Experimental report

17/05/2019

Proposal: 7-03-164 **Council:** 4/2017

Title: Proton vibrational dynamics in Sc-doped BaTiO3 proton conductors

Research area: Physics

This proposal is a new proposal

Main proposer: Adrien PERRICHON

Experimental team: Nico TORINO
Adrien PERRICHON

Local contacts: Monica JIMENEZ RUIZ

Samples: BaTi0.2Sc0.8O3H0.8
BaTi0.84Sc0.16O3H0.16
BaTi0.8Sc0.2O3H0.2
BaTi0.9Sc0.1O3H0.1
BaTi0.67Sc0.33O3H0.33
BaTi0.5Sc0.5O3H0.5
BaTi0.3Sc0.7O3H0.7

Instrument	Requested days	Allocated days	From	To
IN1 LAG	5	2	20/06/2018	22/06/2018

Abstract:

Proton conducting BaTi1-xScxO3Hx perovskites are promising materials as fuel cell electrolyte for intermediate temperature devices (400-800°C). Compared to BaZrO3-based materials, Sc-doped BaTiO3 materials undergo a phase transition between the cubic perovskite structure at high doping level, and a 6H hexagonal perovskite phase a low doping level, associated with a drop in proton conductivity. In order to link the macroscopic conductivity behavior to the structures and microscopic diffusion mechanism, we aim to characterize the proton vibrational dynamics and, subsequently, the local environments of the proton sites, for several compositions of both the hexagonal and cubic phases. The proton dynamics being characterized by wag and stretch modes at about E=100-120 meV and E=430-450 meV respectively, the IN1 Lagrange spectrometer is the most suited spectrometer for this investigation. The experimental results will be valuable not only to understand the change in behavior with the phase transition, but in a larger view, will provide insights on the effects of acceptor-doping in proton conducting perovskites over a large composition series.

Experimental report for experiment 7-03-164 on IN1 Lagrange, from June 20 to June 22, 2018

PI – Adrien Perrichon
LC – Mónica Jiménez-Ruiz

We have measured about 5 g of proton-conducting perovskite-based $BaSc_{0.7}Ti_{0.3}O_3H_{0.7}$ (70ScBTO) and $BaSc_{0.2}Ti_{0.8}O_3H_{0.2}$ (20ScBTO) oxide materials. Beyond the content in scandium and hydrogen, these two materials differ by their crystal structure, primitive cubic for 70ScBTO and hexagonal for 20ScBTO. The INS spectra, measured at $T = 10$ K, are reported in Fig. 1. The spectra are featured by three main bands, the fundamental hydroxide wag bands, δ(O-H), in the range 100–140 meV, the overtone of δ(O-H) at 200–280 meV, and the hydroxide stretch bands, ν(O-H), in the range 400–420 meV. The presence of a broad yet single δ(O-H) band for cubic 70ScBTO indicates that only one type of proton environment is present in the material, associated to intra-octahedral hydrogen-bond geometries with relatively weak hydrogen bonding strength, manifested by a ν(O-H) of about 420 meV. Conversely, the hexagonal 20ScBTO is featured by multiple δ(O-H) bands, associated to at least three distinct proton environments, and by and overall strengthening of the hydrogen bonding, manifested by a ν(O-H) of about 400 meV. First-principle simulations are ongoing to determine the spectral contributions of the different proton sites proposed in the hexagonal structure.

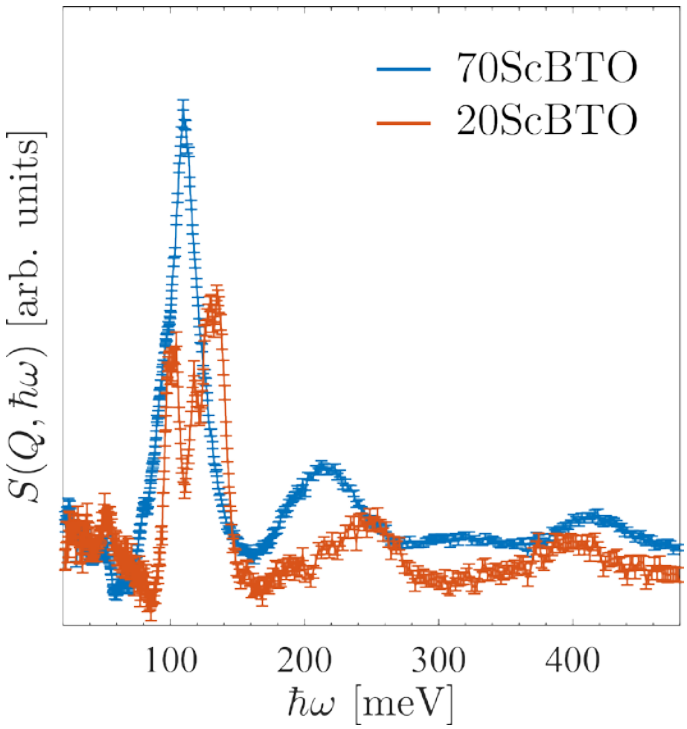

Figure 1 – INS spectra of the 70ScBTO and 20ScBTO samples, measured at 10 K with the Cu220 monochromator.