SYNTHESIS AND ELECTROCHEMICAL DELITHIATION OF $Li_{17}Sn_4$ DOPED BY BORON

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Intermetallic compounds with high Li content are widely used as anode materials in the Li-ion batteries. Research in the field of accumulation and storage energy is a priority among scientists today. In this work we synthesized the B-doped phase with high content of Li for further study of electrochemical delithiation.

Cleaned Li (metal, 99 wt. %, excess 5-wt. %), pressed Sn (foil, 99.99 wt. %) and powder of B (96 wt. %) were pelletized before preparation. Samples with the nominal compositions $Li_{81}Sn_{19}$ and $Li_{80}Sn_{17}B_3$ were synthesized by arc melting of pellets under purified argon atmosphere and were remelted several times for better homogenization. The alloys are sensitive to air and moisture, so they were stored under a layer of indifferent oil.

Electrochemical delithiation from the structure of undoped and doped by B $Li_{17}Sn_4$ phase was carried out in the Swagelok-type cell using a $LiCoO_2$ powder as a positive electrode. The electrolyte consisted of 1 M $LiPF_6$ solution in the mixture of aprotic solvents (1:1 ethylene carbonate / dimethyl carbonate). All electrochemical measurements (discharge and charge) were carried out in galvanostatic mode using galvanostat MTech G410-2.

Using X-ray phase analysis (DRON-2.0M diffractometer, Fe *Kα*-radiation) and scanning electron microscopy (Tescan VEGA3 LMU microscope, EDX-analyzer with X-Max^{N}20 detector) we came to conclusion that the samples consisted of two phases: ternary one with cubic structure ($Li_{17}Pb_4$-type, space group *F*-43*m*, Pearson`s symbol *cF*420) and minor of tetragonal phase *β*-Sn (space group $I4_1/amd$). Elemental mapping of B and Sn as well as EDX-spectra of the $Li_{80}Sn_{17}B_3$ alloy are presented in Fig. Atomic ratio of Sn/B (5.9/1) is well correlated with the nominal composition. Cell parameters of undoped phase are a = 19.727(5) Å, V = 7677(6) Å^3. B-doped phase is characterized by smaller cell parameters: a = 19.655(4) Å, V = 7593(4) Å^3. Unit cell parameters decreased significantly after delithiation.

Li-deintercalation from the crystal structure of studied alloys was carried out at the potential of 3.9–1.8 V under discharging at 0.5 mA/cm^2. Undoped $Li_{17}Sn_4$ and B-doped alloys as anode materials demonstrated the amount of electrochemically deintercalated lithium more than 3.2 Li/f.u. The boron-doped electrode demonstrated better cyclic reproducibility during both discharging and charging processes.

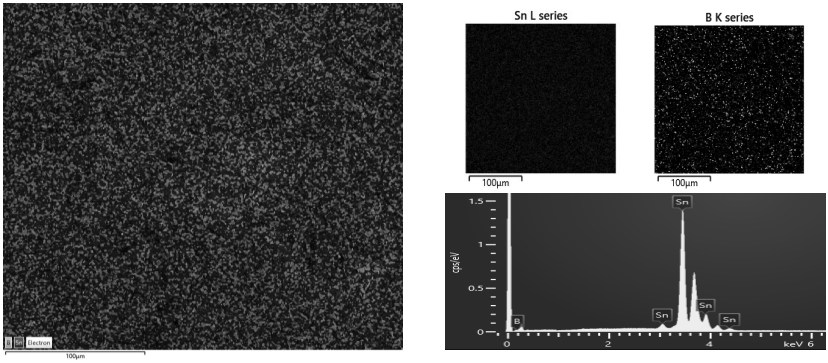

Fig. Elemental mapping of B, Sn and EDX-spectra of the $Li_{80}Sn_{17}B_3$ alloy