Thermodynamic analysis of LiFePO₄ precursor prepared by co-precipitation method

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Abstract: Based on thermodynamics, principles of mass and charge conversion in solution, thermodynamic analysis was carried out in co-precipitation process of FePO₄, a precursor of LiFePO₄ cathode. The relationships between total iron ion concentration (C_Fe), different soluble iron compounds concentrations with pH value in solution, concentrations of H₂PO₄ (C_P) and NH₃ (C_N) were deduced. With the increasing of pH value in solution, C_Fe increased firstly and then decreased with lowest concentration at pH=5.0. pH in solution had different effects on the concentrations of soluble iron compounds: with the increasing of pH, the concentrations of Fe³⁺, Fe(OH)²⁺, Fe₂(OH)₂⁴⁺, Fe₃(OH)₄⁵⁺ decreased gradually; before pH=11.0, the concentration of Fe(OH)³⁺ remained constantly, however, the concentrations of Fe(OH)₃⁻, Fe(OH)₄⁻ increased with the increasing of pH value. C_N had no effect on the concentrations of C_Fe and other soluble iron compounds. During the co-precipitation process of FePO₄, reasonable pH value in solution was 2.4~4.2.

Key words: FePO₄; precursor; coprecipitation; thermodynamics