Overview of Multifunctional Materials

Peter Matic

Multifunctional Materials Branch - Code 6350, Naval Research Laboratory, Washington, DC 20375

ABSTRACT

Multifunctional design has evolved over the past decade, moving away from discrete unifunctional subsystems with clearly defined boundaries, to produce systems design and materials design methods that blend performance in new and innovative ways. This presentation looks at the development of multifunctional design from a systems and a materials perspective. A classification of multifunctional designs is presented, in terms of the decreasing scales at which the boundaries of subsystems, components and materials are blurred. Guidelines for identifying multifunctional opportunities at the system and material scale are also discussed.

Keywords: Multifunctional, systems, performance, materials, properties, design, optimization

1. INTRODUCTION

The word "multifunctional" has more than one meaning. One common usage is interchangeable with the word "interdisciplinary" to signify the blending of people from the traditional technical disciplines in the design process. The word "multifunctional" is also found in consumer product marketing to represent versatility and value. For the purposes of this discussion, "multifunctional" will be used in a technical context as it relates to systems design and the physical performance of materials, where the relationship and synergy of two or more subsystem functions are used to improve system performance.

Multifunctionality has been pursued in a variety of ways for over a decade combining capabilities and performance that captures the notion of versatility, integration and efficiency. Multifunctional designs have moved away from discrete unifunctional subsystems, with clearly defined boundaries, attachments and connections, to produce subsystem designs and materials design methods that blend performance in new and innovative ways. The research and development programs of agencies such as NSF, NASA, ONR, AFOSR, ARO and DARPA, for example, have explored many new avenues to add new subsystems for enhanced performance and combine subsystems for optimization. These efforts are often motivated by the desire for weight reduction, integrated manufacturing, reduced maintenance or "smart" systems potential. Specific information on these programs is well documented in the literature and on the internet.

This presentation discusses in more general terms the development of multifunctional design, differentiates and defines three types of multifunctionality, suggests methods to identify multifunctional opportunities at the systems and material scales, and highlights the need for metrics that quantify multifunctionality. To facilitate clarity and foster concise meaning, the discussion will be developed in terms of system performance, subsystem function, component parameters, and material properties (Figure 1). These definitions highlight the physical scales that constitute the system and the characteristic features at each scale contributing to overall performance. It is hoped that discussing trends and suggesting how to find multifunctional opportunities will be useful to both the systems designer and the materials community.

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2. BASIC FEATURES OF MULTIFUNCTIONAL DESIGN

A few key points about multifunctional design are noted. Multifunctional design is a system performance optimization strategy. It addresses performance descriptions that are generally stated in unifunctional terms. The subsystem function descriptions may be well defined and well established, or they may describe new types of functions needed for the system. New technologies are often the key to achieving multifunctionality, but that need not be a necessity. Mass reduction is often a key multifunctional design objective, and will be referred to a number of times.

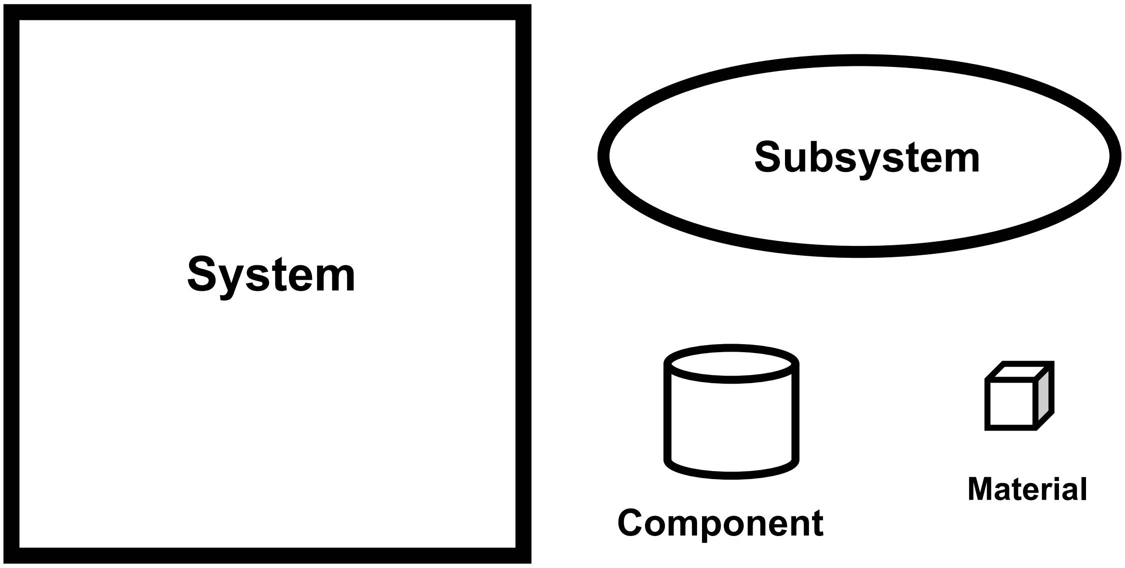


Figure 1 – Hierarchical definitions for multifunctional design and optimization

In its simplest terms, multifunctionality is about reducing the physical distance between subsystems and coupling the functions these subsystems perform. The relative distances vary from system to system, and the strength and symmetry of the coupling may be weak or strong, but these trends in the general sense are used to gain advantages for the system in terms of reduced mass and perhaps volume, too. In addition, the number of components is reduced as the discrete individual parts remain essentially constant, are redesigned and incorporated into integrated components and subsystems.

Miniaturization of components has also been a driving force enabling multifunctionality. Size reductions mean that comparatively high mass and large volume equipment, traditionally viewed as separate and apart from the system itself, could become part of the system. Maintenance related functions are a prime example, where great strides in the reduced size and weight of sensor and signal processing capabilities meant that onboard assessment could be entertained in overall system design. This is particularly true in aerospace systems.

3. THREE CLASSES OF MULTIFUNCTIONALITY

It is convenient and useful to discuss multifunctionality by defining three “types” of multifunctionality. This classification scheme is based on the physical scale and spatial dimensions over which multifunctionality is pursued in the system design process. The difference between these three classes, summarized in Table 1, can be seen as the difference between the *addition of functions* into the system, *union of functions* embedded within a component and the *integration of functions* shared in a volume of material. This classification scheme is described here in more detail.

Type I Multifunctionality: Added Subsystems

- Subsystem addition to provide additional performance
- Connectivity or links between subsystems
- Increased physical or information coupling between subsystems.

Example: Structures with surface mounted health monitoring systems and remote signal processing

Type II Multifunctionality: Co-located Components

- Component co-location to provide packaging integration.
- Reduced dimensionality and complexity of final system.
- Physical distances between subsystems are reduced

Example: Non-load bearing antennas embedded in polymer matrix composites

Type III Multifunctionality: Integrated Materials

- Material selection based on a set of properties to satisfy more than one subsystem function
- Physical volumes of subsystems are combined
- Reduced volume and mass of final multifunctional subsystem

Example: Load bearing polymer batteries with enhanced packaging shaped into airfoils

Table 1 – Multifunctional type definitions.

Type I multifunctionality can be defined as the “addition” of complementary subsystems. It begins with a standard function and adds to it a complementary function to enhance performance. Generally, the standard function is primary or critical in nature while the enhanced function is secondary or non-critical. The distinction between the subsystems is clear, as are the boundaries of the subsystem, while the physical distance between the components of the multifunctional system is often reduced. Only minor modifications are generally made to the primary function.

Many smart structures are examples of Type I multifunctional systems. Useful information about the structural subsystem is gained by the addition of sensors, data acquisition and data processing components that form a damage assessment or health monitoring subsystem. The performance of the structure subsystem is enhanced as information on its physical condition is coupled to the assessment or monitoring subsystem. System mass or cost may be reduced, but not as a result of the added mass and cost of the sensors and instrumentation, but as a result of new design options, operational flexibility or reduced maintenance for the multifunctional structure made possible by the quality of the available information.

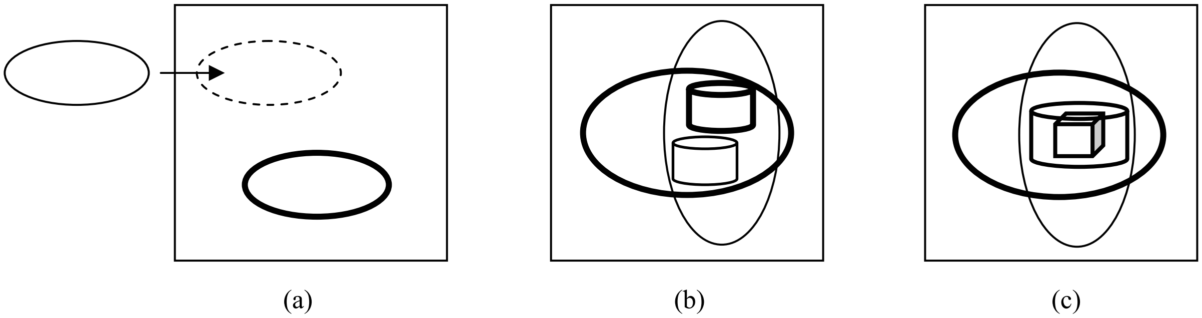
Type II multifunctionality can be defined as the “union” of complementary components into a multifunctional subsystem. The key features of Type II multifunctionality is that the physical distances between subsystem components is significantly reduced. Components with similar geometries can be positioned in a coordinated manner to reduce the dimensionality and complexity of the final subsystem. Component co-location is also useful to facilitate packaging integration. Multifunctional composite materials are often Type II since they can embed a variety of components into a common part. The distinction between subsystems is clear in terms of the materials performing the individual functions. In structural subsystems, load sharing is not yet present. Often, significant modifications are made to the both functions in order to facilitate co-location.

Examples of Type II multifunctionality include the reduction or elimination of interfaces between subsystems where one subsystem is a structural component. The other subsystem components can be such things as electrical wiring, antenna elements, strain sensors, thermal management elements, electronics packages and solar panels. Common themes included the reduction of subsystem dimension to planar forms complementary to flat structural panels.

Finally, Type III multifunctionality can be defined as the designed intersection of functions in a common material. Here, the material selection process is made to satisfy the requirements of more than one subsystem function. Two or more types of energy are managed by the material. The material properties are complementary with respect to these subsystem functions. A successful design reduces the net weight or volume of the multifunction subsystem with respect to the unifunctional subsystems.

Examples of a Type III multifunctional system is a structural subsystem where an embedded antenna or battery power supply subsystem shares the mechanical loads. This example is typical in that parity between the sharing of subsystem functions is not achieved. The passive structure need not be part of the antenna function or battery function, although both of these may in fact contribute back to the structural function.

The common thread between all three classes of multifunctional design is that they progressively blur physical boundaries and blend interfaces, and therefore the distinctions, between system performance and material properties (Figure 2). The emphasis of Type I multifunctionality is on the progressive *selection of subsystems*. Type II focuses on the *breakdown and arrangement of the components* to perform functions that enable performance. The emphasis of Type III multifunctionality is the novel *distribution of functions* within subsystems and components to perform multiple functions. The result of the progressive focus on smaller scales and spacing is greater intrinsic coupling between the subsystems with a greater emphasis on materials properties in Type III than in multifunctional Types I and II.



(a) (b) (c)

Figure 2 – Schematic diagrams of multifunctionality (a) Type I - addition of a subsystem, (b) Type II - co-located components within subsystems and (c) Type III - integrated material function for shared components.

4. FINDING MULTIFUNCTIONAL OPPORTUNITIES IN SYSTEM DESIGN

In order to identify multifunctional opportunities and strategies for new designs, it is useful to look at both required (and existing) system characteristics as well as the intrinsic spectrum of candidate materials and their properties. Here we look at the system level opportunities before looking at materials.

The design of system performance, subsystem functions, component parameters and material properties are developed in the context of candidate technologies at each scale. As discussed above, mass reduction is a significant objective in the multifunctional design process. Multifunctional gains can be found by identifying those subsystems offering the greatest gains from multifunctional designs. Which subsystems to combine and how to combine those subsystems is the key issue.

Preliminary system design based on unifunctional subsystems remains a practical first step for multifunctional design. Available technology, information and experience can be used to establish benchmarks against which to judge any proposed multifunctional design. Unifunctional subsystem characteristics and system constraints can identify subsystem combinations that may offer the greatest potential benefit. Various factors may be useful.

Multifunctionality can be thought of in terms of the way in which the different forms of energy required by the system are managed. Energy, from the point of view of subsystem functions, may come in many forms: electrical, chemical, magnetic, elastic, kinetic, thermal, etc. Energy of one form can flow into the system, be converted from one form into another inside the system, be stored inside the system, or flow out of the system. Unifunctional subsystem design generally deals with one form of energy as the primary design variable, and perhaps another significant form as a byproduct of thermodynamic inefficiency. Multifunctional design tries to combine these energies and manage them at some level in the subsystem.

The mass and energy requirements of the subsystems, components and materials are important factors that can assist in identifying and combining subsystems for multifunctionality. A breakdown and progressive ranking by mass and energy, performed at each level of the hierarchical structure is useful. At some point in this hierarchical breakdown process, similar characteristics and complementary properties and may appear. Even qualitative assessments of common requirements across unifunctional designs such as high stiffness or low thermal conductivity, for example, are useful. These subsets of the system properties and characteristics can be attractive targets for multifunctional design if they can be exploited. Larger mass fractions in the system, with complementary energy functions, will offer the greatest potential for gains if they can be combined.

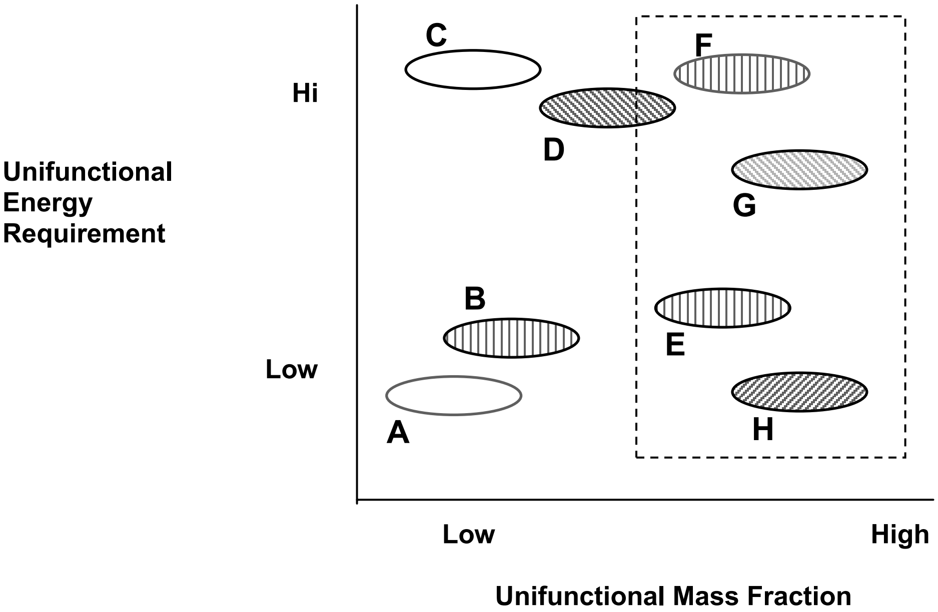


Figure 3 – Schematic diagram energy requirement and mass characteristic breakdown of subsystems, with the forms of energy managed by each subsystem indicated by fill pattern. Candidate subsystems with potential gains from multifunctional design are E,F,G and H due to high mass fraction.

A schematic diagram of this process is shown in Figure 3. The subsystems are plotted based on their mass fraction and relative energy content. The high mass fraction subsystems, i.e. E, F, G and H, offer the greatest potential benefit from multifunctional design. Whether E, F, G and H are suitable would depend on whether the energy management functions could be integrated. One strategy would be to integrate subsystem E or H with subsystem F or G. The disparity in energy requirements might suggest an easier combination if the lower energy content technology could be modified and combined with the higher energy content subsystem. If both technologies are adaptable, combination of the higher content subsystems F and G could be attempted. This process would be repeated at the component and material scales, as well as to identify the appropriate multifunctional design approach.

It is important to recognize that two subsystems, performing two distinct functions, will generally not be equally qualified candidates for modifications or substitutions in order to achieve multifunctionality. The underlying technologies of each subsystem are, of course, different. The constraints on any modifications considered on one subsystem, in order to obtain multifunctionality, will generally be more severe than the constraints on modifications considered to the other. This asymmetry on modifications means that the choice of technologies and multifunctional design baselines for both subystems must be carefully considered to avoid a disproportionate loss in the baseline function of a technology more sensitive to design changes.

5. FINDING MULTIFUNCTIONAL OPPORTUNITIES IN MATERIAL SELECTION

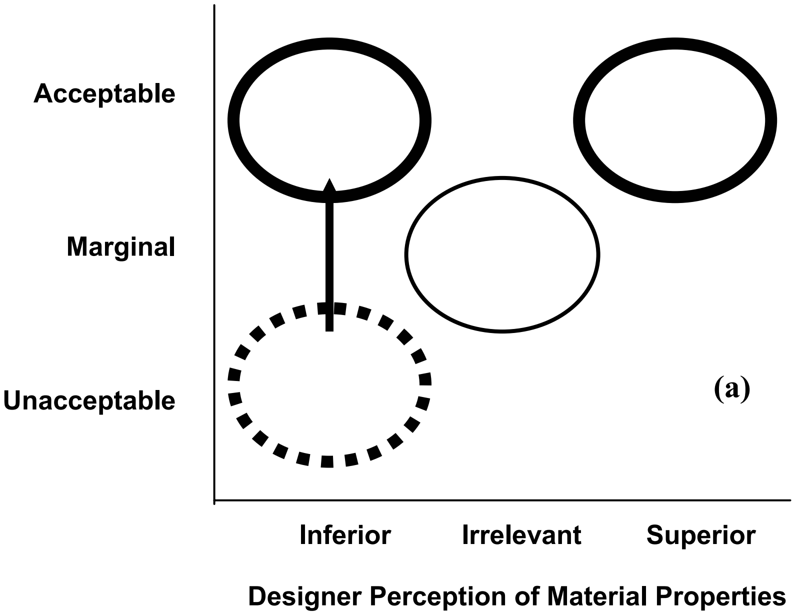
All materials possess a complete set of physical properties that can, in principle, be measured. Specialized technical communities, over a period of time, come to favor specific materials for a comparatively few special properties. Different specialized communities favor different subsets of materials, and optimize the use and combination of these materials.

In practical terms, an individual material selected for use by a technical community is viewed as having subsets of "superior", "inferior" and "irrelevant" properties. With respect to a system, the design decision to employ a material means that it is either "acceptable", "marginal" or "unacceptable". The superior properties of a material explicitly enable engineered system performance. The inferior properties are initially unacceptable and capable of strictly limiting, controlling or even excluding the use of the material in whole classes of applications. The irrelevant properties are marginal and outside the interest of the designers in that specialized community for their current technologies. Figure 4 schematically illustrates this.

The superior and irrelevent material properties classes are related to one another as the outcomes of the initial "best properties" assessments that drive material selection for unifunctional purposes. The inferior properties class is the subsequently distilled from the irrelevant properties by assessement or experience, in response to broader considerations which must be satisfied by design. While unavoidable and of considerable concern in the design process, these inferior properties are generally managed by creative composition, processing, design and life cycle management strategies until they are judged to be acceptable. Successful management of the inferior properties sustains and supports the viability of superior properties. As an example, high stiffness and ductility may drive structural performance. Corrosion of the necessary metal alloy, the inferior property, may be controlled by surface treatments and coatings to ensure that the high stiffness attributes are not eclipsed by problems of cross section thinning or fracture.

Unifunctional design places a premium on identifying a small set of materials with the best superior properties for a single subsystem. This process is repeated independently in parallel across all subsystems and components. System weight is accumulated from each subsystem.

Materials selection to drive a multifunctional design slightly changes this process. Identifying superior material properties is done collectively to satisfy more than one subsystem function. The design for multiple functions may reclassify what were the irrelevant material properties, in their respective unifunctional design processes, into superior properties. While the materials properties may not be the best for any of the functions considered alone, viewed from a unifunctional subsystem perspective, their potential is greater to perform the functions and reduce the net system mass.



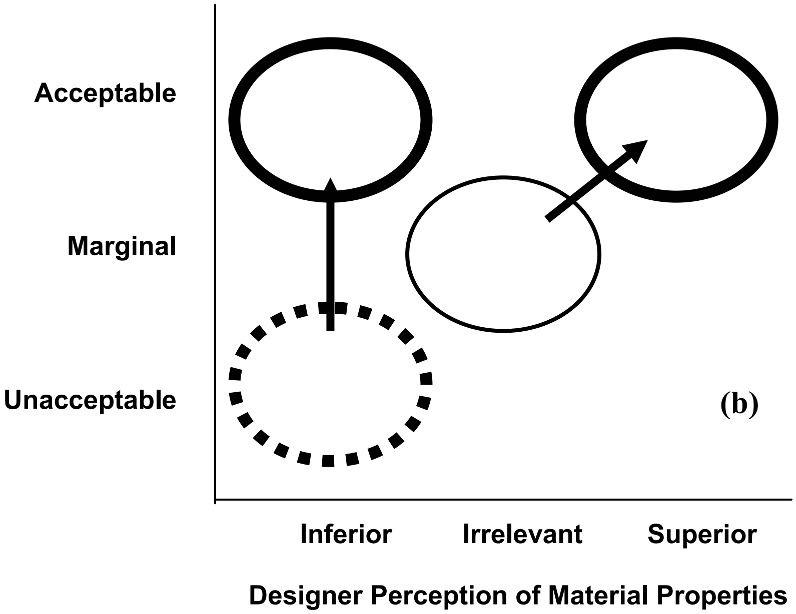


Figure 4 – Schematic diagram of designer perception of "superior", "irrelevant" and "attractive" material properties and their acceptability for use in a (a) unifunctional system and (b) multifunctional system.

Clearly, a material suitable for multifunctional applications must have synergistic properties in some sense. Many of these synergies are documented, some from an understanding of fundamental mechanisms. One approach that may prove useful, in additional to the use of the material performance indices and databases already available and in use for engineering materials, is to reexamine the fundamental properties of elemental and compounds with an eye on multifunctional potential. Energy considerations at the material level, parallel to those at the systems level discussed above, include the electromagnetic, chemical, kinetic, thermal and vibrational forms of energy associated with the atomic mass, charge and bonding.

Review of the periodic table, with the goal of achieving insight into multifunctional opportunities, can provide guidance at the element level (and with regard to compound formation). With the emphasis of this paper on structure as one subsystem and mass reduction a design objective, we focus on element properties in the solid state.

The positive and negative correlations present in physical and chemical properties of elements across the periodic table may point to useful multifunctional material solutions. The general trends in electrical properties are an example of this, and specifically the way in which ionic bonding producing electrical insulators, covalent bonding associated with semiconductors and metallic bonding generating electrical conductors. While the brief discussion here will focus on some trends by elements, the essential spirit in which it is presented also applies to more complex crystals, compounds and engineering materials.

The nuclear mass is responsible for essentially all the material mass, while the outer electrons of the elements dominate so many material properties. It is clear that most multifunctional performance will be engineered, in some sense, by the use of positive and negative correlations in the properties of the outer electrons. A well known elementary example is how the valence electrons of metals, free to move about in the crystalline solid state, are associated with high electrical conductivity, high thermal conductivity, high ductility and high reflectivity to visible light. The potential to bring two or more of these properties to a design, at the expense of only one nuclear mass, is the probably a driving feature of multifunctional design for mass reduction expressed at the atomic scale.

An example of a functional property that the nuclear mass does affect is the thermal conductivity of electrically insulating elements. In these elements, phonons are the transport mechanism for heat. Electron contributions to thermal conductivity are negligible as the atomic lattice vibrations are dominant (in contrast to metals where electrons dominate that property at all but very low temperatures).

The form of the interatomic energy potentials and the characteristics of bonds, at and around the equilibrium interatomic spacing, also yield useful information on material properties. The form of the potentials relates to value of the bond energy and associated trends in the melting point, elastic modulus and the coefficient of thermal expansion. Quantitative expressions, such as the Wiedemann-Franz law relating thermal conductivity, temperature and electrical conductivity modest temperatures ranges around room temperature, may be particularly useful. Relationships of this type highlight the changes in properties that may be expected over an operating range. The point to be made here is that these correlations help to identifying multifunctional combinations that may be useful in applications where similar or opposite property trends contribute to performance.

Other common classes of chemical compounds, such as ceramics and polymers, and composite materials will not be discussed here, although a discussion is clearly not complete without considering them. The polymers bring properties such as their low electrical conductivity, low to moderate elastic modulus, and a wide range of attainable strains. Ceramics feature high elastic modulus, a wide range of dielectric responses and useful thermal properties. These materials, in some ways more complex in their behavior, offer additional opportunities for multifunctional design.

6. SUMMARY

Multifunctional design combines the performance of two or more unifunctional subsystems into a single subsystem to achieve improved global performance and optimization. Multifunctional design can be implemented at the subsystem, component or material scales. These scales are convenient for classifying multifunctionality according to the addition, co-location or integration, respectively, of the way in which the energy required to achieve the desired performance is managed by the subsystem. The technologies employed for unifunctional designs can be useful starting points for multifunctional designs. The combination of unifunctional technologies is one option for multifunctional design, with the caveat that some technologies will be more sensitive than others to any changes in going to a multifunctional design.

Identification of multifunctional opportunities and strategies for new designs can be approached from both system and material ends of the spatial hierarchy. The system features, obtained by progressively breaking it down into constituent mass and energy, can be used to identify complementary groupings that would provide a net benefit from a successful multifunctional design. Positive and negative correlations within and across classes of material properties may be useful for identifying materials whose properties may be more appropriate for multifunctional designs than the materials selected for optimized unifunctional subsystems.