Statistical designs accelerate the optimization of layered 2-D crystals

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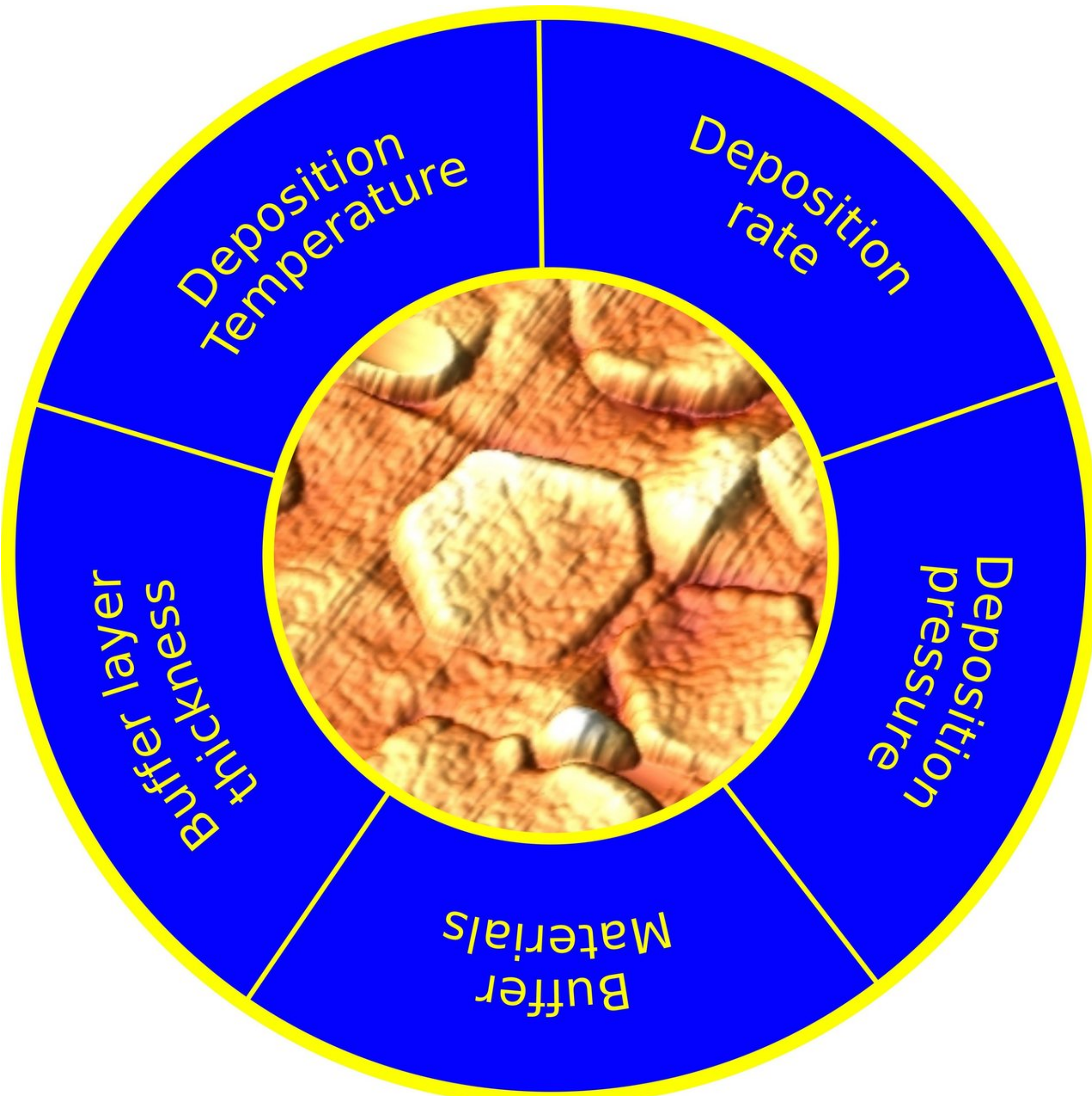

Optimization and growth of texture Sb_2Te_3 crystal by statistical design of experiment (DoE). Statistical significant deposition factors such as temperature, pressure, growth rate, buffer materials, and buffer layer thickness play a crucial role in optimizing van der Waals crystal growth. Credit: Singapore University of Technology and Design (SUTD)

It has been estimated that there are more than 10^{100} possible materials that can be synthesised, grown and optimised. Materials design can be a slow and laborious process, and investigating the full parameter space is a formidable challenge. Machine learning and other advanced statistical techniques will almost certainly accelerate materials development, but many materials scientists are unaware that very basic statistical design methods can accelerate the process. These include the fractional factorial design of experiments, which is more commonly used by product engineers than materials scientists.

Layered chalcogenide materials, such as Sb_2Te_3, have attracted substantial attention in the last decade because of their topologically non-trivial bad structure, and use in thermoelectrics and interfacial phase change memory. High quality crystals of Sb_2Te_3 are required for high-performance memory and energy converting devices. However, efficiently optimising the crystal quality is challenging because it is highly sensitive to a large number of synthesis parameters, such as temperature, pressure, surrounding materials and deposition rate. It is often difficult to determine the parameters that significantly affect the crystal quality, i.e., "we are unable to see the wood in the trees," and therefore, it is difficult to know which design parameter should be prioritised during optimisation.

Researchers from the Singapore University of Technology and Design (SUTD) used the Sb_2Te_3 growth problem to demonstrate the power of fractional factorial design in materials science. After uncovering the statistically significant parameters and interactions that influence the quality of the Sb_2Te_3 crystals, the research team was able to grow high quality layered Sb_2Te_3 crystals over a 4" silicon wafer using sputtering, which is an industrially scalable deposition technique.

SUTD principal investigator, Assistant Professor Robert Simpson said, "Our study demonstrates that these cross-disciplinary statistical optimisation techniques can provide substantial efficiency increases, and it is therefore bemusing that these approaches are not widely used in materials science. Perhaps the reluctance to adopt fractional factorial design is due to the fact that it is purely statistical and does not directly provide information about underlying physics. However, these days, artificial intelligence is fueling a revolution in "black box" optimisation techniques in materials science and teaming them with physical models will undoubtedly provide radical changes to the way that we do materials science."

More information: Jitendra K. Behera et al, Sb2Te3 and Its Superlattices: Optimization by Statistical Design, *ACS Applied Materials & Interfaces* (2018). DOI: 10.1021/acsami.8b02100

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