Designer Disordered Functional Materials via Evolving Wave Networks

Yang Jiao, Arizona State University

Disorder is found in almost all materials, from defects in crystalline solids to amorphous packings of atoms in glassy and non-equilibrium systems. Compared to their crystalline counterparts, the amorphous materials lack conventional long-range translational and orientational order, e.g., there are no Bragg peaks in their scattering intensity. On the other hand, they can possess significant short-range order and inherit the ``isotropy'' property from the preceding high-symmetry (liquid) phase. Traditionally, it was believed that disorder generally has negative impacts on material properties, while recently it has been shown that novel properties and desirable performance, especially associated with photonic applications, can be achieved via properly engineered disorder [1]. However, an outstanding challenge that arises in the systematic design and optimization of disordered materials involves the large number of degrees of freedom associated with the system. In the article "*Evolving scattering network for engineering disorder*" [2], Yu addresses this challenge by developing a novel computational tool for multiscale design of open disordered material system for wave manipulations, bridging network science, computational materials and wave physics.

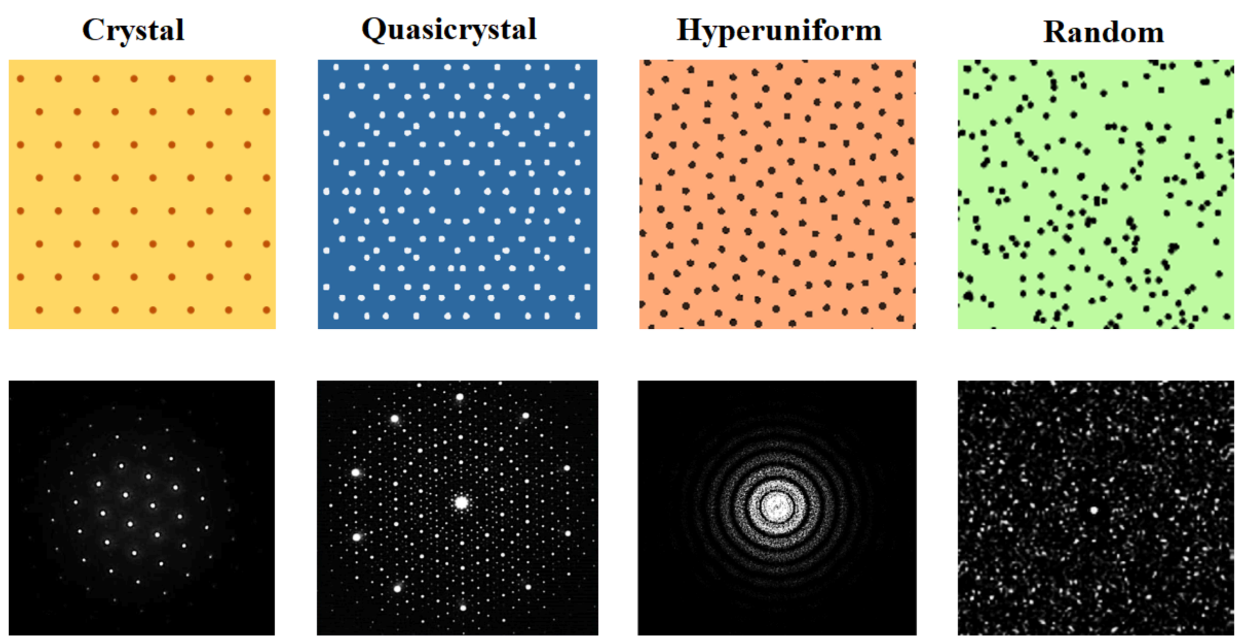

Figure 1*: Material systems with distinct microstructure (i.e., distribution of particles in a matrix, upper panels) and their scattering properties (lower panels). Yu addresses the challenge in multiscale design of open disordered material system for wave manipulations by developing a novel computational tool that bridges network science, computational materials and wave physics.*

The key idea in Yu's approach is to consider a complex open material system as an evolving network --- a mathematical model composed of a collection of "nodes", a subset of which are connected by "bonds". Although conceptually simple, network models have been widely applied in social, economic, biological and physical sciences, successfully unraveling the complexity of these systems. On the fundamental level, a material system is naturally a network --- each atom can be considered as a node, and atoms interacting with one another are connected by bonds, which carry important physical information of their interactions (e.g., the inter-atomic forces). One can easily generalize this reasoning on larger scales. For example, in a composite material in which a number of aluminum spheres are embedded and dispersed in a polymer matrix, it is natural to model each sphere as a node. Under mechanical loading, the embedded spheres “feel” each through the stress field and their “bonds” carry information of their effective elastic interaction through the field.

Here, Yu focused on the matter-wave interactions to design a composite that can scatter lights in a desirable fashion. Scattering, a phenomenon that is responsible for the blue color of our sky, occurs when a light ray is partially deflected in directions deviating from the incident direction as it hits a particle (i.e., a “scatter”) in the composite. Since the composite contains multiple particles, when entering the composite a light ray may be scattered many times by different particles at different spatial locations in the system. Therefore, the overall scattering behavior of the composite is determined by the collective arrangement of all scatters in the system, and one needs to find out an optimal arrangement of particles in order to achieve the desirable scattering behavior.

To solve this challenging design problem, Yu devised a powerful computational tool based on an “evolving scattering network”, which extends the evolution process in network science (e.g., scale-free networks [4]) to wave physics. In this network, each node represents a scatter in the composite. Each bond connecting a pair of scatters is assigned a weight, which characterizes the “interference” effect due to successive scattering by the two scatters. The overall scattering intensity of the material is related to the total sum of bond weights. Armed with this network tool, Yu proceeded with finding the optimal arrangement for the scatters. Instead of simultaneously handling all scatters as done in many optimization approaches, here the particles (i.e., scatters) are sequentially added into the system, i.e., they are placed at their “optimal” locations such that the desirable scattering behavior can be attained. This leads to a dynamically evolving scattering network, which in turn drives the evolution of the material system to the optimal state. The evolving nature of the tool allows one to easily handle open system design, i.e., one with dynamically changing number of particles.

Among other applications, Yu demonstrated the utility of the evolving network approach to design material systems with the remarkable properties of stealthy hyperuniformity. Hyperuniform materials are those that completely suppress scattering of waves with large wavelengths [3]. They possess a unique combination of high-symmetry liquid-like structures on small-scales and crystal-like hidden order on large scales (see Fig. 1), which endow them with many superior physical properties. One of the most striking properties of these hyperuniform materials is the realization of large, complete and isotropic photonic band gaps, blocking all directions and polarizations, which was considered not possible in traditional wisdom and has significant ramifications for realizing electronic and photonic band gaps in disordered materials [1]. Yu’s model enables network-based classification of material phases and screening of microstructures with stealthy hyperuniform materials, which could significantly accelerate the discovery of novel hyperuniform material systems. By employing the concept of preferential attachments in network science (e.g., new nodes are attached to existing ones with more bonds) [4], this model also allows the engineering of the degree distribution of wave networks, achieving exotic material states with distinct particle density and short-range order while preserving hyperuniform long-range order. Although mainly focused on scattering properties, the evolving network model with straightforward generalizations provides a versatile tool for engineering dynamical phenomena in complex material systems.

References:

[1] S. Yu, C. W. Qiu, Y. Chong, S. Torquato, and N. Park, Engineered disorder in photonics, Nature Reviews Materials, 6, 226 (2021).
[2] S. Yu, Nat. Comput. Sci, in press (2023)
[3] S. Torquato, Hyperuniform States of Matter, Physics Reports, 745, 1-95 (2018).
[4] A. Barabási, Scale-free networks: a decade and beyond, Science 325, 412 (2009).