THERMODYNAMIC PROPERTIES OF $LiBH_4$-LiI PSEUDO-BINARY SYSTEM

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The hexagonal structure of the $LiBH_4$ at room temperature can be stabilised by substituting the BH_4^- anion with I^-,[1–3] leading to high Li-ion conductive materials.[1,3] A thermodynamic description of this binary system will be presented in this work. The pseudo-binary $LiBH_4$–LiI system has been explored investigating several compositions, synthetized by ball milling and subsequently annealed. X-ray diffraction and Differential Scanning Calorimetry have been exploited to determine structural and thermodynamic features of various samples. The monophasic zone of the hexagonal $Li(BH_4)_{1-x}(I)_x$ solid solution has been defined equal to $0.20 \leq x \leq 0.55$ at 25 °C. For the formation of the h-$Li(BH_4)_{0.5}(I)_{0.5}$ solid solution, a value of the enthalpy of mixing (ΔH_{mix}) has been determined experimentally equal to -0.59 ± 0.2 kJ/mol of compound. In addition, the enthalpy of melting has been measured for different compositions. Lattice stabilities of $LiBH_4$ and LiI have been determined by ab-initio calculations. Combining results of experiments, literature data and theoretical calculations, the pseudo-binary $LiBH_4$–LiI phase diagram has been determined and assessed in all composition and temperature ranges by the CALPHAD method. Preliminary results on the pseudo-ternary $LiBH_4$–LiI-LiBr system will be also presented.

References

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Short Biography of Author

Asya Mazzucco got her master's degree in industrial chemistry at the University of Turin with a thesis intitled "Thermodynamic properties of the LiBH4-LiI binary system and LiBH4-LiI-LiBr ternary system for applications as solid electrolytes in all-solid-state-batteries" in 2021. Currently she is PhD Student at the University of Turin, Department of Chemistry, working on complex hydride-based Solid-State Electrolytes for Solid State Batteries (lithium and magnesium based).