

**Experiment title:**

Investigation of the crystal structure of TiOCl and TiOBr at the pressure-induced insulator-to-metal transition

Experiment**number:**

HS-3108

Beamline:

ID09A

Date of experiment:

from: 9 Dec 2006

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Date of report:

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Shifts:

9

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Report:

Published paper #1:

C. A. Kuntscher, S. Frank, A. Pashkin, H. Hoffmann, A. Schönleber, S. van Smaalen, M. Hanfland, S. Glawion, M. Klemm, M. Sing, S. Horn and R. Claessen, Phys. Rev. B **76**, 241101(R) (2007):

Abstract:

We investigated the pressure-dependent optical response of the low-dimensional Mott-Hubbard insulator TiOBr by transmittance and reflectance measurements in the infrared and visible frequency range. A suppression of the transmittance above a critical pressure and a concomitant increase of the reflectance are observed, suggesting a pressure-induced metallization of TiOBr. The metallic phase of TiOBr at high pressure is confirmed by the presence of additional excitations extending down to the far-infrared range. The pressure-induced metallization coincides with a structural phase transition, according to the results of x-ray powder diffraction experiments under pressure.

Published paper #2:

C. A. Kuntscher, A. Pashkin, H. Hoffmann, S. Frank, M. Klemm, S. Horn, A. Schönleber, S. van Smaalen, M. Hanfland, S. Glawion, M. Sing, and R. Claessen, Phys. Rev. B **78**, 035106 (2008).

Abstract:

Pressure-dependent transmittance and reflectance spectra of TiOBr and TiOCl single crystals at room temperature suggest the closure of the Mott-Hubbard gap, i.e., the gap is filled with additional electronic states extending down to the far-infrared range. According to pressure-dependent x-ray powder diffraction data the gap closure coincides with a structural phase transition. The transition in TiOBr occurs at slightly lower pressure ($p=14$ GPa) compared to TiOCl ($p=16$ GPa) under hydrostatic conditions, which is discussed in terms of the chemical pressure effect. The results of pressure-dependent transmittance measurements on TiOBr at low temperatures reveal similar effects at 23 K, where the compound is in the spin-Peierls phase at ambient pressure.

Published paper #3:

C. A. Kuntscher, J. Ebad-Allah, A. Pashkin, S. Frank, M. Klemm, S. Horn, A. Schönleber, S. van Smaalen, M. Hanfland, S. Glawion, M. Sing, and R. Claessen, High Pressure Research **29**, 509 (2009).

Abstract:

By pressure-dependent infrared microspectroscopy we observe the filling of the Mott-Hubbard gap in TiOCl and TiOBr above a critical pressure P_c . Concomitant with the gap filling a structural phase transition occurs at P_c . According to our pressure-dependent powder x-ray diffraction data a mixture of the ambient-pressure orthorhombic $Pmmn$ phase and a dimerized, monoclinic $P2_1/m$ phase exists above P_c .