MM 41: Materials design I

Time: Friday 11:00–12:00 Location: H16

MM 41.1 Fri 11:00 H16

A texture component model for predicting recrystallization textures — •Abhijit Brahme, Myrjam Winning, and Dierk Raabe — Max Planck Institute for steel Research, Max-Planck Str. 1 Duesseldorf 40237

We present an analytical model for predicting crystallographic textures and the final grain size during primary static recrystallization of metals using texture components. The model uses a subset of texture components instead of using the entire set of orientations needed to represent the material. The recrystallization kinetics and the texture evolution are governed by the tensorial variant of the Johnson-Mehl-Avrami-Kolmogorov (JMAK) equation. The number of components determines the order of this tensor. Each entry in the tensors represents coupling between the recrystallizing and the deformed components. The growth of a recrystallizing component in to a given deformed component is dependent on various factors like activation energy of nucleation, activation energy for boundary mobility and stored energy (in the deformed region). Main aim of this work is to present a fast and physically based process for simulation of recrystallization texture with respect to processing. We also present preliminary results of application of this method to low carbon steels.

MM 41.2 Fri 11:15 H16

Ab initio calculation of free energies and thermodynamic properties of fcc metals — •Blazej Grabowski, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Deutschland

Phase diagrams are indispensable tools in predicting material evolution during its processing. Current approaches to obtain such phase diagrams (e.g. CALPHAD) are based on an extra- and/or interpolation of experimental data. A crucial issue hampering this approach is the lack/high cost of specific experimental data (e.g. for unstable/metastable phases). For such cases, the replacement of experimental data by ab initio calculations is desirable.

The accuracy of density-functional based ab initio methods is, in principle, only limited by the exchange-correlation (XC) functional. We have therefore evaluated the accuracy of the most commonly used functionals (LDA, GGA) by calculating key thermodynamic properties for a large set of metals (Al, Pb, Cu, Ag, Au, Pd, Pt, Rh, Ir). Great care was taken to ensure that convergence errors due to supercell size, k-point sampling, and energy cutoff are small compared to the error in the XC-functional. Based on the volume and temperature dependence of free energies calculated in the quasiharmonic approximation, thermodynamic quantities such as the thermal expansion or the heat capacity have been derived. The comparison to experiment yields an excellent agreement. A detailed analysis shows that the LDA/GGA results can typically be considered as error bars allowing to estimate the accuracy of the calculation in the absence of experiments.

MM 41.3 Fri 11:30 H16

Thermodynamische Berechnung von Pt-Basis-Legierungen — •Johannes Preussner, Rainer Völkl und Uwe Glatzel — Metallische Werkstoffe, Universität Bayreuth, Ludwig-Thoma-Str. 36b, 95447 Bayreuth

Platinbasislegierungen besitzen einen hohen Widerstand gegen korrosive Medien und gute mechanische Eigenschaften bei hohen Temperaturen. Durch eine geeignete Wahl an Legierungselementen und Wärmebehandlungsparametern kann eine den Nickelbasissuperlegierungen ähnliche Mikrostruktur eingestellt werden: in einer duktilen, Pt-reichen fcc-Matrix lassen sich feine $L1_2$ geordnete Pt_3Al Phasen ausscheiden. Das Legierungssystem Pt-Al-Cr-Ni hat sich dabei als sehr aussichtsreich erwiesen. Die Legierungsentwicklung wird durch thermodynamische Simulation unterstützt, um Vorhersagen über die Phasenbildung treffen zu können. Mit Hilfe von gezielten Experimenten (EDS, XRD) kann die Ausdehnung von Phasenregionen bestimmt werden. Ab-Initio Berechnungen geben hilfreiche Informationen über die Bildungsenthalpien einzelner Phasen. Diese Daten werden zusammen mit Literaturwerten dazu verwendet um die Gibbs-Energien $G(x,T)$ der einzelnen Phasen in Abhängigkeit von der Konzentration der Legierungselemente und der Temperatur zu bestimmen. Besonderes Augenmerk wird dabei auf die Pt-reiche Seite gelegt, da hier die Ordnungsreaktionen zu $L1_2$ stattfinden. Im Rahmen des Vortrags wird insbesondere die Thermodynamik des Systems Cr-Ni-Pt dargelegt.

MM 41.4 Fri 11:45 H16

Theory-guided design of Ti-based binaries for human implants — •Martin Friák[1], Jörg Neugebauer[1], Benedikt Sander[2], and Dierk Raabe[2] — [1]Department of Computational Materials Design, Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany — [2]Department of Microstructure Physics and Metal Forming, Max-Planck-Institut für Eisenforschung, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

The improvement of hip transplants is severely hampered by the lack of suitable materials which are biocompatible in terms of non-toxicity and mechanical properties matched to the bone. The aim of our research has been therefore to identify metallurgical trends for non-poisonous Ti-based alloys employing quantum-mechanical calculations. Specifically, density functional theory (DFT), a plane wave basis set and PAW pseudopotentials have been used. As a first step the thermodynamic stability of Ti-Mo and Ti-Nb binaries has been determined. Second, the Young modulus of the thermodynamically stable alloys has been calculated and an alloy composition that maximally matches human bone has been selected. Guided by the theoretical calculations of phase stability and elastic properties, selected binaries were actually melted, cast, and heat treated to a homogeneous state. The samples have been experimentally characterized by x-ray methods, electron microscopy including crystallographic and chemical analysis, and mechanically tested using ultrasound measurements. The experimental data obtained in these experiments are in excellent agreement with the theoretical predictions.