MM 27: Topical Session: Combinatorial Materials Science III

Time: Tuesday 15:00–16:00 Location: H25

Topical Talk MM 27.1 Tue 15:00 H25

Bulk Combinatorial Design of nanostructured steels: from composition to mechanisms — Hauke Springer, Ivan Gutierrez-Urrutia, Jae-Bok Seol, Tilmann Hickel, Martin Friak, Jörg Neugebauer, and •Dierk Raabe — Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany

We present an approach to the high-throughput synthesis of bulk nanostructured steels including the variation of composition and thermomechanical processing. This method, referred to as Rapid Alloy Prototyping (RAP), uses semi-continuous high-throughput casting, rolling, heat treatment and sample preparation. The method is demonstrated on a group of Fe-30Mn-1.2C- x Al steels which exhibits a wide spectrum of structural and mechanical characteristics, depending on the respective Al concentration: High amounts of Al additions ($>$ 8 wt.%) resulted in pronounced strengthening, while low concentrations ($<$ 2 wt.%) led to embrittlement of the material during aging. Of specific interest is the formation and high thermal stability of nanoscaled (5-50 nm) kappa - carbides (L1'2). These precipitates appear in the high Al containing alloy variants (e.g. 8%Al) in the form of highly ordered and coherent particles that have nano-sized solid-solution channels between them. Atom probe analysis and electron microscopy (TEM, ECCI) is conducted to better understand the interaction between these nano-precipitates and dislocations. The stability of the kappa carbides and corresponding compositional trends are also studied using ab initio methods.

Topical Talk MM 27.2 Tue 15:30 H25

Combinatorics of RuO2 based thermoelectrics — •Denis Music, Felix Basse, and Jochen Schneider — Materials Chemistry, RWTH Aachen University, Kopernikusstr. 10, 52074 Aachen, Germany

RuO2 (P42/mnm, rutile) exhibits interesting transport properties, such as low resistivity, as well as large thermal and chemical stability. It is a promising candidate for thermoelectric devices. The quantum mechanically guided design proposal is based on identifying suitable alloying elements for RuO2 to improve the transport properties and phase stability thereof. Using ab initio calculations, we probed all 4d transition metals and identified Nb and Y to be the best choice. Based on this design proposal, Nb and Y alloyed RuO2 thin films were grown by combinatorial reactive sputtering. Nb and Y can be incorporated in the rutile structure. Nanorods were formed and Nb2O5/Y2O3 coordination appears at increased alloying contents. This may be understood based on our ab initio molecular dynamics data. Surface coarsening on the atomic scale occurs due to O crosslinking of two neighboring Nb-O/Y-O units. Hence, it is reasonable to assume that these units contribute towards the experimentally observed formation of nanorods. Further alloying elements and their influence on structure evolution and transport properties will also be discussed.