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SELF ASSEMBLY IN ADDITIVE MANUFACTURING: OPPORTUNITIES AND OBSTACLES

ABSTRACT

Purpose

Additive manufacturing offers substantial flexibility in shape, but much less flexibility in materials and functionality—particularly at small size scales. A system for automatically incorporating microscale components would enable the fabrication of objects with more functionality. This paper considers the potential of self assembly to serve as an automated programmable integration method. In particular, it addresses the ability of random self assembly processes to successfully assemble objects with high performance despite the possibility of assembly errors.

Methodology

A self-assembled thermoelectric system is taken as a sample system. The performance expectations for these systems are then predicted using modified one-dimensional models that incorporate the effects of random errors. Monte carlo simulation is used to predict the likely performance of self assembled thermoelectric systems and evaluate the impact of key process and system design parameters.

Findings

While assembly yield can drop quickly with increasing numbers of assembled parts, large functional assemblies can be constructed by arranging components in parallel to provide redundancy. In some cases, the performance losses are minimal. Alternatively, sensing can be incorporated to identify perfect assemblies. For small assemblies, the probability of perfection may be high enough to achieve an acceptable assembly rate. Small assemblies could then be combined into larger functional systems.

Value

This analysis identifies two strategies that can guide the development of additive manufacturing processes that incorporate miniature components to increase the system functionality. The analysis shows that this may be possible despite significant errors in the self-assembly process because systems may be tolerant of significant assembly errors.

Keywords: self assembly, thermoelectric, photovoltaic, monte carlo simulation

1) INTRODUCTION

The advent of inexpensive computing has enabled the growth of additive manufacturing (AM) processes in which nearly arbitrary shapes can be built directly from computer models without the need for specialized tooling. These processes take many forms and use many different raw materials including powder, wire, ribbon, drops, and pools. The materials are fixed by freezing, curing, and bonding processes. (Gibson, Rosen & Stucker 2010) Collectively these

processes offer shorter fabrication times for unique objects. These capabilities have changed many existing businesses and created new opportunities.

Significant progress has been made from the early days of AM. Today, many processes use multiple materials. By combining multiple materials, a large number of highly functional devices have been demonstrated including batteries, actuators, transistors, electrical conductors, insulators, and structural elements (Malone et al. 2004, Malone, Lipson 2006, Malone, Lipson 2007). This large number of materials permits the fabrication of very highly functional systems. However, the requirements of each material deposition process impose significant constraints on the materials and the geometries that can be formed. This in turn imposes constraints on the performance of the final objects.

Early in the development of AM processes, people began to insert components produced by other processes into the AM components in order to achieve higher functionalities. This included actuators and sensors in parts produced by shape deposition modeling (Dollar, Wagner & Howe 2006, Weiss et al. 1997). Parts were also inserted into stereo lithography (SLA) components (Kataria, Rosen 2001). These insertion processes have created highly functional components that are not currently feasible using AM processes alone. However, they require manual intervention. This intervention effectively limits the number and size of inserted components based on the skills of the human operator. Processes for automatic insertion of components could dramatically extend the range of systems that can be assembled via AM processes.

Self assembly is one method by which components could be integrated into AM processes. However, self assembly introduces its own complications. This paper reviews some of the advantages of self assembly and then considers some of the new challenges that would be introduced by integrating it into AM processes. The predicted performance of a self-assembled thermoelectric cooler is analyzed and the results discussed in terms of potential strategies for achieving functional self assemblies. Microscale photovoltaic cells are then addressed as a second possible application. The implications of this analysis on the incorporation of self-assembly into AM are then considered.

2) SELF ASSEMBLY

Self assembly is the positioning and bonding of components by random interactions (Whitesides, Grzybowski 2002). This requires the formation of a spontaneous bond between the parts when they assume the desired position. Common bonding forces include chemical (Yan et al. 2003), electrostatic (McCarty, Winkleman & Whitesides 2007), magnetic (Shetye, Eskinazi & Arnold 2009), and surface tension (Syms et al. 2003). Self assembly offers the potential for low-cost assembly (no pick and place robotic systems are required) at a high rate (assembly can occur in parallel). Indeed, promising assemblies have been documented including functional displays (Jacobs et al. 2002), inductors (Scott et al. 2004), and actuators (Fang, Wang & Bohringer 2006). Very fast (>1000 parts /min) assembly rates have also been reported for some applications (Zheng, Buhlmann & Jacobs 2004).

However, progress in moving self-assembly into industrial applications has been slow because significant obstacles remain in transitioning self-assembly from demonstrations to

production. First, bond design becomes very challenging when multiple parts are to be assembled simultaneously. The assembly environment will also impact both the yield and rate of the process. Secondly, errors in the assembly process can substantially reduce the performance of the assembled system. Finally, the assembly rates may drop significantly at the microscale. Careful engineering is required to create feasible microscale self assembly processes.

All of these problems become more serious as the number of parts and the number of part types increases. In order for self-assembly to function as an additive manufacturing process, programmable control of assembly location and timing must be achieved with sufficient speed and yield. This paper considers the yield challenge using stochastic simulations to estimate the performance of self-assembled thermoelectric coolers as a function of device design and assembly process yield.

Some have shown that these processes can often be modeled as first order reactions, but they typically require experimentally determined parameters. (Hosokawa, Shimoyama & Miura 1994, Zheng, Jacobs 2005) Much work remains to develop predictive kinetic models of microscale self-assembly systems. However, most assembly processes can be characterized by the probability of parts assembling. In the common case of assembling parts to sites on a substrate, this would be the fraction of the available sites that are filled. The assembly probability is a function of the process time, the number of parts available to bond, and the way in which the parts are brought together. This work will consider how the assembly probability impacts the performance of the self-assembled systems. The 1D performance models are used to exploreing both the scaling characteristics of self-assembled systems and the impact of different process control methods.

3) CASE STUDY IN THERMOELECTRIC DEVICES

Thermoelectric materials can convert electrical energy into thermal energy and vice versa. Thermoelectric systems are used both to generate electricity from an available heat source (car exhaust, process heat, thermal batteries for deep space probes) and to provide temperature control (small refrigerators, lasers, infrared detectors) (Bell 2008). One application of recent interest is in localized cooling of silicon chips for potentially improved performance and/or system energy efficiency (Bell 2008, Wang, Yang & Bar-Cohen 2009, von Windheim 2007). These applications favor the use of small elements. In many applications, the ideal element size is too small to be assembled via “pick and place” methods but too large for film-based manufacturing. Thus, self-assembly is an attractive alternative (Crane et al. 2009).

High performance thermoelectric materials are typically semiconductors. A thermoelectric device is formed by arranging an alternating series of N-and P-type thermoelectric elements electrically in series and thermally in parallel as illustrated in Figure 1(a). The tops and bottoms of the device must be covered with an electrically insulating material such as alumina. Thermal resistance will further increase due to contact resistance between these plates and the heat source/sink. A current is applied across the elements to provide cooling or heating as required. A thermal resistance model of the device is shown in Figure 1(b). An energy balance at the cold and hot junctions of the thermoelectric device provide a 1D estimate of the device performance (Miner 2007).

Take in Figure 1

Figure 1 Basic thermoelectric schematic. (a) Physical arrangement of the components. (b) One dimensional thermal resistance model.

In practice, every thermoelectric element in the device is typically connected in series electrically. One bad connection or missing element renders the device inoperable. However, self-assembled systems are prone to errors due to missing components. This might be addressed by incorporating redundant electrical paths as illustrated in Figure 2. The redundancy (r) is defined as the ideal number of parallel electrical paths through each group of elements. A 1D model has been developed that accounts for the impact of arranging elements in parallel with the possibility that some of these elements may be missing.

Take in Figure 2

Figure 2 Illustration of a thermoelectric device with redundant electrical paths. The elements are arranged in groups of four ($r = 4$) to form 10 macro elements ($m = 10$). The top thermally insulating plate is not shown for clarity.

The junction temperature can be found by writing the energy balance equations at the cold and hot junctions following the method of Miner [20]:

Where,

T_H, T_C	Hot and cold junction temperatures respectively
T_A, T_S	Ambient and source temperatures respectively
J_e	Electrical current flux through the elements if all are present
K	Thermal conductance of the thermoelectric elements, $K = k/d$
ρ	Electrical resistivity of the thermoelectric material
d	Thickness of the thermoelectric elements
c_i	The number of elements on sites with a redundancy of i

r	The ideal number of electrically parallel elements on a site
K_{CE}, K_{HE}	Equivalent entry and exit thermal conductances including effects of thermal contact resistance between the substrate and thermoelectric elements
f	Fraction of the area filled with thermoelectric elements
S	Seebeck coefficient

The heat flux (Q) is given by

The simulation parameters are summarized in Table 1. These parameters represent a cooling application using bulk Bi_2Te_3 materials, but the general principles of self-assembly impacts are applicable to systems made from other materials as well.

Table 1 Summary of Simulation Parameters

Parameter	Value
S	240 $\mu\text{V/K}$
k	2.0 W/mK
ρ	$10^{-5} \Omega\text{-m}$
d	250 μm
T_a	300 K
T_s	285 K
K_{CE}	$10^5 \text{ W/m}^2\text{K}$
K_{HE}	$10^5 \text{ W/m}^2\text{K}$
f	0.9

Simulation Results

The most basic performance question is whether the device will have the electrical connectivity to function. This can be judged by whether there is an open circuit. Figure 3 compares the fraction of functional assemblies for different numbers of parts and different levels of redundancy. These calculations were made assuming that each individual element has a 99% probability of successfully assembling.

The assembly process was simulated by generating a random number between zero and one for each element location in the thermoelectric device. If the random number is less than the probability of an element assembling (ρ_e) then the location is filled. The resulting device is

modeled with the 1D equations. This process was repeated 10,000 times to estimate the distribution of likely assembly outcomes.

These results show that assembly yield decreases very rapidly with increasing numbers of parts. However, modifying the design to include multiple elements in parallel ($r > 1$) dramatically improves the yield and increases the number of parts that can feasibly be self-assembled.

Take in Figure 3

Figure 3 Fraction of functional thermoelectric coolers assuming 99% process accuracy. As the number of parts increases, the probability of a missing element increases. Adding redundant elements increases the yield.

While these results are promising, it is expected that the system performance will be affected by missing elements. To assess the magnitude of the performance impacts, the performance of each test case was estimated using the 1D model to simulate the impact of missing elements on different device configurations. In each test case, the optimal current was found to maximize the heat flux through the thermoelectric device. Monte Carlo simulation was used to generate 10,000 test cases for each condition. The number of series macro elements was varied from 1024 to 64 and the redundancy from 1 to 16 so that a perfect assembly in each case would contain 1024 elements ( ). The probability of an element assembling was varied from $>99\%$ to $<20\%$. The results are summarized in Figure 4.

Take in Figure 4

Figure 4 Variation in average thermoelectric performance for different assembly accuracies and redundancy levels. The number of parallel elements is given by the redundancy (r).

In Figure 4, positive heat flux indicates a functioning cooler that is removing heat from the cold side. Negative heat fluxes indicate passive conduction of heat from the ambient to the cold reservoir in an open circuit device. For each curve, it is seen that at high element assembly probability there is a positive heat flux, but as the element assembly probability decreases it transitions to negative as an increasing fraction of the thermoelectric coolers have open circuits. There are two limiting conditions: the higher performance condition where all of the assemblies function and a low performance assembly in which none of them do.

Increased redundancy has a powerful affect in producing high performance assemblies at lower element assembly probabilities. In this case, the heat flux decreases very little with decreasing element assembly probability and even increases slightly over some regions. While this is not always the case, it illustrates that if assembly probability can be included in the initial design, it may be possible to achieve high performance thermoelectric systems from relatively low yield self-assembly processes.

This thermoelectric application is an attractive case for the self-assembly trials because it is very tolerant of errors. It is possible that self-assembled systems could be likewise designed to accommodate errors. However, this may not be possible in many systems. In these cases, the results of Figure 3 suggest another alternative. Yield is higher for smaller numbers of elements. Therefore, if the system can be separated into a series of smaller sub-assemblies, then the yield of perfect assemblies is increased. Further, if process feedback is incorporated to detect and harvest just the perfect assemblies, the process yield could approach 100%. Small sub-assemblies could then be combined into larger systems with increased functionality.

This effect is seen in Figure 5 for the case of 80% element assembly probability. With 1024 total elements ($m \cdot r = 1024$), four elements must be arranged in parallel ($r = 4$) in order for ~80% of the assemblies to have a positive heat flux. However, with just 16 total elements, similar yield can be achieved with just two parallel elements. Additionally, with no parallel elements ($r = 1$), approximately 5% of the assemblies are fully functional. While 5% or even 80% success would be poor on its own, selective “harvesting” of the successful assemblies from the process could create high yields of perfect assemblies. The remaining assemblies could be left in the assembly system until they are properly assembled as well. This approach could yield a stream of perfect assemblies from a very imperfect process for those systems where redundancy is infeasible.

Take in Figure 5

Figure 5 Cumulative distribution of thermoelectric device performance with an 80% probability of each element assembling. (Left) 1024 thermoelectric elements (Right) 16 thermoelectric elements.

4) APPLICATIONS TO PHOTOVOLTAICS

Recent work has been done in the fabrication of micro-scale photovoltaic (PV) devices (Nielson et al. 2009). Each PV cell is approximately 500 μm wide and 2-20 μm thick depending on the material used. When used with concentration, these systems have many unique scaling benefits that may permit them to compete with current grid power prices. However, a method is required to integrate these separate devices onto substrates and make the necessary electrical connections.

Self-assembly is attractive for manufacturing solar modules out of the micro-scale PV cells. The ability to assemble many components at a time would increase production speed and reduce costs. It has the potential to allow “roll-to-roll” production of high-efficiency PV modules, a highly desirable manufacturing method for PV modules.

Preliminary studies of solar modules and systems comprised of these micro-scale PV cells indicate that the sensitivity of the module performance to cells missing from an assembly site depends on the method of connection (i.e., series or parallel) of the initial cell group [22]. Similar to the thermoelectric devices, it is important to design the lowest cell grouping as a collection of several cells connected in parallel to reduce the sensitivity of system performance to missing cells. This is fairly straightforward since a typical module comprised of the micro-scale cells would require tens of thousands of cells.

5) IMPLICATIONS FOR ADDITIVE MANUFACTURING

Additive manufacturing depends on flexible forming processes that can produce many different structures. In contrast, the self-assembly processes closest to production readiness assemble one or two part types in repeated arrays. (Mastrangeli et al. 2009) One key limitation is the difficulty of designing a self-assembly system to create an arbitrary geometry. However, these obstacles could be addressed through the repeated assembly of basic units analogous to the building process of additive manufacturing processes themselves.

While self-assembly is attractive at the microscale, there are many obstacles to widespread implementation. Chief among these is the challenge of high yields for large assemblies. This paper has considered how element assembly probability could impact the performance of one self-assembled device: a thermoelectric cooler. This analysis shows that incorporating redundant elements can dramatically improve yield. Under some conditions, missing components may not have a strong impact on system performance. For the test case presented above, effective cooling could be achieved with just 50% of the elements assembled with the proper system design. Similar characteristics have also been observed in models of photovoltaic systems. Where system performance is sensitive to assembly errors, partitioning the assembly into smaller sub-assemblies is a promising route for improved performance. This strategy would also be amenable to additive manufacturing as the subunits could be incorporated on demand.

Both of these approaches permit a high yield of self-assembled systems from a process that has relatively low yields at the component level. Although there are performance tradeoffs, these may be acceptable in situations where self-assembly enables unique capabilities. One potential application area will be in the incorporation of specific functionality on or perhaps into an AM component. For example, self-assembled thermoelectric elements could be integrated into a prosthetic socket to improve temperature control ~~for and~~ reduced issues with skin breakdown on the residual limb. (Peery et al. 2006) Photovoltaic cells might be added to the surface of a component to provide embedded power. Eventually these specific functionalities could be combined with integrated computation and/or energy storage to begin creating more functional systems.

Self-assembly will become more of an AM process when multiple part types can be assembled in arbitrary patterns under computer control. In order for this to be possible, assembly processes will be required to control the location and sequence of the parts that are assembled. While self-assembly programming has been theorized (Hogberg, Olin 2006, Napp, Burden & Klavins 2006) and demonstrated at larger scales (Klavins 2007), very limited programming has been demonstrated at the microscale (Chung et al. 2006)). Large scale programmable self-assembly could be implemented by creating small sub-assemblies on a programmable tool and then combining the sub-assemblies as illustrated in Figure 6. Assembling one part type at a time could reduce many types of assembly errors. This process could be used by itself or in combination with AM processes or other manufacturing methods.

Take in Figure 6

Figure 6 Illustration of a programmable self-assembly process that could achieve the flexibility of additive manufacturing.

6) CONCLUSIONS

While integration of microscale components into additive manufacturing can increase the performance capabilities of these processes, automated assembly of small components is still very limited. Self assembly is a promising approach, but concerns about assembly accuracy and control remain. This paper has shown that component and process design can be used to achieve good performance despite errors. These results will have broader application to additive manufacturing when self assembly control methods are developed to enable the flexible assembly of a variety of components in varied positions. When these challenges are addressed, self-assembly methods may provide new avenues for additive manufacturing. Until then, self assembly may be useful in incorporating common substructures into AM components.

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