Structural colors: toward AI design and low-cost fabrication

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Structural colors made of inorganic elements contrasts the natural dye pigments, and they are environmental-friendly and offers long-term stability[1]. However, a large class of structural colors relies on precision patterning techniques, which limits their large-scale applications. Another category that is based on multilayer thin film structures are more scalable, but currently depends on vacuum deposition processes[1]. The design of such layered structures requires accumulated experience, thus creates high entry barriers to many. This talk will describe our efforts to address the above challenges.

To design a thin film structure that can produce the desired color, we formulate the task as an inverse design problem, i.e. design multilayer structures to achieve a certain optical response, such as reflection spectrum of a target color. However, the design process can be non-trivial because for each layer both material selection and thickness need to be considered. To make this easier, many optimization-based methods have been devised. But these methods are usually based on heuristic searching, which can lead to suboptimal performance. We applied Reinforcement Learning (RL) algorithm to treat the multilayer structures as a sequence generation process, which after training can automatically design the structures given input[2].

To illustrate, we design a structure to mimic the chrome-appearance. Decorative chrome plating is ubiquitous in creating highly appealing chrome-finish. However, the fabrication uses hazardous process with adverse health effects for the workers and causes significant environmental impact. To overcome these challenges, we employ reinforcement learning to generate multilayer structures to mimic chrome's reflection spectrum; and the structures are made entirely with environmentally benign materials and deposited using PVD process on a variety of substrates. Furthermore, we show another unique functionality by making a chrome-look coating transparent to RF waves, which is not possible with traditional chrome coatings. This is achieved by removing metals from consideration during the design process using reinforcement learning algorithm[3].

To reduce the cost of making layered structural colors, we develop a full solution-based method to fabricate multilayer thin film structures, which contrasts with the conventional vacuum-based physical vapor deposition process. We chose copper/dioxide/copper as a model system due to its simple structure and wide color tunability, and carried out systematic investigation for each layer to ensure good film quality as well as its compatibility with all previous layers[4].

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2. H. Z. Wang, Z. Zheng, C. G. Ji, L. J. Guo, "Automated Optical Multi-layer Design via Deep Reinforcement Learning," *Mach. Learn.: Sci. Technol.* ***2,*** *025013*, 2020.
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4. W. J. Feng, C. G. Ji, L. J. Guo, "Primary and Secondary Reflective Color Realized by Full-Solution-Processed Multi-Layer Structures," *Adv. Opt. Mater*. 11, 2300456, 2023.

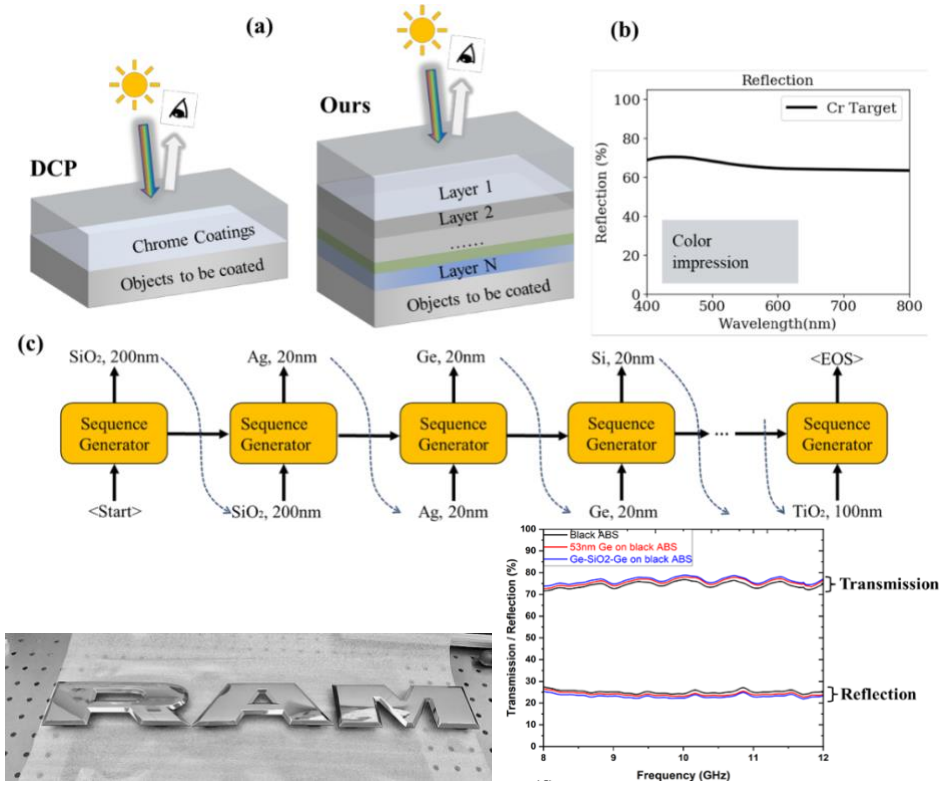

Figure 1. (a) Layered structure to mimic the Chrome reflection spectrum and without any Cr in the material selection. (b) Reflection spectrum and visual appearance of a chrome layer. (c) Sequential design process used by Reinforcement learning algorithms. Photo of fabricated sample showing chrome-finish appearance and exhibits RF transparency measured in 8-12 GHz range.

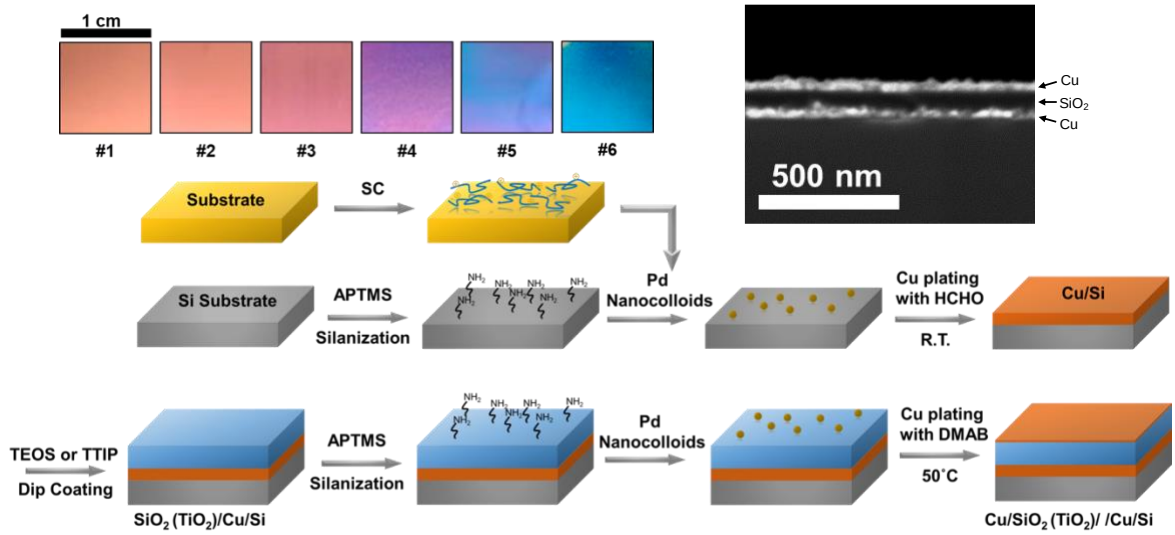

Figure 2. Pictures of solution processed colored samples and cross-section SEM of the cooper/SiO_2/cooper layer trilayer stack. Schematic of steps used in all-solution process to fabricate the individual layers, ensuring each compatible with the previous layer.