MM 23: Topical Session: Combinatorial Materials Science II

Time: Tuesday 11:45–13:00 Location: H25

Topical Talk MM 23.1 Tue 11:45 H25

A combinatorial materials science approach to the development of new functional thin film materials — •Ulf Jansson[1], Fang Mao[1], Tomas Nyberg[2], Urban Wiklund[2], and Mattias Klintenberg[3] — [1]Department of Chemistry-Ångström, Uppsala University, Sweden — [2]Department of Engineering Science, Uppsala University, Sweden — [3]Department of Physics and Astronomy, Uppsala University, Sweden

Combinatorial materials science (CMS) enables a rapid discovery of new materials for various applications. Compared with conventional methods, CMS is a powerful tool for time-saving development of new materials. This paper will present a platform for CMS including rapid methods for theoretical modelling, sputtering of gradient films, analysis equipment as well as tools to evaluate mechanical, tribological and electrical properties.

Two examples of screening for new materials will be presented. The first is rapid theoretical screening of M-B-C materials (M=early transition metal) for wear-resistant coatings where new phases based on e.g. tungsten give improved properties. The other example is sliding electrical contacts which must combine low resistivity and contact resistance with low wear rate and friction and high corrosion resistance, a combination of properties which is very difficult to meet simultaneously. We have initiated studies of Ag-based alloys, Ag-M-X, (M and X = selected metals and nonmetals) and with CMS demonstrated that addition of Al together with other metals can increase hardness and reduce friction but still maintain good electric properties.

MM 23.2 Tue 12:15 H25

Polyhedron-based structure maps for pd-bonded systems — •Arthur Bialon, Thomas Hammerschmidt, and Ralf Drautz — ICAMS, Ruhr-Universität Bochum, Germany

Structure maps are an approach to identify the governing factors that determine whether a mixture of elements will form a compound and which crystal structure is to be expected. Here, we present new structure maps for the pd-bonded systems that are footed on databases of experimentally observed structures. Our new structure maps depend on atomic properties and on the local environment of the crystallographic Wyckoff sites. The latter is determined by a polyhedron analysis that decomposes the atomic environment into corresponding coordination polyhedra. This enables us to identify trends in the favorite coordination number and relationships between the global compound and the local coordination polyhedron composition for the p-block elements. The information from the polyhedron analysis enters the order parameters that represent the axes of the structure maps. As a result, we find very good separation between different crystal structures. The chosen order parameters are also able to account for fractionally occupied Wyckoff sites.

MM 23.3 Tue 12:30 H25

Oxygen Incorporation in Cr2AlC Investigated by Combinatorial Thin Film Synthesis and X-Ray Stress Analysis — •Lin Shang, Moritz to Baben, Jens Emmerlich, and Jochen M. Schneider — Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany

The oxygen incorporation in Cr2AlC was studied by combinatorial thin film synthesis. Thin films with chemical concentration gradient were deposited by DC magnetron sputtering from elemental targets, and oxygen was intentionally introduced. Ab initio calculation results indicate that oxygen is incorporated interstitially in the Al layer of Cr2AlC, even for carbon-deficient Cr2AlC. Two phase-regions of Cr2AlC and Cr2Al were investigated in order to study oxygen incorporation in carbon-deficient Cr2AlC. X-ray stress analysis data indicate that the a and c lattice parameters increase with increasing oxygen content. These trends are in good agreement with the change in lattice parameters predicted by ab initio calculations and therefore corroborates the notion of interstitial oxygen incorporation in Cr2AlC. A metastable solubility limit for oxygen of 3.5 at% was determined. This is the first report on interstitial oxygen incorporation in MAX phases and may be of relevance to the initial stages of oxidation.

MM 23.4 Tue 12:45 H25

Ab initio study of single-crystalline and polycrystalline elastic properties of Mg-substituted calcite crystals — Li-Fang Zhu[1], •Martin Friak[1], Helge Fabritius[1], Pavlina Hemzalova[1], Andreas Ziegler[2], Svetoslav Nikolov[3], Anna Janus[1], Dierk Raabe[1], and Joerg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]University of Ulm, Ulm, Germany — [3]Bulgarian Academy of Sciences, Sofia, Bulgaria

We employ ab initio calculations and investigate the single-crystalline elastic properties of (Ca,Mg)CO_3 crystals covering the whole range of concentrations from pure calcite $CaCO_3$ to pure magnesite $MgCO_3$. Studying different distributions of Ca and Mg atoms, our theoretical results show that the energetically most favorable configurations are characterized by elastic constants that nearly monotonously increase with the Mg content. Based on the first principles derived single-crystalline elastic anisotropy, the integral elastic response of (Ca,Mg)CO_3 polycrystals is determined employing a mean-field self-consistent homogenization method. As in case of single-crystalline elastic properties, the computed polycrystalline elastic parameters sensitively depend on the chemical composition and show a significant stiffening impact of Mg atoms on calcite crystals in agreement with experimental findings.