EVALUATION OF THERMODYNAMIC PROPERTIES OF PALLADIUM AND NEODYMIUM INTERMETALLIC COMPOUNDS

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A pyrochemical process for reprocessing spent nuclear fuel (SNF) is currently being developed in the Russian Federation. One of the objectives is to create thermodynamic models for each stage of SNF reprocessing. Spent nuclear fuel has a complex composition, and reliable thermodynamic data are not available in the literature for all compounds, even the most important ones.

The aim of this study is to evaluate thermodynamic data on NdPd, $NdPd_3$, and Nd_3Pd_4 intermetallic compounds, which are formed during the electrolytic reduction of spent nuclear fuel. Accounting for these intermetallic compounds is important for the proper distribution of rare earth and noble metal flows.

The enthalpies of formation of NdPd and $NdPd_3$ are available in [1]. The enthalpy of formation of Nd_3Pd_4 was estimated as $\Delta H_f(Nd_3Pd_4) = 1.036 \cdot \Delta H_f(NdPd)$ based on the general trend of similar palladium alloys [2]. The entropy and heat capacity were estimated using the Neumann–Kopp rule. The heat capacity was approximated by the generally accepted equation:

$$C_p(T) = A + 10^{-3}BT + 10^5 CT^{-2}$$

The obtained data on the enthalpy of formation and entropy, as well as the coefficients of the heat capacity equation are given in the table.

Thermodynamic properties of Nd and Pd intermetallic compounds

Intermetallic compound	ΔH^0, kJ/g-atom	ΔH^0, kJ/mol	ΔS^0, J/(mol·K)	Coefficients of the equation		
				A	*B*	*C*
NdPd	-77.2 [1]	-154.4	108.91	38.942	32.709	4.479
$NdPd_3$	-73.3 [1]	-293.2	184.56	87.5	44.263	4.479
Nd_3Pd_4	-80.0	-560	364.55	141.106	103.905	14.437

The data obtained are used in thermodynamic modeling of processes for the pyrochemical technology being developed for spent nuclear fuel reprocessing.

1. Guo Q., Kleppa O.J. Standard enthalpies of formation of neodymium alloys, Nd + Me (Me - Ni, Ru, Rh, Pd, Ir, Pt), by high-temperature direct synthesis calorimetry. Metall Mater Trans. (1995) 26B pp. 275–279.

2. Colinet C., Pasturel A. Thermodynamic properties of metallic systems. Ch. 134 in: Handbook on the Physics and Chemistry of Rare Earths, 1994 Vol. 19, pp. 479-647.