displacement of the oxygen atoms from the linear O-Re-O chains of cubic ReO_3 to a "hinged" arrangement at the oxygens. This necessitates a doubling of the lattice and a change from simple cubic to a body centered geometry.

Until now, due to a large X-ray form factor mismatch, design limitations in X-ray single crystal pressure cells and a limited range in accessible pressure for the neutron powder measurement, no direct evidence of the high pressure ReO_3 structure has been obtained. For the first time, we have been able to obtain direct structural information at 15 kbar using the newly designed single crystal neutron diffractometer at WNR. This was accomplished by developing a novel geometry for the high pressure experiment which maximizes the available information using time-of-flight techniques and does not require the sample to be remounted in order to solve the structure (good for high symmetry systems > orthorhombic, with possible extensions to lower symmetry groups). This method consists of a cylindrical high pressure cell mounted along the beam axis (i.e. mounted on the incident beam collimator) so that the incident beam enters through the bottom of the cell. The sample is isolated inside a hydrostatic fluid chamber and the diffracted beam is scattered at 90° to the incoming beam.

As predicted, ReO_3 does undergo a lattice doubling with a hinging of the oxygen atoms. At ~15 kbar, the Re-O-Re angle is 165.4° (Re-Re-O 7.3°) with almost no change in the Re-O distance from the zero pressure structure. The "compressibility collapse", therefore, results from a rotation of Re-O octahedra.

13.5–4 ANTIFERROMAGNETIC STRUCTURE OF $LaFeO_3$ FROM HIGH RESOLUTION NEUTRON DIFFRACTION. By T. Peterlin-Neumaier and E. Steichele, Fakultät für Physik der Technischen Universität München, E 21, D-8046 Garching, BRD.

The rare earth orthoferrites belong to the orthorhombically distorted perovskite structures (space group D_{2h}^{16} - Pbnm) and show an antiferromagnetic ordering of the iron ions at room temperature. The determination of the Fe^{3+} moment direction from the intensities of magnetic Bragg peaks may become difficult from powder measurements when some of the relevant reflexions overlap. This problem is most serious with the light rare earth perovskites, as here the difference of the cell edges a and b is very small. For $LaFeO_3$ the a/b ratio is only 1.002, compared to 1.0175 for $PrFeO_3$. With a high resolution time-of-flight neutron diffractometer (E. Steichele and P. Arnold, Phys. Letters (1973) 44A, 165) and a carefully prepared sample the orthorhombic splitting could be resolved.

The sample was prepared from a 1:1 molar mixture of La_2O_3 and Fe_2O_3, pressed to pellets with force of 15 tons, subsequently heated twice to 1420° C with grinding of the pellets in between. The diffractometer resolution could be improved to $\Delta d/d \approx 4 \times 10^{-4}$ for the (101) and (011) reflexions, which are purely magnetic peaks.

Diffraction measurements were performed in the fixed backscattering geometry between $\lambda = 2d = 9.2$ Å and $\lambda = 2d = 3.4$ Å, where the experimental resolution was 1×10^{-3}. For higher order reflexions no magnetic contributions could be observed due to the reduced magnetic form factor of the iron ion. Individual peaks were fitted with a combined Gauss-Lorentz function (Lorentzian in the peak and Gaussian in the tails), which approximated well the expected triangular resolution function. The result of such a least squares fit for the (101) and (011) reflexions is shown in the figure below. The experimental linewidth is about twice the instrumental resolution and the relative splitting of the clearly separated peaks is 1.2×10^{-3}.

For a pure G_x - type configuration mostly found in rare earth perovskites one would expect an intensity ratio R = {011} : {101} = 3 : 1, whereas our experimental result is $R_{exp} = 2.32 \pm 0.12$. This implies that the spin must be canted with respect to the x-axis. From the experimental result two extreme orientations can be derived: With the moment in the xz-plane the deviation from the x-axis would be ≈ 27 ± 4° and with the moment in the xy-plane the deviation from the x-axis would be ≈19 ± 4°. In order to design the spin a unique orientation in space the intensities of other magnetic peaks are being evaluated. We also find that the magnetic peaks are by about 20% wider than the purely nuclear peaks probably due to finite magnetic domain sizes.

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