Improved Conductivity for AlSb Used as the Anode Material for Lithium-Ion Batteries

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As functionality increases in portable electronic devices, there occurs a corresponding demand for increased energy density batteries. Carbon, and in particular graphite, now dominates the anode materials employed in lithium-ion batteries. Suppliers readily provide graphite materials exhibiting near-theoretical values (372 mAh/g). Therefore, a new class of materials is required to advance the energy density of lithium-ion battery anodes. This new class of materials, either individually or combined with graphite in the form of composite materials, should improve energy density while maintaining other key performance features including cycle life, high rate capability and safety.

Metal anodes have shown promise as high energy density materials, especially with potential to dramatically improve volumetric energy density. Such is the case for metal alloys such as InSb and AlSb. These compounds offer theoretical gravimetric capacities of 227 and 360 mAh/g respectively, assuming an ability to incorporate up to 2 lithium per formula unit. Both values are below the theoretical value of graphite. However, considering the high density of these materials (5.77 and 4.26 g/cm^3 respectively) relative to graphite (2.2 g/cm^3), opportunity exists for improved volumetric capacity. We have estimated in-electrode volumetric capacities for these materials to be at 880 mAh/cm^3 for InSb and 1035 mAh/cm^3 for AlSb. In addition to 2 Li per formula unit, this estimate assumes electrode fabrication with 90% active material loading and a coating density of 75% versus material density, both realistic estimates based on current graphite-based electrodes. For both materials, the volumetric energy density improvements are dramatic versus that demonstrated with graphite (~550 mAh/g).

Previous work demonstrated the ability of these materials to reversibly incorporate lithium, showing InSb able to incorporate up to 2.6 Li. InSb also showed superior cycling characteristics versus AlSb and GaSb.[1] TIAX density-of-states calculations indicate that low conductivity provides one possible reason for poor performance with AlSb [Figure 1]. Poor conductivity can limit the amount and rate of lithium incorporation at potentials suitable for lithium-ion batteries. Conductivity and performance can further decrease with cycling due to passivation of particles from reactions with electrolyte and electronic isolation of particles as a result of large volume changes during cycling. Modeling work in our group suggested the opportunity to improve conductivity in AlSb by using transition metal doping and hence offer an opportunity for improved performance in lithium-ion battery application.

We successfully improved conductivity using Cu, Zn and Sn incorporated during high temperature synthesis at levels of a few percent. Figure 2 shows conductivity for pressed pellets of AlSb powders synthesized with and without dopants present. Elemental analysis confirmed the presence of dopants in two tested doped samples. Elemental analysis did not show any significant level of impurities (unintentional doping) in the synthesized AlSb powder.

These conductivity-enhanced materials are undergoing electrochemical evaluation. Methods for further conductivity improvements are also being explored. We will present data on the synthesis of AlSb powders of improved conductivity and their evaluation for use as the anode material in lithium-ion batteries.

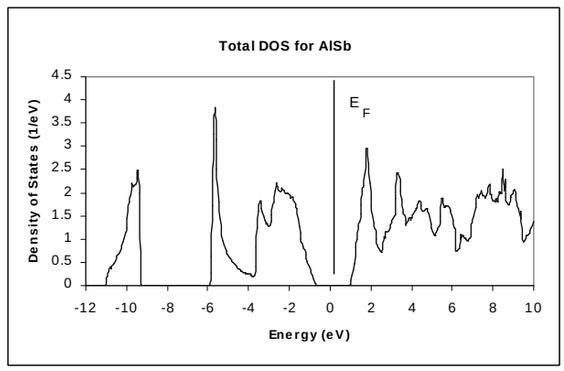

Figure 1. Density-of-states calculation for AlSb.

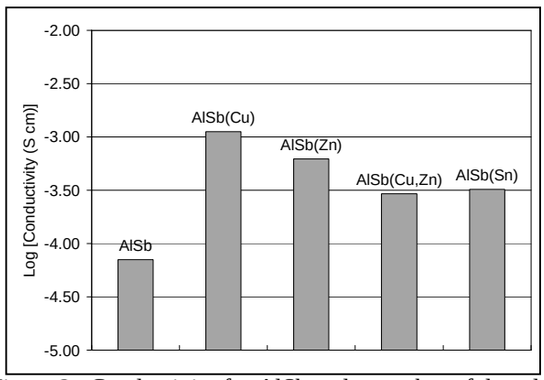

Figure 2. Conductivity for AlSb and a number of doped AlSb powders. Measurements were made on pressed pellets using PVDf binder (2%).

[1] Vaughey, J. T.; et. al., *J. Power Sources*, v. 97-98, 194, 2001.