Directed 3D Self Assembly of Reconfigurable Materials

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Basic research on the directed assembly of 3D materials using reconfigurable or switchable elements could revolutionize the processing of future materials and deliver unprecedented advances in performance.

These are exciting times for materials scientists. The field of materials science is undergoing a transformation in the way it will engineer new materials in the future. Recent research advances in the bottoms-up assembly of materials have the potential for providing exquisite control over the local chemistry and properties of a material, and thereby enhancing our ability to engineer much greater functionality and complexity into future material systems. Work over the past several decades has demonstrated the feasibility of using tailored interactions between small molecules to drive the assembly of inorganic nanoparticles, molecules, and biological entities (e.g. DNA and proteins) into larger structures spanning multiple length scales and functionalities.\(^1\)\(^-\)\(^3\) Similarly, dynamic assembly processes have been initiated in which the bonding and network structures undergo disassembly and reassembly in route to their final structures.\(^4\)\(^,\)\(^5\) Finally, recent advances in computational power are enabling material engineers to move beyond simple trial and error methods of materials development to the point where they are able to predict the evolution of material microstructures and properties based on first principle calculations. Future developers will design new materials based largely on the predictions of computational and phenomenological models. We stand at the dawn of a new paradigm for materials development that promises new opportunities for discovery, and new approaches to material design and synthesis. In particular, these new capabilities will allow material scientists to more efficiently explore hierarchical approaches to materials design (e.g. biological systems) and the integration of disparate materials technologies (e.g. biological, electronic and structural materials) into multifunctional systems with unprecedented properties and characteristics.

To date, we have witnessed some major breakthroughs in the area of self-assembly. But they fall far short of the ultimate goal: the design and assembly of complex 3D structures that involve multiple techniques linked into a sequential assembly process that culminates in materials with specifically targeted properties. This still remains well beyond our grasp. Nonetheless, the potential payoffs could be great, and therefore the Materials by Design Subfield at ARO is actively supporting research to advance this exciting field of science. Success will require the continued exploration of approaches for manipulating the self-assembly process by utilizing aspects of shape, intermolecular interactions, induced conformation changes, functionalized adduct and site specific binding groups, molecule-to-substrate interactions, and external fields. But, that will not be enough. To move forward, we need to also refine our ability to incorporate building blocks into these systems that are capable of dynamically altering their configuration, varying their coupling interactions, and switching between physical states. The potential for using these elements to dynamically tune the developing template architecture and to alter the
binding interactions that are expressed during different stages of the directed-assembly process must be better understood. This will permit the design of new, more robust assembly processes to produce structures that would be impossible to achieve in a strictly linear assembly process. In addition, understanding how we might exploit the presence of these actuation elements to yield materials that can dynamically alter their properties under operating conditions in response to external command signals or environmental cues could reap huge dividends in the context of system weight reductions and performance enhancements. Studies will be needed to determine appropriate feedback mechanisms for controlling the response as well as identify feasible avenues for the capture, conversion, and/or transduction of various forms of energy that will be needed to power the desired assembly and reconfiguration processes. Finally, the issue of structural defects must be addressed through various schemes of repair and/or enhanced tolerance. Only then will we be close to enabling the bottom-up design and fabrication of highly complex multifunctional materials that deliver new and unprecedented materials performance. Some of the new technologies emerging from these activities could include the development of active camouflaging systems that mimic natural systems, negative index composites with optical cloaking properties or new classes of smart materials that can alter their behavior in response to environmental stimuli.

References