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Symmetry and anisotropic properties of β-PbO2 studied by DFT as well as SR and neutron diffraction

Tuesday, 21 March 2023 16:00 (2 hours)

The structural and electronic properties of the rutile-type oxide beta-PbO2 (plattnerite) are studied by neutron and synchrotron radiation powder diffraction and first-principles density functional theory (DFT) calculations~[1]. The motivation to study the electronic properties of beta-PbO2 gained some additional impact related to the possible existence of topologically nontrivial [2,3] semimetallic states. Both diffraction measurements and DFT calculations show that beta-PbO2 has a CaCl2-type orthorhombic structure (space group Pnnm) instead of the widely accepted beta-PbO2 rutile-type tetragonal structure (space group P42/mnm).

This symmetry lowering in beta-PbO2 is a robust effect observed at ambient pressure at temperatures between 100 and 400 K. The orthorhombic symmetry rules out the possibility of a semimetallic symmetry-protected state in beta-PbO2. Both diffraction measurements and DFT calculations show an anisotropy of thermal expansion, atomic vibrations and elastic constants of β-PbO2 along the [100] and [010] directions.

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[3] B. Peng, I. Bravic, J. L. MacManus-Driscoll, and B. Monserrat, Phys. Rev. B 100, 161101(R) (2019).

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