MS16-P8 Structural phase transitions in (Ce,La)$Pd_2Al_{(2-x)}Ga_x$ series

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Tetragonal CeT_2X_2 compounds (T: d-block element and X: p-block element) exhibit interesting physical properties such as pressure-induced superconductivity, valence fluctuating phenomena or strong crystal field exciton-phonon coupling leading to the formation of a new quantum state in $CePd_2Al_2$ [1]. The CeT_2X_2 compounds generally crystallize in centrosymmetric $ThCr_2Si_2$- or $CaBe_2Ge_2$-types with tetragonal crystal structure. Compounds crystallizing in the $CaBe_2Ge_2$ structure are frequently reported to undergo transition to structures with lower-symmetry at low temperatures. $CePd_2Al_2$ and $CePd_2Ga_2$ compounds exhibit such a structural transition from tetragonal $CaBe_2Ge_2$-type structure to an orthorhombic structure at 13.5 K [1] and to a triclinic structure at 125 K [2], respectively. Moreover the same structural phase transition was observed also in their non-magnetic La analogues [1,2].

The present study focusses on the examination of lattice distortion in (Ce,La)$Pd_2Al_{(2-x)}Ga_x$ compounds with Ga doping at low temperature. The type of transition and transition temperature within the series were investigated by low-temperature powder X-ray diffraction. Complementary the measurements of temperature dependent magnetization, specific heat, electrical resistivity and electrical resistivity under hydrostatic pressure were performed on selected compounds, including $CePd_2Al_2$ single crystal, and are discussed from the thermodynamic point of view. The structural transition temperature in the $CePd_2Al_{(2-x)}Ga_x$ compounds increases with Ga content (more steeply for $x > 0.8$), whereas the opposite development is observed for La counterparts. The low-temperature orthorhombic crystal structure (Cmma 67) has been found in the whole series. The evolution of the crystal structure in the studied composition series is discussed in the context of other tetragonal CeT_2X_2 compounds.

[1] L.C. Chapon, E.A. Goremychkin, et al., Physica B 378-380, 819 (2006)

[2] J. Kitagawa, M. Ishikawa, Journal of the Physical Society of Japan, 2380-2383, 68 (1999)

Keywords: (Ce,La)Pd2Al(2-x)Gax, structural phase transition, CaBe2Ge2 structure, low temperature powder diffraction

MS16-P9 SUBGROUPS: A novel program in the Bilbao Crystallographic Server for the analysis of distorted structures

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A new program has been added to the Bilbao Crystallographic Server (www.cryst.ehu.es), which greatly extends its capabilities concerning the analysis of group-subgroup relations of space groups and the symmetry characterization of distorted structures. The main task of this online freely available tool is to derive all the symmetries that are possible for a distorted phase, provided that the relation of its lattice with respect to the one of the parent undistorted structure is known. For a given parent space group and a supercell defining the lattice maintained by the distortion, SUBGROUPS generates all possible subgroups of the parent space group whose translational symmetry corresponds to the observed lattice. The group-subgroup hierarchy among all the calculated possible symmetry breaks is visualized through group-subgroup trees, and their physical equivalence is monitored by their classification according to conjugacy classes. The program can work with parent symmetries described in non-standard settings and the supercell input can be substituted by the introduction of the (commensurate) modulation wave vectors (one or more) involved in the distortion. The search can be truncated up to some specific subgroup, or filtered according to the crystal system, point group, etc. A much more interesting filter is also available, which permits to identify the subgroups that can be realized if the primary distortion corresponding to the transition order parameter transforms according to one irreducible representation (irrep) of the parent space group. Thus, the so-called irrep isotropy subgroups (or irrep epikernels and kernels) for any space group and any irrep (and their group-subgroup hierarchy) can be obtained. Some examples of application of this computational tool to the characterization of distorted structures will be presented.

By default SUBGROUPS only provides the space groups that are possible for the observed lattice of the distorted phase, but optionally all intermediate subgroups can also be derived. In this way the program can be applied to obtain the full hierarchical tree of intermediate subgroups relating any group-subgroup pair of space groups.

Keywords: Bilbao Crystallographic Server, distorted structures, group-subgroup relations, isotropy subgroups, epikernels, irreducible representations