skin assemblies.
Keywords: residual stress, welded structures, aerospace alloys

MS42.26.2
Acta Cryst. (2005). A**61**, C57
Crystallographic Texture of Semi-finished Products
Heinz-Günter Brokmeier[a,b], [a]*Institute of Materials Science and Engineering, Clausthal University of Technology, Germany.* [b]*GKSS Research Center Geesthacht (GeNF), Geesthacht Germany.* E-mail: brokmeier@gkss.de

Texture measurement is widely used to characterize any type of materials such as metals, ceramics and rocks. In the case of industrial applications not only the texture of the material itself described in the three dimensional orientation space is of importance but also texture gradients in real products. Commonly used techniques are based on sample destruction to prepare a set of ideal samples for a diffraction experiment, see for instance the EBSD orientation stereology by Bunge and Schwarzer [1] or the texture mapping of melt grown YBaCu samples by Jung and Brokmeier [2]. The investigation of semi-finished products or real components has to be carried out sometimes non-destructively. Thus, a beam with a high penetration power is necessary available at neutron or synchrotron sources. A number of experiments have been done at TEX-2 the neutron texture diffractometer at GeNF (GKSS-Research Center Geesthacht, Germany) and at the high energy beam line BW5 at HASYLAB (DESY, Hamburg, Germany). Due to the grains size, the sample geometry and the scattering behavior one has to use hard X-rays or neutrons to investigate tubes, rings, extrusion profiles, turbine blades, implants, etc.

[1] Bunge H.J., Schwarzer R.A., *Advanced Engineering Materials*, 2001, **3**, 25.
[2] Jung V., Brokmeier H.-G., *Crystal Research and Technology*, 2000, **35**, 321.
Keywords: texture analysis, neutron diffraction, synchrotron X-ray diffraction

MS42.26.3
Acta Cryst. (2005). A**61**, C57
Dynamic Diffraction Effects in X-ray and Neutron Stress Analysis
I. C. Noyan[a], Ersan Ustundag[b], Mark Daymond[c], HanFei Yan[a], [a]*Department of Appl. Phys. And Appl. Math., Columbia University.* [b]*Mat. Sci. & Engg. Iowa State Uinversity, Ames, Iowa, USA.* [c]*Mat. Sci.& Engg, Queens University, Ontario, Canada.* E-mail: icn2@colubia.edu

We present time-of-flight neutron and x-ray diffraction data from thick perfect Si single crystal samples showing dynamic double diffraction effects associated with finite crystal size. In this mode constructive interference occurs solely from thin layers bounded by the front (entry) and back (exit) surfaces of the sample with no scattering originating from the layers in between. This results in two distinct peaks for each reflection. If the instrument resolution is insufficient, these two peaks convolve and cause peak-shape aberrations which can cause significant errors in parameters obtained from diffraction analysis.
Keywords: dynamic diffraction, single crystals, stress analysis

MS42.26.4
Acta Cryst. (2005). A**61**, C57
Charge Ordering and Magnetic Structure in Fe_3BO_5
Pierre Bordet[a], Emmanuelle Suard[b], [a]*Laboratoire de Cristallographie CNRS, Grenoble, France.* [b]*Institut Laue-Langevin, Grenoble, France.* E-mail: Pierre.bordet@grenoble.cnrs.fr

The structure of $(Fe^{2+})_2(Fe^{3+})O_2BO_3$ ludwigite (space group Pbam, a=9.462Å, b=12.308Å, c=3.075Å) is made of zigzag walls of edge-sharing FeO_6 octahedra, connected by BO_3 triangular groups. It contains two types of 3-leg ladders of Fe cations: ladder 1 with only Fe^{2+} cations and ladder 2 formed by Fe^{3+} cations with one additional electron per rung delocalized at high temperature. This leads to a quite complex physical behavior. Two magnetic ordering transitions are observed at 112K and 70K. Specific heat shows a plateau between ≈100K and 250K, and a change of slope of resistivity is observed close to room temperature. Using single crystal x-ray diffraction, we have shown that it is due to a partial localization of the Fe 3d electrons on ladder 2, accompanied by a superstructure doubling the c-axis.

We report here the investigation of the magnetic ordering, using neutron powder diffraction on I.L.L. D20 between 300K and 10K. Based on the superstructure found with x-rays, both magnetic structures were solved and refined by the Rietveld technique. Between 70K and 110K, only ladder 2 is ordered. The coupling is ferromagnetic in the rungs and antiferromagnetic between them. At 70K, ladder 1 orders as a canted antiferromagnet in the rungs which are ferromagnetically coupled. This also leads to a partial reorientation of the spins of ladder 2. A strong magnetic background increasing from room temperature to 110K could be related to short range correlations in both magnetic sub-units.
Keywords: magnetic structure determination, superstructure, spin ladder

MS42.26.5
Acta Cryst. (2005). A**61**, C57
Determining Pb/Bi Distributions using High-Energy Resonant Scattering at K Edges
Peter L. Lee[a], Yuegang Zhang[a], Sarvjit D. Shastri[a], Deming Shu[a], Duck-Young Chung[b], Mercouri G. Kanatzidis[b], Angus P. Wilkinson[c], [a]*XOR, Advanced Photon Source, Argonne National Laboratory,Argonne, IL 60439, USA.* [b]*IDepartment of Chemistry, Michigan State University, East Lansing, MI 48824, USA.* [c]*School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30332, USA.* E-mail: pllee@aps.anl.gov

Powder diffraction data collected at just below both the Pb and Bi K edges (88.005 keV and 90.526 keV respectively), and ~86 keV on an imaging plate detector have been used to examine the Pb/Bi distribution over the 11 crystallographically distinct sites in $Pb_5Bi_6Se_{14}$. Specialized x-ray optics with excellent energy resolution and stability were used for the experiment. Even with the relatively low scattering contrast that is available at the K edges, it was possible to determine the Pb/Bi distribution and probe the presence of cation site vacancies in the material. The current results indicated that resonant scattering measurements at high-energy K edges are a viable, and perhaps preferable, route to site occupancies when neutrons provide insufficient contrast and absorption from the sample or sample environment/container is a major barrier to the acquisition of high-quality resonant scattering data at lower energy edges.
Use of the Advance Photon Source was supported by the U.S. Department of Energy, Office of Sciences, Office of Basic Energy Sciences, under Contract No. W-31-109-Eng-38.
Keywords: synchrotron powder diffraction, anomalous scattering method, high-energy X-ray diffraction