MS42-O2 Neutron Diffraction Studies of Gas Hydrates

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The gas hydrates are a group of compounds which are of wide importance. They are model systems for the study of interactions between water and other molecules and can thus provide fundamental insight into such interactions. Gas hydrates also provide a cheap and environmentally benign way to store and transport gases and are thus potentially crucial to the task of decarbonising the energy economy. Finally, gas hydrates are common in nature and their behaviour affects phenomena as diverse as the Earth's paleoclimate and the magnetic fields of Uranus and Neptune.

High pressure studies of gas hydrates provide valuable insight into all of these areas. At low pressures most gas hydrates adopt one of three related cage structures. The application of modest pressures reveals a rich and varied structural landscape that provides deeper insight into water-gas interactions. New gas hydrate structures provide potential new materials for hydrogen storage and carbon sequestration. And, information on high pressure is directly relevant to models of planetary formation and evolution. In my talk I will ilustrate some of these aspects with recent neutron diffraction studies of gas hydrates.

Keywords: neutron, diffraction, high-peressure

MS42-O3 Matrix transformation temperature in boron containing Co-Re alloys for high temperature gas turbine applications

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Co-Re-based alloys [1] are being developed to supplement single crystal Ni-based superalloys in future gas turbines which will operate with increased gas entry temperatures. The stability of the matrix at the foreseen metal operation temperatures (≥1200°C) is a very important concern for the alloy development.

Neutron diffraction was proved to be a valuable tool to study both the matrix transformation and minority phases stability in situ at high temperatures. Neutron measurements showed in the past that the low temperature hcp Co-solid solution matrix undergoes an allotropic transformation to a fcc structure above 1100°C [2]. The transformation temperature depends on the alloy composition.

It is known that an addition of boron (50-1000 ppm) to the alloy largely increases its ductility, which is desirable for the application of the Co-Re alloys. The boron influence on structure and microstructure was therefore tested on Co-17Re-23Cr alloy. The alloy contains, beside the matrix phase, only sigma phase (Cr2Re3) and (for boron containing alloy) also borides.

First, it was found in situ at high temperatures using neutron difraction (MLZ Garching) that the boron content changes significantly the hcp -> fcc transformation temperature. For the reference alloy (Co-17Re-23Cr) without boron, the transformation hcp -> fcc starts at around 1400°C on heating, while a small addition of boron to the reference alloy lowers significantly the transformation temperatures by more than 50K [3].

As the cycling through the hcp-fcc transformation temperature during operation of the components produced from the alloy could be a problem for the microstructural stability, the boron-content influence on the matrix transformation temperature deserved more attention. Therefore, its influence on the hcp-fcc transformation temperature was investigated in more detail using neutron diffraction.

It was found by studying samples with boron content 0-1000 ppm (wt.) that the temperature of hcp-fcc transformation in Co-Re alloys is not changing monotonically with increasing boron content. After the initial decrease, the temperature significantly increases for the samples with high content of boron. Possible reason could be an interplay between amount of boron in the matrix and amount of sigma phase which binds hcp-stabilizing element Re.

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Keywords: High-temperature materials, Co-Re alloys, Neutron scattering

MS42-O4 Neutron Total Scattering of Crystalline Materials in the Gigapascal Regime

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Neutron total scattering of disordered-crystalline materials provides direct experimental access to the local (short-range) structure. The ways in which this local structure agrees (or disagrees) with the average (long-range) crystal structure can provide important insight into structure-property relationships. High-pressure neutron diffraction using the Paris-Edinburgh (P-E) pressure cell allows experimenters to explore the ways in which materials are affected by pressure, can reveal new synthetic routes to novel functional materials and has important applications in many areas, including geology, engineering and planetary science. The combination of these two experimental techniques poses unique challenges for both data collection and analysis. In this paper it is shown that, with only minor modifications to the standard P-E press setup, high-quality total scattering data can be obtained from crystalline materials in the gigapascal pressure regime on the PEARL diffractometer at ISIS. The quality of the data is assessed through the calculation of coordination numbers and the use of reverse Monte Carlo (RMC) refinements. The time required to collect data of sufficient quality for detailed analysis is assessed and is found to be of the order of 8 hours for a quartz sample. Finally, data from the perovskite LaCo0:35Mn0:65O3 is presented and reveals that PEARL total scattering data offers the potential for the extraction of local structural information from complex materials at high pressure.

Keywords: neutron, high-pressure, total scattering