

MS19-P18 A new high flux neutron backscattering spectrometer for research into the ns-dynamics of battery, fuel-cell and hydrogen storage materials.

Bernhard Frick¹, Markus Appel¹

1. Institut Laue-Langevin, Grenoble

email: frick@ill.fr

The new neutron backscattering spectrometer IN16B at the Institut Laue-Langevin, Grenoble, with highest flux and signal-to-noise ratio for a high energy resolution spectrometer of its kind, is perfectly suited for studying diffusion and relaxation processes on the nanosecond time scale. In this poster we also present some instrumental aspects, but will mainly give examples to illustrate the possibilities for spectroscopy on materials which are of interest for fuel cells, battery materials or hydrogen storage.

IN16B has a standard energy resolution with Si11 analysers in backscattering of FWHM ~ 0.75 μeV in an energy transfer range of ± 30 μeV , thus exploring simultaneously a momentum transfer (Q) range between 0.2 and 1.8 \AA^{-1} . The Q-range can be doubled by using Si311 analysers and the resolution can be halved by using unstrained small crystals on the analyser sphere. Ongoing projects aim for an energy transfer range extension by a factor of 10 with BATS, Backscattering and Time-of-flight Spectrometer and a decade improvement of the energy resolution.

Keywords: neutron spectroscopy, energy related materials, dynamics, relaxation

MS20 Materials for energy conversion and harvesting

Chairs: Manuel Hinterstein, Siegbert Schmid

MS20-P1 Organic-inorganic hybrid perovskite $\text{CH}_3\text{NH}_3\text{PbI}_3$: structural consequences of water absorption

Alla Arakcheeva¹, Dmitry Chernyshov², Massimo Spina¹, László Forró¹, Endre Horváth¹

1. Laboratory of Physics of Complex Matter, Ecole polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

2. SNBL, ESRF, 71 Avenue des Martyrs, 38043 Grenoble Cedex 9, France

email: alla.arakcheeva@epfl.ch

The organic-inorganic hybrid perovskite-like $\text{CH}_3\text{NH}_3\text{PbI}_3$ (MAPbI₃) is intensively studied owing to its role in energy conversion. In this compound, the linear methyl ammonium (MA⁺) cation is located in the centre of the cuboctahedra formed by I-atoms. Hence, statistical disorder over its different orientations can be expected. This allows a high flexibility of the structure symmetry with pressure, temperature and other conditions affecting the weak N-H...I hydrogen bonds, which maintain this cation inside the cubooctahedron. Indeed, the different tetragonal space groups, such as *I4/mcm* [1-4], *I4cm* [5,6] and *I4/m* [7], were reported previously even in the room temperature phase. MAPbI₃ is structurally unstable at ambient conditions. Air humidity provokes its gradual decomposition. We have studied the mechanism for the decomposition. Crystal structure of the pristine (I) and in wet air aged (II) samples has been investigated at 293 K with high precision single crystal XRD experiments using synchrotron radiation. We show [8] that different space groups, *I422* and *P4₂2*, characterize I and II, respectively. Both of them are subgroups of *I4/mcm*, which is commonly adopted for MAPbI₃. The difference appears due to the changes in H-bonds induced by the H₂O inclusion in the structure of the aged crystal II. This inclusion initiates the crystal decomposition, which can be described by the chemical reaction: $\text{CH}_3\text{NH}_3\text{PbI}_3 + (\text{H}_2\text{O}) = \text{CH}_3\text{NH}_2 + \text{PbI}_2 + (\text{H}^+ + \text{I}^- + \text{H}_2\text{O})$. The dashed contour in the figure 1 indicates the atomic part, which most probably leaves the structure leading to the decomposition.

[1] Y. Kawamura *et al.*, Journal of the Physical Society of Japan, **71**(7), 1694 (2002).

[2] Y. Yamada *et al.*, Journal of the American Chemical Society, **137**, 10456 (2015).

[3] Y. Dang *et al.*, CrystEngComm, **17**, 665 (2015).

[4] M.T. Weller *et al.*, Chem. Commun. **51**, 4180 (2015).

[5] C.C. Stoumpos *et al.*, Inorg. Chem. **52**, 9019 (2013).