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In situ PDF and solid-state NMR studies of antimony anodes for Na-ion batteries

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Sodium-ion batteries have attracted attention in recent years because of the natural abundance of sodium compared to lithium, making them particularly attractive in applications such as large-scale grid storage where low cost and sustainability, rather than light weight is the key issue [1]. Several materials have been suggested as cathodes but far fewer studies have been done on anode materials and, because of the reluctance of sodium to intercalate into graphite, the anode material of choice in commercial lithiumion batteries, the anode represents a significant challenge to this technology. Materials which form alloys with sodium, particularly tin and antimony, have been suggested as anode materials; their ability to react with multiple sodium ions per metal-atom give potential for high gravimetric capacities[2]. However, relatively little is known about the reaction mechanism in the battery, primarily due to drastic reduction in crystallinity during (dis)charging conditions, but also because the structures formed on electrochemical cycling may not be alloys known to exist under ambient conditions. In this study, we present a study of antimony as an anode in sodium-ion batteries, using in situ pair distribution function (PDF) analysis combined with ex situ solid-state nuclear magnetic resonance studies. PDF experiments were performed at 11-ID-B, APS using the AMPIX electrochemical cell [3], cycling against sodium metal. Inclusion of diffuse scattering in analysis is able to circumvent some of the issues of crystallinity loss, and gain information about the local structure in all regions, independent of the presence of long-range order in the material. This approach has been used to probe local correlations in previously uncharacterised regions of the electrochemical profile and analyse phase progression over the full charge cycle. This analysis has been linked with ex situ 23Na solid-state NMR experiments to examine the local environment of the sodium; these show evidence of known NaxSb phases but indicate additional metastable phases may be present at partial discharge.

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