MM 26: Topical Session: Data Driven Materials Science - Machine Learning for Materials Properties

Time: Tuesday 14:15–15:30 Location: BAR 205

MM 26.1 Tue 14:15 BAR 205

From Atom Probe Tomography to CALPHAD modeling: Estimating T_c from local concentration fluctuations — •Marvin Poul, Sebastian Eich, and Guido Schmitz — Universität Stuttgart, Stuttgart, Germany

One way to determine the extent of the miscibility gap and the associated critical solution temperature T_c in binary alloys from Atom Probe Tomography (APT) is to prepare nano-layer stacks, anneal them and determine the respective layer concentrations, which mark the boundaries in the phase diagram. Since this relies on diffusion, it can be problematic when T_c and atomic mobilities are low, such as in Cu/Ni, leading to long annealing times.

This work proposes a novel methodology based on statistical mechanics to extract T_c from histograms of thermodynamically inherent local concentration fluctuations annealed above T_c, i.e. in the region of complete miscibility. The same formalism allows to extract relative chemical potential differences from two or more samples with different mean concentration. Given enough data to span the full concentration range it is even possible to non-parametrically recover the excess free energy of mixing $g_{ex}(c)$, which allows a direct approach to a CALPHAD parametrization.

The approach is benchmarked using Embedded Atom Monte Carlo simulations of Cu/Ni and applicability to experimental histograms from APT is discussed.

MM 26.2 Tue 14:30 BAR 205

Analysis of magnetic properties in the Fe-Si system using first principles calculations — •Matteo Rinaldi, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany

Magnetic steels containing small amounts of silicon have been used extensively as soft magnetic materials in various technological applications. The behavior of magnetic materials can be simulated at the macroscale using a micromagnetic model whose key parameters, such as exchange stiffness constants and magnetic anisotropies can be derived from first-principles electronic structure calculations. In our work, we employ Korringa-Kohn-Rostoker (KKR) Green's function calculations together with a Wannier-based tight-binding (TB) method to investigate the dependence of the spin-wave stiffness and the first coefficient of the cubic magneto-crystalline anisotropy on the Si concentration. These two methodologies give a chemical and structural description of the changes in the micromagnetic parameters caused by the addition of Si. The KKR method is used in conjunction with the Coherent Potential Approximation to simulate chemical disorder while the TB method addresses local relaxations induced by the presence of Si in a supercell framework. The role played by the hybridization between the Si and Fe orbitals turned out be decisive to explain the trends in the micromagnetic parameters. Our calculated values are in excellent agreement with available experimental data.

MM 26.3 Tue 14:45 BAR 205

Machine learning modeling of magnetic ground state and Curie temperature — •Teng Long, Nuno Fortunato, Yixuan Zhang, Oliver Gutfleisch, and Hongbin Zhang — Institute of Materials Science, Technical University of Darmstadt, Darmstadt 64287, Germany

Magnetic materials have a plethora of applications ranging from information and communication technologies to energy harvesting and conversion. However, their functionalities are often limited by the magnetic ordering temperature. In this work, we performed machine learning on the magnetic ground state and the Curie temperature (T_c), with generic chemical and crystal structural descriptors. Using 2805 known intermetallic compounds, a random forest model is trained to classify ferromagnetic and antiferromagnetic compounds and to predict the T_c of the ferromagnets, with only 15 and 23 descriptors used, respectively. The resulting accuracy is about 86% for classification and 92% for regression (with a mean absolute error (MAE) of 55K). We found that composition based features are sufficient for both classification and regression, whereas structural descriptors improve the performance. Using the trained model, we predicted the magnetic ordering and T_c for the intermetallic magnetic materials in the Materials Project, with a MAE of 73K in comparison to the experimental reported T_c that has been collected by us. This work paves the way to accelerate the discovery of new ferromagnetic compounds for technological applications.

MM 26.4 Tue 15:00 BAR 205

Automatization of magnetic properties calculation using AiiDA-FLEUR — •Vasily Tseplyaev, Jens Bröder, Daniel Wortmann, Markus Hoffmann, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Magnetic properties of thin films, e.g. magnetic anisotropy, Heisenberg exchange and Dzyaloshinskii-Moriya interaction constants define material quality for possible use in state-of-the art memory and other devices. These parameters can be determined via *ab initio* theory and the FLEUR [1] code. Together they provide precise simulations with the necessary predictive power. The current state of computational resources allows for high-throughput screening of materials, which means similar calculations are repeated for a large set of possible magnetic film structures that can be promising for further experimental study. Automated computing, data storage, provenance and thus reproducibility are provided by the open science platform AiiDA [2], when key-turn solutions for aforementioned magnetic calculations are implemented as AiiDA-FLEUR plugin. In this talk, we report the current state of AiiDA-FLEUR development, which covers the implemented architecture of general and magnetic workflows and other utilities.

We acknowledge the Center of Excellence MaX – Materials Science at the Exascale (EU H2020-INFRAEDI-2018) for financial support.

1. https://www.flapw.de
2. G. Pizzi *et al.*, Comp. Mat. Sci. **111**, 218 (2016).

MM 26.5 Tue 15:15 BAR 205

Screening impurity effects in topological insulators with the AiiDA-KKR plugin — •Philipp Rüssmann[1], Fabian Bertoldo[1,2], Phivos Mavropoulos[3], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Technical University of Denmark, Kgs. Lyngby, Denmark — [3]Physics Department, National and Kapodistrian University of Athens, Greece

The ability to utilize the predictive power of *ab initio* calculations through automated computing enables scanning of the material space with subsequent materials/properties optimization. We present the *AiiDA-KKR* plugin [1] which enables high-throughput calculations using the Jülich full-potential relativistic Korringa-Kohn-Rostoker Green function method (KKR) [2] to the AiiDA framework [3]. The KKR method allows, for instance, to calculate the electronic structure of defects embedded into crystalline solids. We applied this scheme to screen the effect of impurities in the strong topological insulator Sb_2Te_3. Several thousand impurities have been considered, taking into account both the distance of the impurity to the surface as well as the effect of possible changes in the host material's Fermi level. Our data reveals chemical trends relevant, for example, to transport properties in topological insulators. – We acknowledge the Center of Excellence MaX (EU H2020-INFRAEDI-2018) for financial support.

[1] https://github.com/JuDFTteam/aiida-kkr
[2] https://jukkr.fz-juelich.de
[3] G. Pizzi, *et al.*, Comp. Mat. Sci. **111**, 218-230 (2016).