ABSTRACT

While additive manufacturing processes typically integrate functionally identical building blocks, biological growth depends on the precise assembly of molecular building blocks to achieve the remarkable functionality observed in living systems. This paper considers potential performance benefits and challenges of producing systems by controlled assembly of functional components. The work will consider the impact of self-assembly errors in two energy applications: miniature thermoelectric devices and microscale photovoltaic cells. In both, high performance is possible by assembling microscale components. While assembly errors can reduce system performance, performance models show that high levels of system performance can be achieved through system design and/or self-assembly process control.

INTRODUCTION

The advent of inexpensive computing has enabled the growth 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 powders, wire, ribbon, drops, and pools. The materials are fixed by freezing, curing, and bonding processes. However, collectively these processes offer shorter fabrication times for unique objects. These capabilities have changed many existing businesses as well as creating new opportunities.

An early mantra AM was “any material, anywhere.” Significant progress has been made from the early days of AM. Today, many processes do use multiple materials. Some research has demonstrated a large number of highly functional materials including batteries, actuators, transistors, electrical conductors, insulators, and structural elements [1-3]. This large number of materials permits the fabrication of very highly functional systems. However, the requirements of any material deposition processes 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 [4, 5]. Parts were also inserted into stereo lithography (SLA) components [6]. 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 components to be inserted based on the skills of the human operator. Processes for automatic insertion of components could dramatically extend the range of systems that could feasibly 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 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 high functionality self assemblies. Microscale photovoltaic cells are then addressed as a second possible application.

**SELF ASSEMBLY**

Self assembly is the positioning and bonding of components by random interactions [7]. This requires the formation of a spontaneous bond between the parts when they assume the desired position. Common bonding forces include chemical [8], electrostatic [9], magnetic [10], and surface tension [11]. 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 [12], inductors [13], and actuators [14]. Very fast (>1000 parts /min) assembly rates have also been reported for some applications [15].

However, progress in moving self-assembly into industrial applications has been slow because significant obstacles remain in transitioning self-assembly for 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, at larger size scales, the assembly rates may drop significantly at the microscale. Careful engineering will be required to create feasible microscale assembly processes.

All of these problems become more serious as the number of parts and 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. These models are used for exploring both the scaling characteristics of self-assembled systems and the impact of different process control methods.

**CASE STUDY IN THERMOELECTRIC DEVICES**

Thermoelectric materials can convert electrical energy into thermal energy and vice versa. Thermoelectric systems are used both for energy generation from an available heat source (car exhaust, process heat, thermal batteries for deep space probes) or provide temperature control (small refrigerators, lasers, infrared detectors) [16]. One application of recent interest is in localized cooling of silicon chips for potentially improved performance and/or system energy
efficiency [16-18]. 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 [19].

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 [20].

![Figure 1 Basic thermoelectric schematic. (a) Physical arrangement of the components. One dimensional thermal resistance model.](image)

In practice, every thermoelectric element in the device is commonly arranged in series. One bad connection or missing element renders the device entirely inoperable. 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.

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

$$K(T_H - T_C) = \frac{J_e ST_C}{mr} \left( \sum_{i=1}^{r} \frac{c_i r^2}{i} \right) - \frac{(T_s - T_C)}{f} \frac{J_e \rho d}{mr} \left( \sum_{i=1}^{r} \frac{c_i r^2}{i^2} \right)$$

$$K(T_H - T_C) = \frac{J_e ST_H}{mr} \left( \sum_{i=1}^{r} \frac{c_i r^2}{i} \right) + \frac{(T_A - T_H)}{f} \frac{J_e \rho d}{mr} \left( \sum_{i=1}^{r} \frac{c_i r^2}{i^2} \right)$$
Where,

\[ \begin{align*}
T_{H}, T_{C} & \quad \text{Hot and cold junction temperatures respectively} \\
T_{A}, T_{S} & \quad \text{Ambient and source temperatures respectively} \\
J & \quad \text{Electrical current flux through the elements if all are present} \\
K & \quad \text{Thermal conductivity of the thermoelectric elements} \\
\rho & \quad \text{Electrical resistivity of the thermoelectric elements} \\
d & \quad \text{Thickness of the thermoelectric elements} \\
c_{i} & \quad \text{The number of sites with a redundancy of } i \\
r & \quad \text{The targeted number of electrically parallel elements on a site} \\
K_{CE}, K_{HE} & \quad \text{Equivalent entry and exit thermal conductances including effects of thermal contact resistance} \\
f & \quad \text{Fraction of the area filled with thermoelectric elements} \\
S & \quad \text{Seebeck coefficient}
\end{align*} \]

The heat flux \( Q \) is given by

\[ Q = (T_{S} - T_{C})K_{CE}A_{tot} \]

The performance of self-assembled thermoelectric coolers was simulated using Monte Carlo simulation. A series of coolers is created based on an assumed probability of assembly. The 1-D performance of each cooler is calculated. The distribution of the resulting performance numbers provides an estimate of the system performance. The simulation parameters are summarized in Table 1. These parameters represent a cooling application using bulk Bi₂Te₃ materials commonly available, but the general principles of self-assembly impacts are applicable to systems made from other material as well.

**Table 1 Summary of Simulation Parameters**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S )</td>
<td>312 ( \mu )V/K</td>
</tr>
<tr>
<td>( K )</td>
<td>2.0 W/mK</td>
</tr>
<tr>
<td>( \rho )</td>
<td>( 10^6 ) ( \Omega )-m</td>
</tr>
<tr>
<td>( d )</td>
<td>200 ( \mu )m</td>
</tr>
<tr>
<td>( T_{a} )</td>
<td>325 K</td>
</tr>
<tr>
<td>( T_{s} )</td>
<td>300 K</td>
</tr>
<tr>
<td>( K_{C} )</td>
<td>( 10^6 ) W/m²K</td>
</tr>
<tr>
<td>( K_{H} )</td>
<td>( 10^6 ) W/m²K</td>
</tr>
</tbody>
</table>
SIMULATION RESULTS

The most basic question is whether the device will function at all. This can be judged by whether there is an open circuit. Figure 2 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.

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.

![Figure 2 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 reduces the errors.](image)

While these results are promising, it is expected that the system performance will be affected by missing elements. 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 1000 test cases for each condition. All test conditions contained 1024 thermoelectric elements. The number of parallel elements \((r)\) was varied from 1 to 512 while the probability of an element assembling was varied from >99% to <20%. The results are summarized in Figure 3.
Figure 3 Variation in average thermoelectric performance for different assembly accuracies and redundancy levels. The number of parallel elements is given by $r = 2^{(p-1)}$.

In Figure 3, 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. It is clear that higher heat fluxes are achieved with higher assembly accuracy values for a particular level of redundancy. However, higher values of redundancy ($p$) are more powerful in increasing the heat flux. In this case, the heat flux is not optimized for the fully assembled version and so heat flux actually increases as the assembly accuracy decreases as long as there is sufficient redundancy to maintain electrical continuity. This occurs because a fewer elements results in less conduction from the hot side through the elements back to the cold side. As the probability of an open circuit increases, the average performance decreases and reaches a lower limit controlled by the rate of heat conduction from the hot side to the cold side through the elements. In the case of the 1D model, there is no significant penalty for missing elements. Three-dimensional models are currently being analyzed to assess the local impact of missing thermoelectric elements.

This thermoelectric application is an attractive case for the self-assembly trials because it is very tolerant of errors. Performance actually increased with some missing elements. 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 2 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 is increased. Further, if process feedback is incorporated to detect and harvest just the complete assemblies, the yield could approach 100%. Small sub-assemblies could then be combined into larger systems with increased functionality.
This is seen in Figure 4. Despite only a 62% probability of an individual element assembling, there is more than 40% chance of an assembly being functional with just two parallel elements. If the assembly probability were 90%, then 60% of the assemblies would be perfect at steady state with all the elements in series. While 40% and 60% success would be poor on its own, selective removal of the successful assemblies could create high yields. The remaining assemblies are left in the assembly system until they are properly assembled as well.

Figure 4 Cumulative distribution of thermoelectric device performance for the case of 16 elements and a 62% probability of each element assembling.

APPLICATIONS TO PHOTOVOLTAICS

Recent work has been done in the fabrication of micro-scale photovoltaic (PV) devices [21]. Each PV cell is approximately 500 µm wide 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 making 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 productions 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 into 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]. To reduce the sensitivity to missing cells, it is important to design the lowest cell grouping as a collection of several cells connected in parallel. This is fairly straightforward since a typical module comprised of the micro-scale cells would require tens of thousands of cells.
CONCLUSIONS

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 this might impact the performance of one self-assembled device: a thermoelectric cooler. Analysis shows that incorporating redundant elements can dramatically improve yield and that missing components may not have a strong impact on system performance under the proper conditions. Where system performance is sensitive to assembly errors, partitioning the assembly into smaller sub-assemblies is a promising route for improved performance.

When these challenges are addressed, self-assembly methods may provide new avenues for additive manufacturing. The ability to integrate components produced by other manufacturing processes will enable increased functionality.

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REFERENCES


