

## MM 39: Phase Transformations: Simulation and Machine Learning

Time: Thursday 11:45–13:15

Location: SCH A 215

MM 39.1 Thu 11:45 SCH A 215

**Simultaneous structural and thermal characterisation of Zr-based bulk metallic glasses via synchrotron X-ray diffraction and fast differential scanning calorimetry** — ●ŠTEFAN T. STANKO<sup>1</sup>, JÜRGEN E.K. SCHAWÉ<sup>1,2</sup>, and JÖRG F. LÖFFLER<sup>1</sup> — <sup>1</sup>Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — <sup>2</sup>Mettler-Toledo GmbH, Analytical, 8606 Nänikon, Switzerland

Fast differential scanning calorimetry (FDSC) experiments were performed to measure time-temperature-transformation (TTT) diagrams of Zr-based bulk metallic glasses used for additive manufacturing. The alloys were measured in powder and bulk form, and multiple crystallisation events upon cooling were observed in both cases. The fast differential scanning calorimeter was modified to allow its integration into a synchrotron X-ray beamline and thus to characterise *in situ* metastable phase transformations. With the *in situ* setup it was possible to simultaneously investigate the structure of the phases involved and their transformation kinetics. The results were correlated with the oxygen content of the alloys, with the aim of optimising the additive manufacturing process of metallic parts.

MM 39.2 Thu 12:00 SCH A 215

**Measurement and simulation of cooling times in pump-probe experiments of phase transitions with latent heat** — ●DANIEL KAZENWADEL, NOEL NEATHERY, and PETER BAUM — Universität Konstanz, Konstanz, Germany

Ultrafast pump-probe experiments are often limited by the need to wait for a sample's back reaction to take place between adjacent laser pulses. Here we investigate by experiments and simulations how the sample geometry influences the cooling rate of VO<sub>2</sub>, a strongly correlated phase-transition material with substantial latent heat. We measure back reaction times of milliseconds, microseconds and nanoseconds in free-standing thin-films, coated substrates and bulk crystals, respectively. A simple latent heat model reproduces the behavior of all geometries and can therefore be used to predict the speed of the back reaction in other phase-change materials as well.

MM 39.3 Thu 12:15 SCH A 215

**Ab initio thermodynamics and atomistic modeling of NiTi SMA with machine learning interatomic potentials** — ●PRASHANTH SRINIVASAN and BLAZEJ GRABOWSKI — Institute for Materials Science, University of Stuttgart, Germany

Equiatomic Nickel-Titanium (NiTi) possesses interesting properties such as pseudoelasticity and shape memory effect that arise from a reversible transformation between the austenite (B2) and the martensite phase (B19'). Other competing phases (B19 and B33) make modeling of NiTi challenging. *Ab initio* molecular dynamics (AIMD) calculations have shown that B19' and B2 phases are entropically stabilized (Haskins et. al., 2016), but the calculations were restricted to a single DFT exchange correlational functional (XC). Studying the kinetics of phase transformation using only DFT is also severely expensive.

In this work, we address both challenges. Using a recently developed thermodynamic integration technique (Jung et. al., 2022) aided with machine-learning based moment tensor potentials (MTPs, Shapeev 2016), it is possible to efficiently compute high-temperature thermodynamic phase stability to DFT accuracy. We perform such calculations to analyze three different XCs (GGA, LDA and SCAN). We also perform large-scale molecular dynamics (MD) simulations using the MTPs to study the kinetically-driven phase transformation behavior in each of these cases. Preliminary results show the necessity of having a high *k*-point density in the underlying DFT calculations. When fitted to such a training set, the MTPs predict highly accurate thermodynamic

properties and phase transformation behavior.

MM 39.4 Thu 12:30 SCH A 215

**Prediction of quantum paraelectricity and quantum phase transitions using ab initio self-consistent lattice dynamics and machine learning** — ●QUINTIN MEIER<sup>1</sup>, AMBROISE VAN ROEKEGHEM<sup>2</sup>, and NATALIO MINGO<sup>2</sup> — <sup>1</sup>Université Grenoble Alpes, CNRS, Institut Neel, 25 Av. des Martyrs, 38042 Grenoble — <sup>2</sup>Université Grenoble Alpes, CEA, LITEN, 17 Rue des Martyrs, 38054 Grenoble, France

Anharmonic interactions of the lattice are essential for understanding the temperature-dependent behavior of many materials. Here we present a method combining DFT and the active learning of interatomic potentials to obtain the necessary sets of forces to calculate the temperature dependent force constants using the quantum self-consistent lattice dynamics formalism [1]. A particularly strong anharmonicity has been shown in incipient ferroelectrics like KTaO<sub>3</sub>. We show that our method can be used to accurately and efficiently compute the strongly anharmonic low temperature behaviour of the soft mode in quantum paraelectric KTaO<sub>3</sub>, and we study its stability range under pressure and uniaxial strain.

[1] Van Roekeghem, A et al, Comp. Phys. Commun, Vol 263 (2021)

MM 39.5 Thu 12:45 SCH A 215

**Atomic cluster expansion for modelling of transition metal carbide systems** — ●MINAAM QAMAR — ICAMS, Ruhr University Bochum, Bochum, Germany

Atomic cluster expansion (ACE) provides an alternative to classical and machine learning potentials by modelling the local environment of an atom with a mathematically complete descriptor. We present an ACE potential for the Mo-C system, which is parametrized over an exhaustive dataset of important phases and defect structures. The resulting ACE is shown to be accurate with respect to the DFT reference data and computationally efficient which allows us to perform large scale finite temperature applications.

MM 39.6 Thu 13:00 SCH A 215

**Structure-mapping workflow for the investigation of solid-solid phase transitions** — ●ARTEM SAMTSEVICH, CHRISTOPH SCHEURER, and KARSTEN REUTER — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Solid-solid transformations are common in nature and in the aging of functional materials. It is thus crucial to understand the origin of these complex phenomena at the atomistic level. The involved activated processes can be modeled as transitions between basins on a high-dimensional free energy landscape (FES). Using the harmonic approximation to transition state theory (hTST), one can estimate reaction rate constants from the location of saddle points on the FES. The chain-of-states method optimizes presumed pathways between two structural endpoints towards the minimum energy pathway (MEP), yielding transition state estimates. The generation of the initial pathway requires the mapping of atomic structures onto each other, which can be achieved either by purely geometrical methods (mapping of atomic positions and cells) or by the topology-based method, which maps the graphs of interatomic bonds. Both approaches are complementary to each other and generate a diverse set of mappings.

The combination of mapping algorithms with the chain-of-state method has recently been merged into a generalized workflow. We will present applications to phase transitions in high-energy-density and superhard materials [1,2] as well as catalyst aging.

[1] Wang, Y., Bykov, M., et al., Nat. Chem. 14, (2022).

[2] Kvashnin, A. G., Samtsevich A.I., Jetp Lett. 111, (2020).