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MAGNETIC AND CRYSTAL STRUCTURES OF THE FRUSTRATED LAVES PHASES AND THEIR HYDRIDES UNDER VERY HIGH PRESSURES

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We have studied magnetic and crystal structures of magnetically unstable Laves phases RT_2 (R = rare earth, T = transition metal) and their hydrides. Laves phases have very unusual topology of the T sublattice resulting in a fully degenerated magnetic ground state. The topological frustration can stabilize partial magnetic disorder (short-range order) at T = 0 K. Moreover, the T sublattice is close to the instability limit between localized and itinerant states. Interplay between the magnetic instability and the topological frustration results in highly unusual physical phenomena: giant magneto-volume anomalies, magneto-structural transitions, etc. We have searched for exotic magnetic and structural phenomena in the wide ranges of pressures $0 < P < 45$ GPa and temperatures $1.5 < T < 300$ K. We also used hydrogen doping in order to expand the lattice 'negative pressure'. In order to obtain complete information on metal, hydrogen and magnetic sublatticies we combined neutron and X-ray diffraction techniques. We used sapphire and diamond anvil cell high-pressure setups.
We found very original magnetic and structural phenomena. In $GdMn_2$ and $Ho(Mn_{0.9}Al_{0.1})_2$ we observed sequences of magnetic transitions with pressure. Short range magnetic orders 'crystallize' into canted magnetic structures and finally transform to a simple ferromagnetic structure. In the hydrides RT_2H_x we observed pressure induced chemical segregation in the hydrogen sublattice accompanied by a magnetic collapse in the Mn sublattice.

Keywords: PRESSURE, MAGNETISM, DIFFRACTION

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QUANTUM-MECHANICAL STUDIES OF MINERALS AT HIGH PRESSURES AND TEMPERATURE

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Ab initio simulations are an important tool in studying materials under extreme P-T conditions. Here we will briefly review methods based on density functional theory and discuss examples of recent studies of Earth-forming minerals at the extreme conditions of the Earth's deep interior.
The examples will include the latest theoretical results on: MgO (structural stability, equation of state and anharmonicity), $MgSiO_3$ perovskite (stability, elasticity, and dynamics of crystal structure), SiO_2 polymorphs (structural stability at high pressures), Al_2SiO_5 polymorphs, FeO and (Mg,Fe)O (high-pressure behavior and magnetic collapse). Geophysical implications will be highlighted; in particular, it will be shown how these results allowed us to construct a model of the thermal structure of the Earth's mantle.

Keywords: MINERALS, EXTREME CONDITIONS, QUANTUM THEORY

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PHOTO-EXCITED CRYSTALLOGRAPHY OF DIPLATINUM COMPLEX BY MULTIPLE EXPOSURE IMAGING PLATE METHOD

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Light-induced excited state crystallography requires high accurate measurements of diffraction intensity changes induced by photo-irradiation. We have developed a special data collection system, the multiple exposure imaging plate (IP) method, by which both diffraction patterns from a crystal under light irradiated (light-on) and non-irradiated (light-off) conditions are recorded on the same IP frame, and installed it in the low-temperature vacuum x-ray camera at SPring-8 BL02B1 beamline. The first x-ray exposure at the light-off stage is followed by the second one at the light-on after a slight shift (10-20mm) of IP, and these steps are repeated several times in order to minimize effects of IP image fading and decreasing of SR beam intensity. We have applied this method to the photo-excited crystal structure analyses of a dinuclear Pt(II) complex, $(n\text{-}Bu_4N)_2H_2[Pt_2(pop)_4]$ (pop = $P_2H_2O_5$) under blue laser (442 nm) illumination at 65 K. Difference Fourier syntheses using Fon-Foff values after corrections for fading and temperature effects gave significant residual peaks and holes located around Pt atoms. Positional and occupancy refinements of two independent Pt atoms based on the intensity changes (Ion-Ioff/Ion) revealed that 1.3% of Pt atoms are shifted about 0.3 Å from the ground-states positions, and the Pt---Pt distance of 2.70 Å at the excited-states is 0.22 Å shorter than that of the ground-states. The shrinkage of the Pt---Pt bond suggests that electron transfer from antibonding $d\sigma^*$ to bonding $p\sigma$ inter-metallic orbital occurs associated with photo-excitation processes.

Keywords: PHOTO-EXCITED STATES, SYNCHROTRON RADIATION, PLATINUM COMPLEX

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HOW TO GET A PROTOTYPIC GROUP OF ALL THE CRYSTAL STRUCTURES

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A simple method was discovered which enables us to get a finite prototypic group of all the crystal structure types. In a crystal, a parallelepiped made of 3*3*3 primitive cells is chosen arbitrarily and all the atoms in it are numbered. Symmetry operations such as rotations or reflections are regarded as the permutations of the atoms using the periodic boundary conditions. With this definition, we can connect any two operations into a new permutation of the atoms. All these combinations are closed within the group of all the permutations of atoms. Therefore a finite prototypic group can be always found.
For example, Bravais lattices are related as the figure. The order of the new prototypic group is 11232, which is far fewer than that of the previous one(2799360).[1]
References
[1] M.Hosoya: Acta Cryst. (2000). A56, 259-263. Erratum ibid.(2002).A58,208

Keywords: CRYSTAL STRUCTURE BRAVAIS-LATTICE PROTOTYPIC GROUP