From Machine Learning to Discovery of New Family Member

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A recent study in which machine learning was applied to suggest potential high-temperature superconductors predicted that $Ba_3In_2O_6$ should superconduct at around 46 K [Z.-L. Liu *et al.* *APL Mater.* **8**, 061104 (2020)]. Though no barium indate superconductors are known, $Ba_3In_2O_6$ has a crystal structure that resembles $YBa_2Cu_3O_7$ and other well-known cuprate superconductors.

Thin films of $Ba_3In_2O_6$ had never been made and **PARADIM researchers were able to grow the desired phase** using a new variant of molecular-beam epitaxy (MBE), suboxide MBE, developed in PARADIM. In addition to succeeding in the growth of the targeted phase, $Ba_3In_2O_6$, **PARADIM researchers also discovered a new barium indate phase** with an even simpler crystal structure, $Ba_4In_2O_7$, that is analogous to the first high-temperature cuprate superconductor discovered, $(La,Ba)_2CuO_4$.

These phases are shown at the right in both cartoon form and high-resolution electron microscope images of the thin films grown. These phases are n = 1, 2, and ∞ members of a family of structurally related phases known as Ruddlesden–Popper phases with general formula $Ba_{n+1}In_nO_{2.5n+1}$ of which the n=1 member was previously unknown. The high-temperature superconducting cuprates also belong to this same family of structures. In addition to $Ba_3In_2O_6$, $Ba_4In_2O_7$ also warrants study as a potential high-temperature superconductor when doped with electrons or holes. This will be the subject of future work.

F.V.E. Hensling *et al.* *J. Vac. Science & Technol. A* **40**, 062707 (2022).