

Protective and High-temperature Coatings Room Town & Country D - Session MA4-2-TuM

Boron-containing Coatings II

Moderators: Martin Dahlqvist, Linköping University, Sweden, Anna Hirle, TU Wien, Austria

8:00am MA4-2-TuM-1 Tuning Structure and Mechanical Properties of TaB_x

Films using HiPIMS, Kateryna Smyrnova
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Both experimental and theoretical studies have reported TaB_x to be promising for high-temperature and wear-resistant applications due to its exceptional hardness and oxidation resistance. However, achieving dense, nanocrystalline TaB_x with controlled stoichiometry remains a challenging task. To date, TaB_x films have been deposited only by conventional magnetron sputtering and high target utilization sputtering. This study demonstrates the pressure-controlled structure transformation of TaB_x films deposited by HiPIMS.

TaB_x coatings were deposited from a TaB₂ target in an Ar atmosphere at 340 °C using HiPIMS. Three groups of films were grown under three pressures (0.3 – 0.9 Pa) and two substrate bias conditions. The target current density was maintained at 1 A/cm² by adjusting the pulse frequency. The microstructure was analyzed using XRD and TEM. TaB_x films exhibited an amorphous structure at low pressure, a nanocomposite nature at moderate pressure, and a dense nanocrystalline structure at high pressure. This work presents the first systematic investigation into how energy flux controlled by pressure influences phase evolution in TaB_x deposited by HiPIMS. Cross-sectional SEM confirmed uniform thicknesses and sufficient adhesion. The chemical composition, as determined by WDS, showed that the B/Ta ratios rose from 1.05 to 1.4. This might be attributed to the reduced resputtering of B by thermalized reflected Ar neutrals at higher pressure. The nanoindentation method yielded a nanohardness of 26.2 GPa and Young's modulus of 344.6 GPa for amorphous films, improving to 42.4 GPa and 469.8 GPa for nanocrystalline ones. Fracture toughness (K_{IC}) was also determined by cantilever fracture testing in SEM.

These results establish working pressure in HiPIMS as a powerful parameter for controlling the crystallinity, stoichiometry, and mechanical properties of refractory borides. This study clarifies how changes in microstructure affect the densification and hardening of boron-rich films. The demonstrated ability to obtain dense, hard, and tough TaB_x films by HiPIMS highlights its potential for preparing next-generation materials for extreme environments. This work was funded by the Slovak Research and Development (No. APVV-24-0038) and the European Union under grant agreement No. 101158464 (COLOSSE).

8:20am MA4-2-TuM-2 Solid Self-Lubrication Mechanism of B₂O₃ in Boride Based Thin Film Materials Under Various Atmospheres, Daniel Pözlberger

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Transition metal borides (TMBs) represent a highly promising family of materials for functional coatings due to their abundance, cost-effectiveness, and exceptional mechanical properties. These include a high melting point, hardness of up to 60 GPa, excellent chemical and thermal conductivity, and outstanding resistance to wear. Their distinct self-lubricating behavior arises from the formation of boron oxide, which reduces friction, although the fundamental mechanisms behind this tribo-reaction remain not fully understood, particularly for TMB-based thin films. Temperature and atmosphere play a significant role in boron oxide formation, making it essential to understand the oxidation behavior of physical vapor-deposited boride based films to interpret their friction and wear performance at elevated temperatures. Tribological tests reveal that

sputter-deposited super-stoichiometric TiB_{2.9} exhibits a significantly lower friction coefficient (~0.3) than sub-stoichiometric TiB_{1.5} (~0.4) at 500°C, attributed to the higher oxidation rate of TiB_{2.9} and the presence of B-rich tissue phases at column boundaries. Similarly, α-WB_{2+z} coatings display self-lubrication via boron oxide formation, although growth related sub-stoichiometry limits boron availability during oxidation. The surrounding atmosphere further influences friction behavior: in oxygen-depleted conditions, oxidation and lubrication are minimal, whereas under humid conditions, water vapor reacts with boron oxide to form boric acid with layered, lubricious properties. To investigate these processes, we conducted ex-situ and in-situ oxidation studies of the TMB based thin films using elastic backscattering spectrometry (EBS) over a temperature range from room temperature to 940°C. The oxidation data, correlated with tribological, X-ray photoelectron spectroscopy, X-ray diffraction, and transmission electron microscopy analyses, provide new insights into the temperature-dependent lubrication mechanisms of boron oxide in TMB thin films.

8:40am MA4-2-TuM-3 Super-Ordered MAB Phases: Theoretical Design of Novel Boron-Containing Materials with Simultaneous in-Plane and Out-of-Plane Chemical Ordering, Martin Dahlqvist [martin.dahlqvist@liu.se], Johanna Rosen, Materials Design Division, Linköping University, Sweden

Chemical ordering in layered materials, such as MAX and MAB phases, enables precise tailoring of functional properties through structural motifs like in-plane (*i*-MAB, *i*-MAX) and out-of-plane (*o*-MAB, *o*-MAX) configurations. This study introduces super-ordered MAB phases (*s*-MAB), a novel structural material combining simultaneous in-plane and out-of-plane chemical ordering, previously unreported in synthesized MAB phases. Using first-principles density functional theory, we systematically investigated the thermodynamic stability of hypothetical quinary *s*-MAB phases with 314 (M₁M₂M₃M₃Al₃B₁₂) and 416 (M₁M₂M₃M₃Al₃B₁₈) compositions (M₁, M₃ = transition metals; M₂ = Sc, Y) against a comprehensive set of competing phases, including ternary and quaternary MABs, disordered configurations, and binary/ternary borides at 2000 K. Our calculations predict 27 thermodynamically stable *s*-MAB compositions, predominantly featuring M₁ = Cr, Mo, W, Mn, Fe and M₃ = V, Nb, Ta, with M₂ = Sc or Y promoting the combined in-plane and out-of-plane order. Notably, 416 structures exhibit conditions favoring partial or complete disorder, highlighting the nuanced stability landscape. These *s*-MAB phases offer a theoretical roadmap for synthesizing novel boron-containing compounds with precisely controlled atomic arrangements, potentially yielding unique mechanical, thermal, and electronic properties. Additionally, stable *s*-MABs can serve as precursors for 2D boridene (MBene) synthesis, expanding compositional flexibility for property tuning compared to existing boridenes. This work establishes a framework for designing advanced boride-based materials, with implications for high-temperature coatings, structural components, and electronic devices. Future experimental efforts should prioritize optimizing synthesis conditions to validate predicted chemical ordering and explore application-driven property enhancements.

Author Index

Bold page numbers indicate presenter

— D —

Dahlqvist, Martin: MA4-2-TuM-3, **1**

— G —

Gachot, Carsten: MA4-2-TuM-2, **1**

— H —

Hahn, Rainer: MA4-2-TuM-1, **1**; MA4-2-TuM-2, **1**

— K —

Kutrowatz, Philip: MA4-2-TuM-2, **1**

— M —

Mikula, Marián: MA4-2-TuM-1, **1**

— N —

Ntemou, Eleni: MA4-2-TuM-2, **1**

— P —

Pözlberger, Daniel: MA4-2-TuM-2, **1**

Primetzhofer, Daniel: MA4-2-TuM-2, **1**

— R —

Riedl, Helmut: MA4-2-TuM-1, **1**; MA4-2-TuM-2, **1**

Roch, Tomáš: MA4-2-TuM-1, **1**

Rosen, Johanna: MA4-2-TuM-3, **1**

— S —

Salvadores Farran, Norma: MA4-2-TuM-2, **1**

Satrapinsky, Leonid: MA4-2-TuM-1, **1**

Smyrnova, Kateryna: MA4-2-TuM-1, **1**

Šroba, Viktor: MA4-2-TuM-1, **1**

Švec, Peter: MA4-2-TuM-1, **1**

— T —

Truchlý, Martin: MA4-2-TuM-1, **1**

— W —

Wojcik, Tomasz: MA4-2-TuM-2, **1**