MM 21: Microstructure and Phase Transformations I

Time: Tuesday 11:45–13:15 Location: H38

MM 21.1 Tue 11:45 H38

Undercooling behavior of the nucleation of liquid-liquid phase — •Christian Simon[1], Yikun Zhang[2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48155 Münster — [2]State Key Laboratory of Advanced Special Steels, Shanghai University, Shanghai, 200072, China

A wetting transition from partial wetting to complete wetting is possible in alloys with a liquid miscibility gap. At a temperature T_p below the critical temperature T_c, the alloy separates in a two-phase liquid system which plays an essential role in the microstructure formation of monotectic alloys. A thermal cycling in the liquid state allows observing the mixing and the demixing transition. This allows a monitoring of the statistical behavior of the phase transition temperatures over a large number of cycles. We present data of the copper-cobalt and the copper-iron system obtained by classical DTA experiments. The copper-cobalt and the copper-iron system have a metastable miscibility gap. The interest is here in the observation of the undercooling behavior. Thus, the dependence of the mixing and the demixing transition on processing parameters and cycle number including the undercooling behavior of the demixing transition can be investigated. This allows a new access to the nature of nucleation of the bimodal phase separation process.

MM 21.2 Tue 12:00 H38

Time-resolved investigation of the liquid-solid phase transitions in supercooled liquid Argon and Krypton — •Alexander Schottelius[1], Björn Beyersdorff[2], Tiberio Ezquerra[3], Stephan Roth[2], and Robert Grisenti[1] — [1]Universität Frankfurt, Frankfurt am Main, Germany — [2]Deutsches Elektronen Synchrotron (DESY), Hamburg, Germany — [3]Instituto de Estructura de la Materia CSIC, Madrid, Spain

We will present new experimental results imaging the crystallization process in the two Lennard-Jones liquids, Argon and Krypton, using Small Angle and Wide Angle X-Ray Scattering (SAXS and WAXS). The sample was provided by a strongly supercooled micro-liquid jet inside a low pressure environment at cooling rates of up to 10^8 K/s. Due to the fact that the axial distance of the jet to its source can be translated into time scale, we were able to obtain a full movie of the phase transition by X-Ray scattering. In particular, while most of the final solid samples displayed the expected fcc- crystal structure, the WAXS diffraction patterns provide evidence of a hcp- structured crystal fraction for both Systems, Argon and Krypton.

MM 21.3 Tue 12:15 H38

Microstructure development of aluminum based alloys in additive manufacturing revealed from differential fast scanning calorimetry and metallographic studies — •Bin Yang[1], Olaf Kessler[2], and Christoph Schick[1] — [1]Institute of Physics, University of Rostock, Rostock, Germany — [2]Faculty of Mechanical Engineering and Marine Technology, University of Rostock, Rostock, Germany

To obtain the desired additive manufacturing (AM) fabricated aluminum-based alloy parts, the rapid solidification processes need to be investigated in-situ. Based on the calorimetric method (differential fast scanning calorimetry) developed for the study of metal particles, the solidification process of aluminum-based alloy powder-particles, i.e. AlSi10Mg, was studied, for the very first time, under AM relevant heating and cooling rate conditions. A preliminary series of DFSC heating and cooling experiments was conducted, applying cooling rates as high as 80,000 K/s. The differential fast scanning calorimeter traces revealed that the material undergoes a two-stage melting and solidification processes depending on heating and cooling rates. In particular, the solidification structure of the real time quenched single droplet was observed and analyzed with focused ion beam (FIB), scanning electron microscopy (SEM) and high resolution transmission electron microscopy (HRTEM). This research proposed a new approach to research the solidification structure of single aluminum-based alloys particles used in AM technologies with precisely controlled size and extreme cooling rate.

MM 21.4 Tue 12:30 H38

Pressure-induced spin transition of Fe^{2+} in magnesio-siderite solid solution and siderite studied by x-ray Raman scattering — •Christopher Weis[1], Christian Sternemann[1], Max Wilke[2,3], Valerio Cerantola[4], Christoph J. Sahle[5], Georg Spiekermann[2,6], Yury Forov[1], Hendrik Rahmann[1], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, 44221 Dortmund, GER — [2]GeoForschungsZentrum(GFZ), 14473 Potsdam, GER — [3]Universität Potsdam, 14469 Potsdam, GER — [4]Bayerisches Geoinstitut, 95440 Bayreuth, GER — [5]ESRF, 38043 Grenoble Cedex 9, FRA — [6]DESY, 22607 Hamburg, GER

Owing to the low solubility of carbon in Earth mantle silicate phases, carbonate minerals may form as evidenced by inclusions found in diamonds formed in the Earth's mantle. Here, Siderite ($FeCO_3$) forms a complete solid solution with magnesite ($MgCO_3$). Pressure-induced high-spin (HS) to low-spin (LS) transitions of such carbonates at conditions of the inner Earth and the associated change of its magnetic properties largely influences the materials characteristics such as sound velocity and density. In contrast to diffraction experiments, high-pressure optical Raman studies found indication for the coexistence of HS and LS state in a transition range in siderite as well as in the solid solutions. We investigated the spin transition of a siderite and magnesio-siderite single crystal for pressures up to 50 GPa using diamond anvil cell by x-ray Raman scattering at the iron $M_{2,3}$-edge and $L_{2,3}$-edge. The course of the spin transition will be discussed and confronted with optical Raman, x-ray emission and Mössbauer studies.

MM 21.5 Tue 12:45 H38

Confocal Raman microscopy for noncontact and nondestructive characterization of carbon fibers — •Sergej Shashkov, Valery Kopachevsky, Alexander Gvozdev, and Alexander Grigorenko — SOL instruments LTD., Minsk, Belarus

Confocal Raman microscopy is a nondestructive technique in materials characterization that provides valuable structural information, and allows monitoring changes in molecular bond structure. In this paper,confocal Raman microscopy with high spatial resolution and high sensitivity has been used for carbon fiber research. We present Raman measurement results of several types of carbon fibers. The graphitization level of fibers has been estimated.

MM 21.6 Tue 13:00 H38

Anharmonic quantum nuclear vibrations and the stability of hexagonal ice — Edgar Engel, •Bartomeu Monserrat, and Richard Needs — TCM Group, Cavendish Laboratory, 19 JJ Thomson Avenue, Cambridge, CB3 0HE, UK

We use a recently developed vibrational self-consistent field approach in conjunction with first-principles density functional theory (DFT) calculations to calculate anharmonic quantum nuclear vibrations in the hexagonal and cubic forms of water ice. The very similar free energies of hexagonal and cubic have so far prevented even state-of-the-art first-principles quantum mechanical calculations using non-local DFT and quantum Monte Carlo methods from reproducing, let alone explaining, the stability of hexagonal ice. We show that, although the static lattice and harmonic vibrational energies are almost identical, anharmonic vibrations crucially stabilise hexagonal ice compared with cubic ice by at least 1.4 meV/H2O, in agreement with experimental estimates. The difference in anharmonicity arises predominantly from the difference in vibrational frequencies of the O-H bond stretching modes, which is in agreement with recent IR absorption measurements for stacking disordered ice. We account for proton-disorder and relate our results to recent IR absorption measurements for partially proton-ordered cubic ice. Moreover, we trace the difference in anharmonicity back to the difference in structure.