Protective and High-temperature Coatings
Room Palm 5-6 - Session MA5-1-WeA

Boron-containing Coatings I
Moderator: Anna Hirle, TU Wien, Austria

11:00am **MA5-1-WeA-10 Metal Boride Nanocrystal Inks for Applications in Extreme Environments***, **Loredana Protesescu [l.protesescu@rug.nl]**,* RUG, Netherlands **INVITED**

How can boron-rich nanocrystalline films be optimized to meet the stringent mechanical demands of extreme environment applications?

Modern advances in clean energy, hypersonic travel, and nuclear technologies place extraordinary demands on materials' thermal and mechanical durability. High-stakes fields, such as aerospace and space exploration, require materials that withstand extreme conditions, often exceeding 4,000 °C, with substantial mechanical strength and oxidation resistance. Refractory materials like ultra-high temperature ceramics (UHTCs), while promising, are limited by high production costs and challenging synthesis processes. This study seeks to address this challenge by exploring nanoscale metal boride materials—specifically, strontium hexaboride (SrB6) nanocrystals (NCs)—as a cost-effective, mechanically robust alternative.

Nanocrystals (NCs) offer unique advantages due to their high surface area, tunable crystallization, and the ability to form films with nanoscale precision, which is critical for enhancing mechanical properties in thin coatings. Here, we investigate the potential of surface-modified SrB6 NCs, blade-coated onto silicon and sapphire substrates, as a pioneering solution for boron-rich, super-hard thin films. Through ligand modification with BF4 and BI3, these NCs achieve distinct structural formations on different substrates, significantly impacting their mechanical performance.

Our findings demonstrate that SrB6-BI3 films on silicon reach up to 10 GPa hardness and a Young's modulus between 180 and 200 GPa. In comparison, SrB6-BF4 films attain 5 GPa hardness and 170 GPa modulus on silicon, with a notably higher modulus of 300 GPa on sapphire, suggesting enhanced stiffness through substrate optimization. Atomic force microscopy (AFM) revealed crystallization patterns where SrB6-BI3 formed micron-sized crystals on silicon, while SrB6-BF4 created spherical clusters, further affecting mechanical properties.

This study highlights that by optimizing ligand choice, substrate selection, and minimizing defects, boron-rich metal boride nanomaterials can be tailored for demanding applications. These findings position SrB6 NC-based films as a promising, cost-efficient alternative to conventional super-hard materials like diamond, with potential breakthroughs in extreme environment applications.

11:40am **MA5-1-WeA-12 Dos and Don'Ts When Performing Theoretical Predictions for Identification of Stable Metal-Boride Materials (MAN Phases)***, **Martin Dahlqvist [martin.dahlqvist@liu.se]**,* Linköping University, IFM, Materials Design Division, Sweden

The number of atomically laminated boron-based materials (MAB phases) have grown significantly since their discovery in the 1960s and in the last decade we have seen the realization of their two-dimensional derivatives, boridene. MAB phases are versatile in terms of chemical composition, which facilitate controlled and tailored properties. Widening and enhancement of these materials requires an enlarged palette of compositions. Alloying through the addition of elements is one way for expanding the compositional space of MAB phases and, in turn, their attainable properties. This has traditionally been realized through solid solutions upon metal alloying and recently through the formation of chemically ordered metal layers. This is where theory can be used for accelerating the exploration of next-generation MAB phases. It will be demonstrated how predicted stability can be used to identify the most promising novel material candidates to be used as guidance for synthesis experiments. The importance of considering both chemically ordered structures and disordered solid solutions for reliable predictions will also be discussed. is required. Results will cover ternary and quaternary MAB phases, the latter with metal disorder and order (in-plane *i*-MAB and out-of-plane *o*-MAB).

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