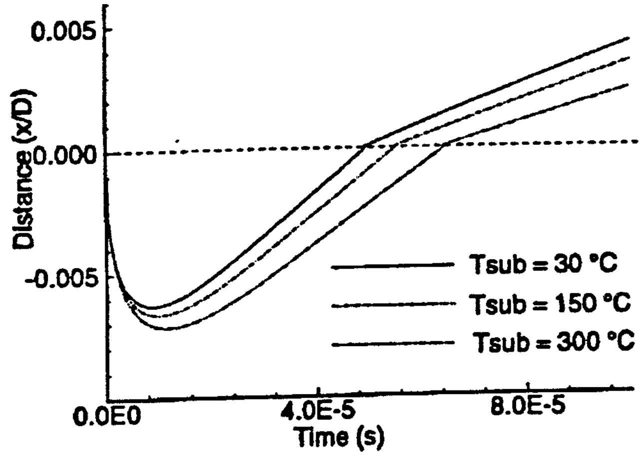
Estimates of the droplet cooling and solidification time scales can be obtained based on the thermal conductivity, λ, thermal diffusivity, α, initial temperatures of the substrate and molten droplet, T, substrate and droplet material properties, impinging velocities, v, and droplet size, r. In the range of operating parameters for which an individual droplet strikes the pre-solidified substrate and spreads much more rapidly than it solidifies ($t_{solidification} >> t_{spreading}$), the dynamic effects of the flattening process are considered a precursor to the thermal process, which is uncoupled from the fluid dynamics and simplified to a heat transfer problem. Because of the discrete nature of the Shape Deposition microcasting deposition process, a one-droplet model is used. The governing equation is given by:

$$\rho c_p \frac{\partial T}{\partial t} = \lambda(T)\ \nabla^2 T + \frac{\partial \lambda}{\partial T}\ (\nabla T)^2 \qquad (1)$$

For the materials and temperature ranges considered, temperature-dependent thermal properties are used, but we neglect as a second order effect the derivative of thermal conductivity with respect to temperature. Equation 1 is valid for both the liquid and the solid regions. At the top of the molten droplet, combined convective and radiative boundary conditions are imposed. The energy balance is applied at the moving interface between the liquid and solid regions, balancing the energy flux into and out of the interface with latent heat release:



a. Effect of Steel Droplet Impact Temperature for an Ambient Temperature Substrate



b. Effect of Steel Substrate Temperature for an Impinging Steel Droplet at 2300°C

Figure 6: Substrate Remelting Thickness as a Function of Time

$$\rho L \frac{\partial n}{\partial t} = \lambda_{sol} \frac{\partial T}{\partial n} - \lambda_{liq} \frac{\partial T}{\partial n} \tag{2}$$

where n is the normal to the direction of the melting front. At the lower boundary of the substrate, a constant temperature is maintained.

Equation 1 is discretized using a mixed Lagrangian-Eulerian explicit formulation. The explicit temporal discretization is used for its simplicity, despite the need for meeting numerical stability criteria. The remelting process is sufficiently rapid (on the order of 10^{-3} seconds) that small time steps imposed for stability do not present a significant calculation burden. To track the location of the melting front during solidification, a three-point Lagrange interpolation formula (Amon *et al.*, 1993a; Crank, 1984) is used that permits the tracking of mesh points corresponding to the melting front. The Lagrangian formulation used for temperature calculations for nodes preceding the melting front is:

$$\frac{\partial^2 T}{\partial n^2} = \frac{T_{melt}}{p(p+1)} - \frac{T_j}{p} + \frac{T_{j-1}}{(p+1)} \tag{3}$$

The melting parameter, p, represents the melting front location between the fixed, Eulerian, mesh points and is recalculated after each iteration using a discretized spectral-element form of Equation 2.

For the initial interface temperature, when the droplet first strikes the solid substrate, the analytical Stefan interface solution approximates the temperature as follows:

$$T_{inter} = \frac{rT_{liq} + T_{sol}}{1 + r} \tag{4}$$

where

$$r = \left(\frac{(\lambda c_p \rho)_{liq}}{(\lambda c_p \rho)_{sol}}\right)^{\frac{1}{2}} \tag{5}$$

We assume that both liquid droplet and substrate initial temperatures are either known from the experiments or calculated as a function of the wire feed rate, plasma power, and heat transfer from the droplet to the environment during flight. We have performed numerical simulations for models with low-carbon steel, stainless steel, and zinc droplets landing on similar substrates (Amon *et al.*, 1993a). These simulations examine the effect of droplet and substrate temperatures on remelting. Results indicate the conditions for substrate remelting are: 1) a substrate several hundred degrees above ambient temperature, 2) for unheated substrates, droplet impact temperatures with significant superheat, or 3) or a combination of the first two conditions. Figure 6.a shows the effect of impinging droplet temperature on the melting front migration versus time for a 1 mm diameter low-carbon steel droplet (1.55% Mn, 0.844% Si, 0.09% C and 0.011% P) landing on an ambient temperature steel substrate. Figure 6.b shows the melting front migration versus time using the same carbon steel materials over a range of substrate preheating conditions. The positive portion of the vertical axis represents the droplet region, while the negative portion represents the substrate. For a steel substrate initially at ambient temperature, substrate remelting occurs when the impinging droplet temperature is superheated to a temperature approaching 1500°C. Below this molten droplet temperature, no remelting occurs unless the substrate is preheated.

For the microcasting Shape Deposition process, depending on the order of magnitude of the droplet spreading and cooling process times, modeling that incorporates multi-dimensional effects, together with the dynamic effects of the droplet impact, is required. Droplet dynamics is important in certain ranges of application parameters typifying the microcasting process because it controls the contact of the molten droplet with the substrate and thus the interface conduction that drives the solidification process. Issues to be covered in the mathematical formulation of the droplet dynamics include the temperature-dependent surface tension, the solidification angle (i.e., the apparent contact angle of the solidified melt) (Gao and Sonin, 1994), the modeling of the droplet spreading and interface contact, the coupling and conjugate heat transfer effects of the droplet and substrate remelting, and droplet characterization at impact from both velocity and convection considerations.

Accurate mathematical modeling and simulation based on the relevant physical phenomena involved makes it possible to determine conditions (or combinations of controlling parameters) that yield partial substrate remelting. These models also enable us to investigate the effect of operating conditions (impinging droplet and substrate temperatures, droplet size, *etc.*) on the properties of the sprayed materials and on the build-up of residual thermal stresses. However, not all relevant physical phenomenon or effects, (e.g., voids, microstructure, and level of oxidation) can be captured by the mathematical and physical models. Therefore, we also perform experiments to verify the accuracy of the numerical predictions and to account for the unmodelled effects of the process parameters for Shape Deposition. Once the mathematical models and numerical approach have been validated by comparing the computed results with the experimental data, then numerical simulations can be used to investigate the microcasting process for a wide range of shape deposition parameters cheaply, efficiently, and quickly. Furthermore, numerical simulations can provide detailed information such as the cooling rates in all droplet and substrate regions which are inaccessible by experimental means.

EXPERIMENTAL VERIFICATION

Experiments on the Shape Deposition microcasting process are necessary to verify droplet impact conditions and to compare model predictions, from DNS and surrogates, with experimental results for temperatures and substrate remelting thickness. Three sets of experiments are being carried out: calorimetry to determine average droplet impact temperatures over a range of Shape Deposition process parameters; thermocouple measurement of the droplet and substrate temperatures to determine cooling rates for different materials and spray conditions; and metallographic examinations of test samples to ascertain remelting depth and material microstructure.

Temperature measurements are performed for the impinging droplets and the substrate using a type C thermocouple (Tungsten with 5% Rhenium/Tungsten with 26% Rhenium) and a type K thermocouple (Nickel with 5% Aluminum/Silicon with 10% Chromium, time constant of approximately 0.003 seconds), respectively. The temperature of the substrate is measured at different depths directly below the location of the droplet impact and at a lateral distance from the droplet impact using the same substrate depths.

As an example, for a carbon steel droplet impinging on a similar substrate, Figure 7 shows the numerical prediction and the experimental measurements of the average temperature as a function of time. Comparing the numerically simulated droplet cooling rate with experimental data, the cooling rate predicted by the model is comparable to the experimental results for the initial time steps; however, the simulated results for later time steps reflect a lower cooling rate than those measured by experiments. This divergence begins at about 1400°C which corresponds to the solidification temperature of the steel droplet. This suggests that the thermal properties produced by rapidly cooled, solidified droplet varies from the tabulated values. For the entire simulation, an underprediction of cooling rate is expected because the model does not account for contact resistance induced by air voids. In addition, droplet temperature underestimation is affected by uncertainties regarding the convective heat transfer due to motion of the liquid within the impacting droplet, as well as unmodelled aspects of the solid-solid (austenite-ferrite) phase transformation of steel.

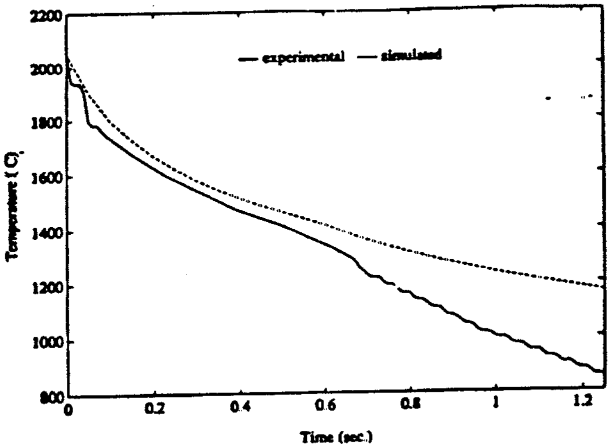


Figure 7: Comparison between Thermocouple Experiment and Numerical Simulation of the Impact Temperature of a Carbon Steel Droplet Impact Droplet Temperature

Comparing the experimental measurements with numerical simulation results shows that the physical model provides useful information about the initial stages of the solidification process, about the conditions required to achieve substrate remelting, and about the relative importance of application parameters. However, it is only modestly successful in predicting temperatures for carbon steel over time. We believe that the main sources of underprediction at large times are due to the neglect of contact resistance of air voids and to the decoupling of droplet fluid dynamics and heat transfer. Including fluid dynamics of the droplet spreading and modelling the contact resistance in future formulations will improve the accuracy of the physical model.

Substrate remelting, which occurs in about 10^{-3} seconds, is verified by metallographic examination of the sample plates used for the substrate temperatures experiments. This allows us to correlate observed remelting with measured temperatures. The exposed surface is polished with 0.05 micron alumina solution and etched with 3% nitric acid. Remelting is measured for each droplet at 50X magnification, while greater magnification at 200X is used to determine the steel microstructure. Figure 8 shows a 50X magnification metallographic examination of a low-carbon steel droplet at 2300 °C solidified on a similar substrate material which was initially at ambient temperature. This figure verifies the numerical predictions of the remelting zone and depicts different regions corresponding to the initial molten droplet, the remelted substrate and the heat-affected substrate. Notice that the grain orientation in the droplet microstructure is perpendicular to the droplet/substrate interface. Since the

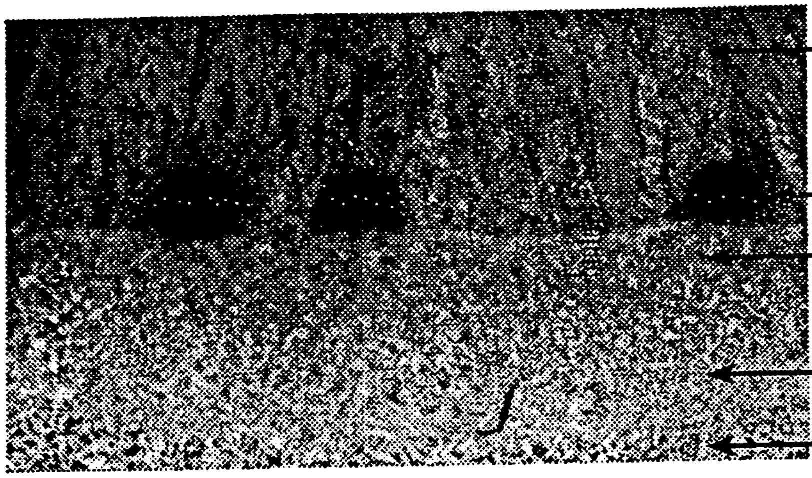


Figure 8: 50X Magnification of Remelt Region of a Low-Carbon Steel Droplet

solidifying material microstructure aligns with the constant temperature lines, this micrograph corroborates the assumptions made in the numerical model, *i.e.*, that the heat flow in the droplet is uni-directional and dominated by the heat transfer at the droplet/substrate interface.

Figure 9 is a 200X magnification of the droplet/interface region. The solidified droplet has a martensite microstructure which is indicative of the rapid cooling. The substrate has a ferrite-pearlite structure at a distance far from any remelting, shifting from a coarse to a fine structure as the droplet is neared. Where remelting has occurred, martensite, lower bainite, and carbide inclusions appear. Cooling rate estimates can be made by examining the microstructure using carbon steel cooling transformation diagrams (Boyer, 1977). Based on the martensitic structure, the droplet cools to below 500 °C in less than 2 seconds. The remelted zone resolidifies and cools below 300 °C in less than 5 seconds.

SURROGATE MODELS

While we are using DNS to model the thermal phenomena in the Shape Deposition process, there are limitations on its use:

- The number of permutations required to find a solution to a process optimization problem is not known *a priori*, so the use of resource-intensive simulations is limited since resources may be exhausted before even a feasible solution is found.
- DNS is inflexible with respect to incorporating modifications and new data. This is a limitation for processes like Shape Deposition which are under development and hence continually evolving.
- DNS inhibits proper incorporation of knowledge obtained from experimental, analytical, and heuristic investigations.
- Multidisciplinary constraints are difficult to incorporate in DNS.

Although the availability of inexpensive, fast computers

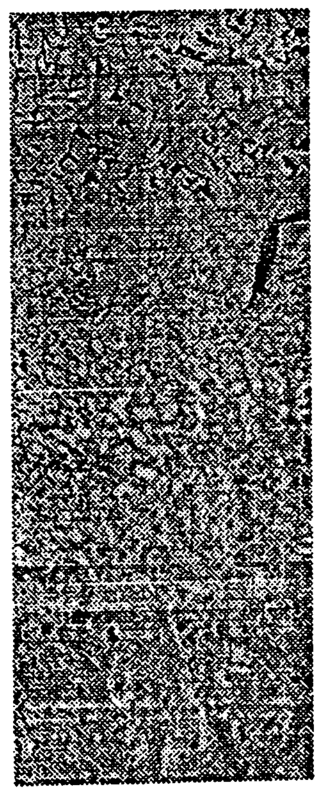


Figure 9: Metallographic Microstructure of a Carbon Steel Droplet

permits numerical prediction of complex thermo-fluid phenomena in manufacturing processes not previously possible (Amon *et al.*, 1993a), the thermal analysis of many such phenomena still remains time-consuming and resource-intensive for rapid prototyping and manufacturing applications. In particular, the large space of parameters associated with novel manufacturing processes prohibits direct numerical simulation of all permutations. To address this difficulty, we use surrogate models which are obtained using statistical methods, numerical simulations and experimental results for a selectively chosen reduced space of parameters. This is based on successive model refinement (Nigen and Amon, 1992) in which we use the relatively expensive DNS simulations to construct and validate surrogate models. Once the parameter space is reduced, successively more complete and accurate models are employed. The model evolution culminates with a conjugate conduction, convection, solidification, and remelting direct numerical simulation of the selected parameter process.

For any manufacturing process, including Shape Deposition, not all relevant physical phenomena can be readily incorporated into mathematical models based on fundamental principles. As an example, the metallographic examination of a low-carbon steel droplet solidified on a similar substrate, shown in Figure 8, indicates the presence of gas voids at the interface. These air bubbles or voids, shown as the dark areas at the interface, have a large effect on the quality of the artifact, and so must be modelled and accounted for; however, these defects cannot be modeled from first principles. Instead, air voids effects are accounted for through contact resistance correlations based on experimental metallographic observations and a statistic approach. These correlations are then incorporated in the mathematical equations for simulations.

In addition to creating surrogate models of the microcasting process, we also create surrogate models of the Shape Deposition process as a whole. Using the same statistical techniques, different surrogate models can be constructed depending on the modeling requirements. For different phases in a product's life cycle, different process parameters may be of interest and different levels of detail may be required. Using surrogate models gives us the flexibility to tailor the models to the user's needs. Furthermore, the modular nature of the subprocesses allows us to substitute one process model for another — thus each subprocess can be modeled at an appropriate level of detail, and changes in the Shape Deposition process can be accommodated easily.

CONCLUSIONS

We have presented a modeling framework for novel manufacturing processes that combines statistical methods, direct numerical simulations and experimental measurements. We have developed a framework for concatenating models of the individual subprocesses to create surrogate models with different levels of resolution and accuracy. The modeling approach is illustrated for thermal spray microcasting — one of the manufacturing subprocesses of the Shape Deposition fabrication. Important factors which control material properties during microcasting are the cooling rates which determine the microstructure, residual thermal stresses, and metallurgic bonding through substrate remelting. Direct numerical simulations based on physical models are performed to predict the thermal history of the deposited materials, cooling rates and the effect of operating conditions, such as substrate and droplet temperatures, on the substrate remelting thickness. Numerical results for low-carbon steel droplets predict that substrate remelting can be achieved for the impact temperatures available in the microcasting thermal spray process and require superheating of the molten droplets or preheating of the substrate. The occurrence of substrate remelting is further verified by metallographic examination. The grain orientation on the steel microstructure indicates that the heat transfer is predominantly one-dimensional, perpendicular to the droplet/substrate interface and that conduction into the substrate is the dominant mode of heat transfer. Experimental temperature measurements are in good agreement with the numerical predictions during the initial stages of the solidification and remelting phenomena; however, we need to model the effect of air void-induced contact resistance at the droplet/substrate interface to accurately predict the long-term cooling process.

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REFERENCES

Amon, C., Prinz, F. B., Schmaltz, K., "Numerical Modelling of Thermal Spray Systems," Technical Report EDRC 24-106-93, Engineering Design Research Center, Carnegie Mellon University, 1993.

Amon, C., Beuth, J., Kirchner, H., Merz, R., Prinz, F. B., Schmaltz, K., Weiss, L., "Material Issues In Layered Forming," *Solid Freeform Fabrication Symposium*, The University of Texas at Austin, Austin, TX, September 1993, pp. 1-10.

Anderson, C. W., Franklin, J. A. and Sutton, R. S., "Learning a Nonlinear Model of a Manufacturing Process using Multilayer-Connectionist Networks," *Proceedings of the 5th IEEE International Symposium on Intelligent Control*, IEEE, Philadelphia, PA, 5-7 September 1990.

Box, G. and S. Bisgaard, "Statistical Tools for Improving Designs," Technical Report, Mechanical Engineering, University of Wisconsin, January 1988.

Boyer, H. E. (ed.), *Atlas of Isothermal Transformation and Cooling Transformation Diagrams*, American Society for Metals, Metals Park, OH, 1977.

Crank, J., *Free and Moving Boundary Problems*, Oxford Press, New York, 1984.

Deckard, C. R. and Beaman, J. J., "Recent Advances in Selective

Laser Sintering," *14th NSF Conference on Production Research and Technology*, University of Michigan, Ann Arbor, MI, October 1987, pp. 447-456.

Donnelly, A. T., "Response-surface Experimental Design," *IEEE Potentials*, February 1992, pp. 19-21.

El-Kaddah, N., McKelliget, J. and Szekely, J., "Heat Transfer and Fluid Flow in Plasma Spraying," *Metallurgical Transactions B*, Vol. 15B, 1984, pp. 59-70.

Fagin, M., "Laminated Object Manufacturing," *The National Conference on Rapid Prototyping*, Center for Advanced Manufacturing, The University of Dayton, Dayton OH, June 1990.

Finger, S., Stivoric, J., Amon, C. H., Gursoz, L., Prinz, F. B., Siewiorek, D. P., Smailagic, A. and Weiss, L. E., "Reflections on a Concurrent Design Methodology: A Case Study in Wearable Computer Design," *submitted to Computer-Aided Design, special issue on Concurrent Design*, 1994.

Gao, F. and Sonin, A., "Precise Deposition of Molten Microdrops: the Physics of Digital Microfabrication," *Proceedings of the Royal Society A*, 1994.

Gioia, S., Miller, G. and Daughton, W., "Application of Statistical Experimental Design to the Development of a One Micron CMOS Process," *Proceedings of the IEEE 1989 National Aerospace and Electronics Conference*, IEEE, Dayton, OH, May 1989.

Gupta, M., Mohamed F. A. and Lavernia, E. J., "Solidification Characteristics of Atomized Al-Ti Powders," *Scripta Metallurgica et Materialia*, Vol. 26, 1992, pp. 697-702.

Gutierrez-Miravete, E., Lavernia, E. J., Trapaga, G. M., Skekely, J. and Grant, N. J., "Mathematical Model of the Spray Deposition Process," *Metallurgical Transactions A*, Vol. 20A, 1989, pp. 71-85.

Hanrahan, J. J. and Baltus, T. A., "Efficient Engineering through Computer-Aided Design of Experiments," *IEEE Transactions on Industry Applications*, Vol. 28, No. 2, 1992, pp. 293-296.

Hartmann, K., Krishnan, R., Merz, R., Neplotnik, G., Prinz F. B., Schultz, L., Terk, M. and Weiss, L. E., "Robot-Assisted Shape Deposition Manufacturing," *Proceedings of the 1994 IEEE International Conference on Robotics and Automation*, IEEE, San Diego, May 1994.

Hauber, D., "Automated Fabrication of Net Shape Microcrystalline and Composite Metal Structures Without Molds," *Manufacturing Processes, Systems and Machines: 14th Conference on Production Research and Technology, NSF*, Society of Manufacturing Engineers, Ann Arbor, MI, October 1987.

Lawley, A., Mathur, P., Apelian, D. and Meystel, A., "Spray Forming: Process Fundamentals and Control," *Powder Metallurgy*, Vol. 33, No. 2, 1990, pp. 109-111.

Mahajan, R. L., Wang, X, A., Xie, H. and Lee, Y. C., "Neural Network and Fuzzy Models for Real Time Control of a CVD Epitaxial Reactor," *SPIE Science of Artificial Networks*, Vol. 1710, 1992, pp. 598-607.

Masters, W., "The Ballistic Particle Manufacturing Process," *The National Conference on Rapid Prototyping*, Center for Advanced Manufacturing, The University of Dayton, Dayton OH, June 1990.

Nadi, F., Agogino, A. M. and Hodges, D. A., "Use of Influence Diagrams and Neural Networks in Modelling Semiconductor Manufacturing Processes," *IEEE Transactions on Semiconductor Manufacturing*, Vol. 4, No. 1, 1991, pp. 52-58.

Nigen, J. S. and Amon, C.H., "Concurrent Thermal Design: Balancing Accuracy with Time Constraints," *IEEE Transactions on Components, Hybrids, and Manufacturing Technology*, Vol. 15, No. 5, 1992, pp. 850-859.

Padmanabhan, P. and Finger, S., "Acquiring Manufacturing Processes Knowledge for Design," Technical Report EDRC 24-112-94, Engineering Design Research Center, Carnegie Mellon University, 1994.

Pawlowski, L., "Temperature Distributions in Plasma-Sprayed Coatings," *Thin Solid Films*, Vol. 81, 1981, pp. 79-88.

Pomerantz, I., "Precision Resolution in Physical Imaging," *The National Conference on Rapid Prototyping*, Center for Advanced Manufacturing, The University of Dayton, Dayton OH, June 1990.

Sachs, E., Cima, M., Corine, J., Brancazio, D., and Curodeau, "Three Dimensional Printing: Ceramic Tooling and Parts Directly from CAD Models," *The National Conference on Rapid Prototyping*, Center for Advanced Manufacturing, The University of Dayton, Dayton OH, June 1990.

Siewiorek, D. P., Smailagic, A., Lee, J. C.Y. and Tabatabai, A. R. A. , "An Interdisciplinary Concurrent Design Methodology Applied to the Navigator Wearable Computer System," *Journal of Computer and Software Engineering*, Vol. 2, No. 2, 1994.

Strojwas, A. J., "Design for Manufacturability and Yield," *Microelectronics Journal*, Vol. 21, No. 2, 1990, pp. 53-66.

Taguchi, G., *System of Experimental Design, vol. 1 and vol. 2*, UNIPUB-Kraus International Publications, White Plains, 1987.

Trapaga, G., Matthys, E. F., Valencia, J. J. and Szekely, J., "Fluid Flow, Heat Transfer and Solidification of Molten Droplets Impinging on Substrates: Comparison of Numerical and Experimental Results," *Metallurgical Transactions B*, Vol. 23B, 1992, pp. 701-718.

Yerramareddy, S., Lu, S. C-Y. and Arnold, K. L, "Developing Empirical Models from Observational Data using Artificial Neural Networks," *Journal of Intelligent Manufacturing*, Vol. 4, No. 1, 1993, pp. 33-41.

Yesilyurt S. and Patera, A. T., "Surrogates for Numerical Simulations; Optimization of Eddy-Promoter Heat Exchangers," *Computer Methods in Applied Mechanics and Engineering*, 1994.