SYMM 1: Magic MAX Phases: Self-healing, Magnetism and the next best Graphene

Time: Thursday 9:30–12:30 Location: H 0105

Invited Talk SYMM 1.1 Thu 9:30 H 0105

From MAX to MXene - From 3D to 2D — •Michel Barsoum — Dept. of Materials Science and Engineering, Drexel University, Philadelphia, PA, USA

By now it is well-established that the layered, hexagonal carbides and nitrides with the general formula, Mn+1AXn, (MAX) where n = 1 to 3, M is an early transition metal, A is an A-group (mostly IIIA and IVA) element and X is either C and/or N * sometimes referred to as polycrystalline nanolaminates because every basal plane is a potential deformation or delamination plane - combine some of the best attributes of metals and ceramics. In the first part of this talk, the MAX phases and their physical and mechanical properties will be reviewed.

More recently we have shown that by simply placing MAX phase powders at room temperature in HF, the A-layers are selectively etched to produce 2D materials that we labeled MXenes to emphasize the loss of the A-group element and their similarities to graphene. Unlike hydrophobic graphene, MXenes are hydrophilic that behave as *conductive clays*, a hitherto unknown combination. MXenes such as Ti2C, V2C, Nb2C and Ti3C2 can be used as electrode materials in high power lithium-ion batteries and supercapacitors. Recently volumetric capacitances of $>$ 900 F/cm3 were obtained. The potential of using MXenes in energy storage and other applications will be highlighted.

Invited Talk SYMM 1.2 Thu 10:15 H 0105

Structure evolution during low temperature growth of nanolaminate thin films — •J.M. Schneider, L. Shang, H. Bolvardi, Y. Jiang, A. Al Gaban, D. Music, and M. to Baben — Materials Chemistry, RWTH Aachen University, D-52074 Aachen

V*Al*C, Cr-Al-C, Ti-Al-C and Mo-B-C and thin films were deposited by magnetron sputtering. The formation temperatures for V2AlC and Cr2AlC during sputter deposition are compared to the amorphous * crystalline transition temperatures in these material systems. The transition temperatures are determined by DSC and XRD. Based on the significantly lower synthesis temperature for Cr2AlC and V2AlC during vapor phase condensation compared to the bulk diffusion mediated amorphous * crystalline transition temperatures surface diffusion is identified as the atomic scale mechanism enabling the low temperature synthesis of MAX phase thin films. This notion is consistent with the phase formation data obtained utilizing HPPMS where the formation of nano-crystalline V2AlC MAX phase is observed in a (V,Al)2Cx matrix. An ion energy flux of $>$5.7 times of the conventional DC magnetron sputtering flux was identified to be prerequisite for V2AlC MAX phase formation. Based on these findings a low temperature synthesis strategy for Mo2BC was compiled. The data underline the potential of HPPMS for the low temperature synthesis of thin film nanolaminates.

15 min break

Invited Talk SYMM 1.3 Thu 11:00 H 0105

Autonomous healing of crack damage in MAX phase ceramics — •Willem G. Sloof — Delft University of Technology, Department of Materials Science and Engineering, Delft, The Netherlands

MAX phase ceramics, atomically layered ternary carbides and nitrides, have a range of advantageous properties that make them attractive candidates for high temperature applications, where the material is exposed to thermal cycles, mechanical loading and oxidation. In some MAX phases crack damage generated during service can be healed autonomously and multiple times. The healing is due to the formation of a stable, well-adhering oxide with a high relative volume expansion and having mechanical properties close to those of the matrix. The MAX phases that exhibit autonomous healing will be identified. The sealing of cracks and recovery of strength will be presented.

Invited Talk SYMM 1.4 Thu 11:30 H 0105

Magnetic MAX phases from first principles and thin film synthesis — •Johanna Rosen — Department of Physics, Chemistry and Biology (IFM), Linköping University, Linköping, Sweden

Inherently layered magnetic materials, such as magnetic MAX phases, offer an intriguing perspective for use in spintronics applications and as ideal model systems for fundamental studies of complex magnetic phenomena. These phases were discovered from an approach based on predictions from theoretical procedures in combination with thin film synthesis and characterization. Using density functional theory and evaluation of phase stability, the first magnetic MAX phases were obtained from alloying Cr2AlC, Cr2GeC, and Cr2GaC with Mn. The materials were synthesized as heteroepitaxial thin films, and were found to have a variety of magnetic properties, including a displayed ferromagnetic response well above room temperature. Advancing beyond alloying, the more recently discovered magnetic Mn2GaC MAX phase displays pronounced structural changes linked to the magnetic anisotropy, and a rich magnetic phase diagram which can be manipulated through temperature and magnetic field. These results indicate that the magnetic state can be directly controlled by an applied pressure or through the introduction of stress. Ongoing research expand the family of magnetic MAX phases, and the different isostructural compositions suggest that they can be combined in a variety of heterostructures, thus making them ideal for the study of the complex magnetism that occur in layered materials.

Invited Talk SYMM 1.5 Thu 12:00 H 0105

Weak Field Magneto-Transport Properties of Mn+1AXn Phases — •Thierry Ouisse[1], Lu Shi[1], Benoit Hackens[3], Benjamin Piot[2], and Didier Chaussende[1] — [1]Univ. Grenoble Alpes, LMGP, F-38000 Grenoble, France and CNRS, LMGP, F-38000 Grenoble, France — [2]LNCMI, CNRS, France — [3]IMCN/NAPS, Université Catholique de Louvain,Louvain-la-Neuve, Belgium

After a review of the published data and open issues about the electronic transport properties of polycristalline MAX phase materials, we focus on single crystals. For such nanolamellar compounds, it is expected that the structural anisotropies result in quite particular transport properties. We propose a general, yet simple model for explaining the weak field magneto-transport properties of the MAX phases in their crystalline form. The relevance of this model is then supported by elementary considerations, analytical computations and a set of experimental data obtained from single crystals of V2AlC and Cr2AlC as a function of temperature and magnetic field, both in the basal plane and along the c-axis.