Determination of the Gibbs Formation Energy of CuGaSe₂ by EMF Method

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The thermodynamic stability of the chalcopyrite CuGaSe₂ compound semiconductor was studied. A solid-state electrochemical cell was employed to obtain the standard Gibbs energy of formation of CuGaSe₂. The reversible EMF data of the following cell over the range of 818 to 950 K were measured: Pt, Ga(l), Ga₂O₃(s) // 15 YSZ // Ga₂O₃(s), Cu₂Se(s), CuGaSe₂(s), Cu, C, Pt. By using Cu₂Se literature data with the EMF results, the following expression for the standard Gibbs energy of formation for CuGaSe₂ was obtained: (ΔG°_f CuGaSe₂) (kJ/mol) = -233.31 + 0.0075T(K) (818 to 950 K). The calculated ΔG°_f function shows that the ternary CuGaSe₂ compound is more stable than the corresponding CuInSe₂ by approximately 10 kJ/mol over the entire temperature range of the present investigation, which is consistent with the current phase diagram information.

Keywords: CuGaSe₂, EMF, Gibbs energy of formation, enthalpy of formation, solid-state electrochemical cell.

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