Structures of Defect Perovskites Suitable for Li Ion Intercalation

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The phase $Sr_7Zr_4Nb_6O_{30}$ in the $SrO\text{-}ZrO_2\text{-}NbO_{2.5}$ system was recently discovered in our laboratories. X-ray diffraction patterns have shown that the compound $Sr_7Zr_4Nb_6O_{30}$ forms a cubic perovskite sub-structure with an additional modulation (satellite reflections at $½<111>_p$). This compound is analogous to the perovskite Sr_xNbO_3, $0.7 \le x \le 1$, which exists over a significant range of composition [1]. In contrast to our new phase Sr_xNbO_3, $0.7 \le x \le 1$, does not display additional ordering (no satellite reflections were found despite intensive searching). Therefore it is likely that the additional reflections for our new phase are due to Nb/Zr ordering.

If x in the Sr_xNbO_3 solid solution equals 1 all the niobium is in oxidation state +IV. Reducing the amount of strontium leads to vacancies on that site and to a corresponding amount of Nb^{+5} required for charge balance. The vacancies on the Sr site allow Li to be intercalated electrochemically. In $Sr_7Zr_4Nb_6O_{30}$, all Nb^{4+} has been replaced by Zr^{4+}, which allows syntheses to be carried out in air at high temperature. Preliminary investigations [2] have shown that a significant amount of Li can be intercalated, which would make that compound suitable as a cathode in a Li ion battery. The apparent reversibility of the intercalation process is another indication that this new phase might be suitable for that application.

[1] Hessen B., Sunshine S. A., Siegrist T., Jimenez R., *Mater. Res. Bull.*, 1991, **26**, 85. [2] Schmid S., Kuhn A., *unpublished*.

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