Department of Materials Science and Engineering,

PhD Defense

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MEM Seminar Room

Synthesis and Characterization of the MAB Phases: Ternary, Nanolayered Transition Metal Borides

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Abstract

The MAB phases are atomically laminated, ternary transition metal borides whose crystal structures are comprised of stacked M-B layers (M = transition metal; B = boron) interleaved by monolayers of Al or Zn, or bilayers of Al atoms. This name stems from the fact that their layered atomic structures resemble those of the nanolaminated MAX phases. Structurally, the MAB phases are anisotropic because the M-B layers contain parallel, covalently-bonded B-B chains and the M-B layers themselves are separated by relatively weaker M-Al bonds. Though nearly all the MAB phase compounds were discovered prior to the 1990s, their properties had remained largely unknown, in part, because of the unavailability of bulk, high purity, polycrystalline samples.

In this thesis, three MAB phases are synthesized to full density and five as powders using reactive powder metallurgy. The ultimate goal was to systematically characterize their physical properties. Some

of these compounds were synthesized in bulk for the first time, while many of their properties were never characterized for polycrystalline samples.

The MAB phases MoAlB, Mn_2AlB_2, and Fe_2AlB_2, like their binary boride counterparts, are found to be good conductors of electricity (0.3-5 $\mu\Omega$m) and highly dependent on the nature of the M atoms. From low-temperature heat capacity studies, the high conductivities are found to be related to the high densities of states at the Fermi level. In turn, the high electrical conductivity of MoAlB translates to good thermal conductivities (28 $Wm^{-1}K^{-1}$ at room temperature), wherein a majority of the heat is transported by electrons. In terms of the elastic properties, the Young's and shear moduli ranged from 250-370 GPa and 100-150 GPa, respectively, and showed weak temperature dependencies up to 1000 ^{o}C. The hardness of these three MAB phases ranged between 8-11 GPa and illustrate that they are significantly softer than their structurally analogous binary monoborides counterparts, whose hardness falls in the 16-23 GPa range. From an in-depth study of the thermal oxidation of MoAlB in ambient air, it was clear that it is the first transition metal boride compound to be highly oxidation resistant and performs comparably to other state-of-the-art alumina-forming alloys and compounds.

Because the unidirectional B-B chains and the face-sharing BM_6 trigonal prism building blocks in the MAB phases are also characteristic of the binary transition metal monoborides, this work endeavored to gain insights on how the Al layers distinguish these two families of solids. The weakly bonded nature of the Al layers was evidenced in several ways: (1) the thermal decomposition of the MAB phases into the corresponding MB phase and elemental Al at high temperatures, (2) the formation of protective aluminum oxide scales on MoAlB when heated in ambient air to high temperatures, (3) considerably lower Vickers

hardness and elastic moduli than the corresponding binary borides, and (4) intra-grain delaminations along basal planes during indentation.

However, there are similarities between the two as well. Both the binary monoborides and MAB phases of the 3d transition metals were found to have their lowest thermal expansion coefficients parallel to the covalently-bonded B-B chains, reflecting their high strengths. Moreover, both Cr_2AlB_2 and Cr_3AlB_4, exhibited Pauli-like paramagnetic behavior, like their CrB and Cr_3B_4 counterparts, and indicated that inserting Al layers into the binaries did not alter the magnetic ground states.