

m44.o03

Topaz: A single-crystal diffractometer for the Spallation Neutron Source

Thomas F. Koetzle^a, Robert Bau,^b Christina Hoffmann,^c
Paula M.B. Piccoli,^a Arthur J. Schultz^a

^aArgonne National Laboratory, Argonne, IL 60439 USA. ^bUniversity of Southern California, Los Angeles, CA 90089 USA. ^cOak Ridge National Laboratory, Oak Ridge, TN 37831 USA. E-mail: tkoetzle@anl.gov

Keywords: single-crystal diffraction, neutron instrumentation, time-of-flight techniques

A single-crystal, time-of-flight Laue diffractometer, Topaz, is under development for the SNS (Spallation Neutron Source). The Topaz instrument design is optimized for studying samples with unit cell repeats up to 50 Å. An innovative bent, focusing neutron guide on an 18 m flight path will produce enhanced flux on sample, while an array of highly pixilated Anger camera detectors will provide coverage over a large volume of reciprocal space. Because the crystal volumes required on Topaz are expected to approach those of typical "X-ray size" samples, the instrument promises to revolutionize the application of single-crystal neutron diffraction as we know it, *particularly from the viewpoint of the practicing synthetic chemist*. Besides conventional structure analysis, Topaz will support the measurement of diffuse scattering to study disordered materials and a polarized beam option to study magnetic systems. Topaz is expected to come on line in 2009. The instrument will be operated in a broadly based user mode, and the Topaz IDT (Instrument Development Team) accordingly welcomes inquiries from all interested parties.

Acknowledgement. The Office of Science, United States Department of Energy, provides financial support for this work. SNS is managed by UT-Batelle, LLC, under contract DE-AC05-00OR22725.

m44.o04

Incommensurate magnetic structure of PrPd₂Ge₂ from powder neutron diffraction

Khalid Halich, Richard Welter

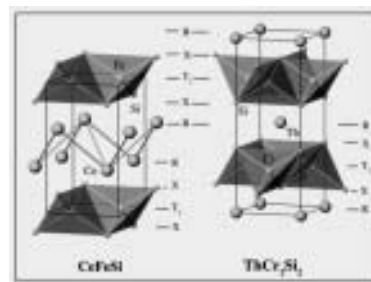
DECOMET lab., UMR-CNRS 7177, Institut de Chimie de l'Université Louis Pasteur Strasbourg I, 4 rue Blaise Pascal, F-67070 Strasbourg Cedex, FRANCE. E-mail: welter@chimie.u-strabg.fr

Keywords: powder neutron diffraction, intermetallic compounds, incommensurate magnetic structure

The magnetic properties of the PrPd₂Ge₂ and NdPd₂Ge₂ (ThCr₂Si₂-type structure[1], S.G. I4/mmm) compounds have been investigated by magnetic measurements, specific heat measurements and neutron diffraction experiments[2]. Recent studies on the magnetic properties of RTX compounds [3-5] with CeFeSi-type structure [6] (this structure is closely related to that of ThCr₂Si₂ with the same "R-X-T₂-X-R" slabs connected by direct and short R-R contact) have shown the large possibility of R-R magnetic coupling in both families. Neutron diffraction studies show that all the RTX studied compounds are characterised by a stacking along the c-axis of ferromagnetic R planes. Furthermore, for a given transition metal T, the R-R interactions through the "BaAl₄" slab are similar to those occurring in the corresponding RT₂X₂ compounds. These results indicate that the R-X-T₂-X-R slab behaves as entities which remain the same magnetic interactions whatever the structural type involved yielding a 'physical support' to its crystal chemistry character

In these materials, the palladium atom is non magnetic. The specific heat measurements clearly detect a low temperature transition for both Pr Pd₂Ge₂ and the NdPd₂Ge₂ compounds, interpreted as a R (Pr, Nd) sublattice antiferromagnetic ordering below 5.0(1) K and 1.3 (2) K.

The magnetic behavior of the PrPd₂Ge₂ compound has been fully characterized. This compound is antiferromagnetically ordered below 5 K (the Pr moments are parallel to the c-axis with a value of ≈2.0 μ_B at 2 K). The incommensurate magnetic structure of the PrPd₂Ge₂ compounds is completely original and, to our knowledge, it is the first magnetic structure characterized by a magnetic cell three times larger than the chemical one by tripling of the c parameter, in the whole ThCr₂Si₂-type compounds family. Moreover, a metamagnetic behavior has been evidenced under weak fields (approximately 2 Tesla).



CeFeSi et ThCr₂Si₂-type structures

CeFeSi et ThCr₂Si₂-type structures

- [1] Z. Ban and M. Sikirica, *Acta Cryst.* 1965, 18(4) 594-599.
- [2] R. Welter and K. Halich, *J.Phys.Chem.Sol.*, in press (PCS-D-05-00015R2).
- [3] R. Welter, G. Venturini and B. Malaman, *J. Alloys Comp.* 1992, 49, 49-58.
- [4] R. Welter, G. Venturini, E. Ressouche and B. Malaman, *Solid State Comm.* 1996, 99(4), 225-229.
- [5] A. Verniere, V. Klosek, R. Welter, G. Venturini, O. Isnard and B. Malaman., *J. Magn. Magn. Mater.* 2001, 234, 261-273.
- [6] O.I. Bodak, E.I. Gladyshevskii and P.I. Kripyakevich. *Izv. Akad. Nauk. SSSR, Ser. Neorgan. Mater.* 1966, 2(12), 2151-2155.