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AXIOMATIC DESIGN OF MULTI-SCALE SYSTEMS

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ABSTRACT

Many of the current research activities are directed towards nanotechnology. The use of nano products requires an integration of nano-scale structures to macro/micro-scale systems. The degree of complexity of multi-scale systems is expected to increase rapidly as the scale order grows. The scale order can be defined in this paper as the relative magnitude of the size of the system to the smallest characteristic length of the system. Production of next generation IC chips and upcoming nanoproducts will have the scale order of 9 or above, which obviously will be a hard challenge with the existing design and manufacturing tools. Axiomatic approach for systems design has been an effective tool to provide new functionalities and better manufacturability of many new engineering products, and is expected to provide better understanding of the complexity of multi-scale systems. The causalities of the systems complexity have been reviewed with respect to design axioms and a hypothetical complexity reduction approach is proposed. The scale decomposition of a multi-scale system into small-scale order domains will reduce the complexity of the system and will subsequently ensure a good design and manufacturing by developing functional periodicity. A novel method of assembling individual carbon nanotube has been developed based on the concept of axiomatic design and complexity theory..

Keywords: nanotechnology, multi-scale systems, complexity, functional periodicity

I. INTRODUCTION

It's been observed that miniaturization without adding new functionalities has been the primary cause of many unsuccessful MEMS devices at the commercialization stage. The axiomatic design approach states that design is a series of top-to-down mapping processes between "What" and "How".[1] "What we want to achieve by shrinking the size of a system" should be defined *a priori* before we work on "how we can miniaturize a system". Tiny products must be designed in a systems context and it's been shown that the axiomatic design can provide a good framework to design and manufacture successful MEMS products.[2] There exist two design axioms, which the mapping process between design domains must satisfy.[2] The first design axiom states that a good design should maintain the independence of the functional requirements (FRs). A MEMS product design which violated the first axiom paid a significant penalty in the fabrication stage as shown in Figure 1.[3] The fabrication of functionally coupled micro-mirror array design took more than 4 years to reach a mediocre result, but decoupled and uncoupled designs took less than 6 months, respectively, to generate much better performances. When a MEMS design has strongly coupled functional requirements (FRs), the design would require very costly iterations of fabrication effort or, sometimes, could not reach the conclusion. Design and manufacture of MEMS would be much more successful if they were designed with the axiomatic framework.

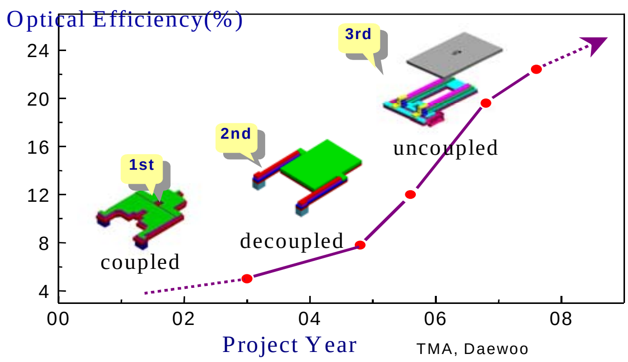

Figure 1. Effect of design couplings to the progress of MEMS-based micromirror array development project. [3]

Design and manufacture of nanostructures require much more precision than that of macro and micro structures. Many research groups have tried to build and control nanostructures bottom-up in this regard. The quantum dots, nanoparticles, nanotubes and nanowires are made with a sub-nanometer accuracy, but have limited repeatability only within a short range order. In other words, nanotechnology is accurate but not precise in a long range order. In order to benefit from the nanotechnology, nanostructures need to be integrated to the micro/macro-scale platforms, where the top-down and bottom-up processes meet.

This makes the design and manufacture of multi-scale systems very complex.

Multi-scale systems are complex. The degree of complexity increases rapidly as the system scale order grows. The scale order can be defined in this paper as the relative magnitude of the size of the system to the smallest characteristic length of the system. Design and manufacture of conventional systems have been able to cover the scale order of up to 4 or 5 reasonably. Precision machining and thin film manufacturing can cover the scale order up to 6. Next generation IC chips and upcoming nanoproducts will require covering the scale order of 9 or above, which obviously will be a hard challenge with the existing design and manufacturing technology. Lessons from the MEMS product development indicate that the axiomatic approach can provide a good framework to define novel functionalities and better manufacturability. The goal of this paper is show how a multi-scale system can be designed well, which includes nano, micro and macro structures. The axiomatic approach is used to understand and deal with complexity of multi-scale systems.

II. What is complexity?

Success of multi-scale systems design may depend on the better understanding of complexity and subsequent reduction of complexity of a design. There have been many different views and approaches to complexity in the fields of information technology, system biology, mathematics, meteorology, economics and many social sciences. It is important to understand "what is complexity" before we try "how to reduce complexity." Efforts to find out absolute measures of complexity, algorithmically, probabilistically and/or computationally, however, have not been helpful in designing a system to have less complexity. A relative measure of complexity has been introduced by Suh [4,5], which has been built on the concept and framework of axiomatic approach of design. In his complexity theory, complexity was defined as a measure of uncertainty in satisfying the functional requirements (FRs) within the specified accuracy. Then four types of complexity were described: time-independent real complexity, time-independent imaginary complexity, time-dependent combinatory complexity and time-dependent periodic complexity. The axiomatic approach to complexity can characterize the nature of complexity much better than the previous efforts by examining the uncertainty associated with the functions of a system rather than its physical entities.

Axiomatic approach with a relative measure would help to design a system with less complexity by introducing functional periodicity.[5] However, there have been some concerns whether the four types of complexity could be orthogonal and the uncertainty could be the only measure for complexity. Consider the case of cutting a rod with a hacksaw to 2 meter in length with 10 nm tolerances. The design range (plus/minus 10 nm) is much smaller than the system range (say plus/minus 1mm), which makes the probability of success is near zero and the information content is near infinite. This design case is very uncertain (or unlikely to happen) but is not really complex. This is because the functional requirement (FR) space of the design is one-dimensional. When the number of FRs (and matching DPs) is large and the information content is very high, however, a design may be regarded as very complex. Information content (uncertainty) alone may not constitute complexity. Consider another case of solving a Bessel function, which is a second order differential equation. Since we know that there exists a solution, this case may not be uncertain. But it's hard for a novice to find a solution. This case is difficult rather than complex or uncertain. For a scholar who has been well educated to solve this kind of problem, this case may not be difficult, but laborious. This kind of difficulty is path dependent, which is similar to the time-independent imaginary complexity from the complexity theory. When there are hundreds of Bessel functions to be solved simultaneously, however, it will be very complex even to an expert without using a computer.

When a system has many FRs and DPs, which are not at their equilibrium states, systems ranges change with time and the system moves toward local or global equilibrium states. This will inevitably make the FRs strongly coupled and increase the information content consequently. It will be very complex, which was described by Suh as the time-dependent combinatorial complexity. [4]

There are subtle differences among the uncertainty, complexity and difficulty in social science.[6] Uncertainty alone may not describe complexity problems in general social problems. This kind of problems in defining complexity can be obviated, however, if the causes of complexity can be found and avoided. Since design axioms have been always true and no counter examples have been observed yet, we may define complexity as a result of design failure to conform the axioms. It's an author's hypothetical proposal to describe complexity by its causal nature with respect to the design axioms. Complexity is a collective outcome when a design doesn't satisfy the design axiom(s).

The causality of complexity can be described as:

- Type I complexity: When a design is coupled. (Independence axiom violation)
- Type II complexity: When a design is uncertain. (Information axiom violation)
- Type III complexity: When a design is decoupled and not solved in the particular sequence. (Lack of knowledge)
- Type IV complexity: When a design has many states (FRs, DPs), which are not at equilibrium and change as a function of time. (Non-equilibrium)

Figure 2 shows that there are four causalities of complexity with respect to the design axioms. Type I complexity is a result of heavy coupling of FRs, which is a violation of the independence axiom. Time-independent complexity is a type II complexity and is a result of the information axiom violation. This kind of complexity has been conceived in social science as "uncertain," such as forecasting weather one year from today. Time-independent imaginary complexity is a type III complexity, which is a result of lack of understanding about the system. This is path dependent and is conceived by people as "difficult," such as protein folding problems. Time-dependent combinatorial complexity is a combined result of Type I, II, and IV complexities, which has been conceived as "a real complex problem" in social sciences, such as the future commodity exchange market in Chicago.[6] Time-dependent periodic complexity is a smaller scale complexity, divided and confined in functionally uncoupled spatial/temporal micro-domains. The functional periodicity accompanies micro-domains, which may have combined types of complexity above, but in a much smaller scale order and is manageable

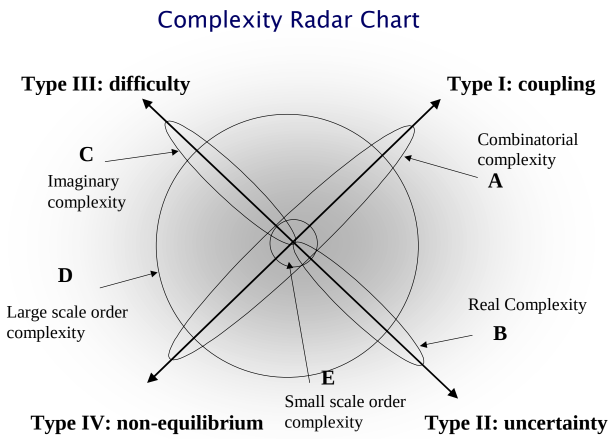

Figure 2. Causality-based Complexity Radar Chart

III. Scale decomposition

The complexity theory suggests that the introduction of functional periodicity can transform a system with time-dependent combinatorial complexity to a system with time-dependent periodic complexity.[5] It may be restated in this paper with the causalities of complexity: functional requirements of a complex system can be satisfied by uncoupled periodic functions of many spatial/temporal micro-domains where the system complexity of all types can be decomposed into smaller scale ones. It will be elaborated further in this section how to scale-decompose a multi-scale system.

The degree of complexity is expected to increase rapidly as the scale order (scale bandwidth) grows. The order of scale can be defined as the relative magnitude of the smallest feature to the largest of the system. For the case of polymer science, the scale order is the number of monomers in a single polymer chain (degree of polymerization). Single chain of ultra high-density polyethylene can have not more than 10^6 monomers at most, which would be very hard to deform due to its very high viscosity. This can be regarded as types I and IV combined complexity (or combinatorial complexity) with a scale order higher than 6. Design and manufacturing of discrete systems, similar to the continuous polymeric chains, cannot easily handle the system with a scale order of 6 or higher.

Time-dependent periodic complexity has a smaller scale order complexity, divided and confined in functionally periodic spatial/temporal micro-domains. One example of utilizing functional periodicity is the nanostructure fabrication using di-block copolymers. A rich variety of nanoscale periodic patterns are fabricated by mixing and micro-separating immiscible block copolymers.[7] Since block copolymers are linked together, either covalently or non-covalently, the linkage prohibits macroscopic separation of immiscible polymers. Instead they form microscopic periodic structures, ranging in size from a few to 100s nanometers, when the Gibb's free energy of mixing has negative slope to trigger spinodal decomposition.[8] The shape and size of micro-domains can be controlled by the composition of copolymers and the length scale of micro-domain periodicity is proportional to the size of the polymer and the radius of gyration, such as;

$$L \propto R_g \propto a\sqrt{N} \qquad (1)$$

where R_g is the radius of gyration of the copolymer chain, a is the length of a characteristic segment, and N is the index number of polymerization.[8] When the micro-separation occurs, the polymer structure tends to minimize the free energy and the size of periodicity becomes proportional to the radius of gyration. Figure 3 shows SEM images of PS-PB diblock copolymer films with spherical micro domains (A) and 20 nm etched holes in silicon nitride film (B). When we consider the length of a characteristic segment length, a, 5 angstrom, and the index number, N, 1000, the radius of gyration, R_g, becomes 15 nm, which is very close to the size of the periodicity observed.

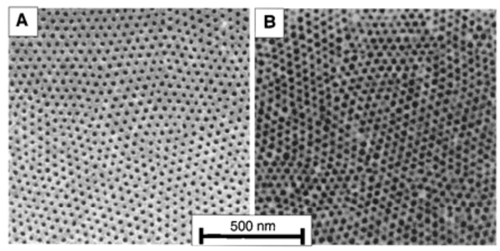

Figure3. SEM pictures of diblock copolymer membrane and nanopatterns transferred on SiNx [7]

IV. Nanopelleting for CNT assembly

To show the effectiveness of the axiomatic approach toward this end, cases of MEMS devices have been developed successfully with a framework of axiomatic design. [9-12] One of the cases involving nano-scale system is a novel concept of carbon nanotube assembly. It is assumed that a discrete multi-scale system behaves similar to a continuous multi-scale system, and will have minimum complexity when the system is divided into micro-domains with a length scale of the functional periodicity proportional to, $a\sqrt{N}$, where a is the characteristic length of a smallest feature, and N is the scale order of the system. For the case of assembling carbon nanotubes on to 1 in^2 area, the scale order is about 6 with the smallest characteristic length of about 25 nm, and the projected periodicity to minimize the complexity is about 25 μm. It suggests that the carbon nanotube assembly on 1 in^2 can be well achieved if the functional requirement can be decomposed into many micro-domains, sized about 25 μm by 25 μm.

Carbon nanotubes (CNTs) is expected to bring big impacts and benefits once a robust, large-scale manufacturing technique is developed. The key challenges to achieve this can be grouped into three categories: growth, handling, and functionalization. The nanopelleting concept, devised by the author, seeks to address these challenges in the context of axiomatic design.[14] A nanopellet consists of a nanostructure embedded in a micro-scale pellet; a CNT embedded in a block of another material shaped to a specific geometry, for example. These micro-scale building blocks can then be readily assembled into pre-defined patterns with high productivity and long-range order, enabling robust, repeatable, and large-scale manufacture of CNT structures. By serving as an assembly vehicle for nanotubes, nanopellets address the complexity of fabrication and assembly of a multi-scale system.

The two basic components of a nanopellet are the CNT and the block that forms the micro-scale pellet. We have developed a process for the creation of these pellets; the process utilizes a subtractive method whereby trenches are created in silicon that then serve as the molds for the nanopellets. (Figure 4)

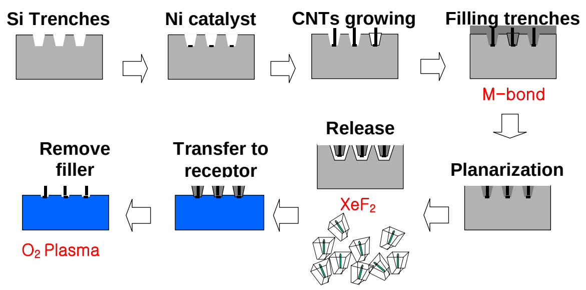

Figure 4. Nanopelleting Process

Pellets are created by coating the wafer surface with the chosen filler, thereby filling the trenches, which are then be planarized until a smooth surface is achieved with filler isolated into the trenches. We have investigated various materials for creating the body of nanopellets with the subtractive method; spin-coated M-Bond epoxy is found to allow selective release of the nanopellets from a silicon substrate utilizing xenon di-fluoride (XeF_2) as well as the selective removal of the M-Bond without attacking the CNT utilizing oxygen plasma etching. The M-bond epoxy was also compatible with a planarization step using a CMP process, which polishes CNTs to an even length. Figure 5 shows a square pellet having a bundle of carbon annotates at the center. [13]

A circular nanopellet has been made and transplanted into a pre-patterned trench as shown in Figure 6 (a) and (b), but anchoring of CNTs onto the substrate was simply done by gluing the pellet. Figure 6 (c) shows a bundle of CNTs after the removal of the filler material via XeF2 etching. It is noted that amorphous carbons have been removed by XeF2 etching and bare graphite nanotubes show much thin trunk at the bottom.

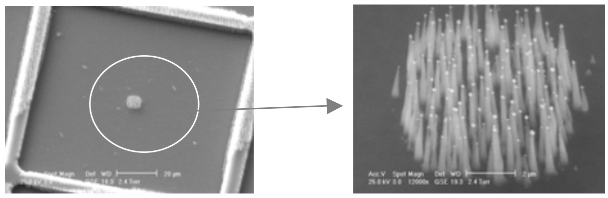

Figure 5. Nanopellet with a bundle of CNT at the center of the patch

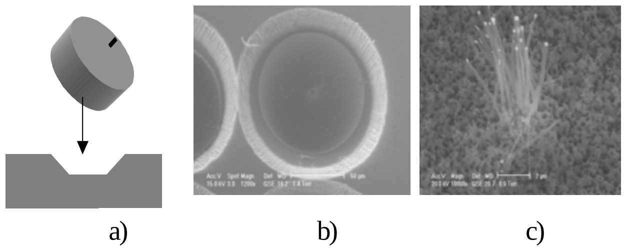

Figure 6. Transplanting of a nanopellet

With the concept of nanopelleting, we have shown the possibility of directly guided assembly of individual nanotube into a long-range ordered two-dimensional array. In order to process high aspect ratio pellets, however, the existing method with trenches would become very complex. Based on the scale decomposition described earlier, a new nanopelleting process has been developed. It doesn't require CNT growth in deep trenches and the subsequent CMP process, thus allowing more flexibility regarding the shape and the height of the nanopellets. Most of all, it will be less complex. Using this new process, high-aspect-ratio nanopellets, "nanocandles", are designed to have the diameter of the nanocandle, 25 μm. Nanopellets of aspect ratio, 5:1, have been fabricated easily and will be scaled up to 15:1.

The new type of nanopellet, "nanocandle" has less complexity in achieving the functionality of a multi-scale system. A nanopipette by assembling single-strand carbon nanopellet to a nanoprobe is under development, as an immediate application, which will enable minimally invasive *in vivo* and *in vitro* biomedical sampling.

V. CONCLUSIONS

It is shown that the axiomatic approach can provide a good framework to design multi-scale systems. It is proposed in this paper that complexity can be reduced by conforming design axioms and decomposing the system into smaller uncoupled micro-domains. The scale decomposition of a multi-scale system into smaller-scale periodic systems can reduce the complexity of the whole system and subsequently ensure a good design and manufacturing by generating functional periodicity as was proposed in the complexity theory. The causalities of complexity were discussed with respect to the design axioms. Type I complexity is a result of heavy functional coupling. Type II complexity is a result of the information axiom violation, which increases uncertainty. Type III complexity is a result of lack of understanding of the functionally decoupled system. This is path dependent. Type IV complexity is a result of non-equilibrium of the design solution, with which systems ranges change with time. Time-dependent combinatorial complexity is a combined result of Type I, II, and IV complexities, which has been conceived as "a real complex problem" in social science. When the scale order is large, all types of complexity become larger. Time-dependent periodic complexity is a smaller scale complexity, divided and confined in functionally uncoupled spatial/temporal micro-domains. The functional periodicity requires micro-domains, which may reduce and confine complexity in much smaller scale orders. A new process for the assembly of carbon nanotubes has been designed based on the axiomatic framework to reduce the system complexity.

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