Ni – Ru (Nickel – Ruthenium)

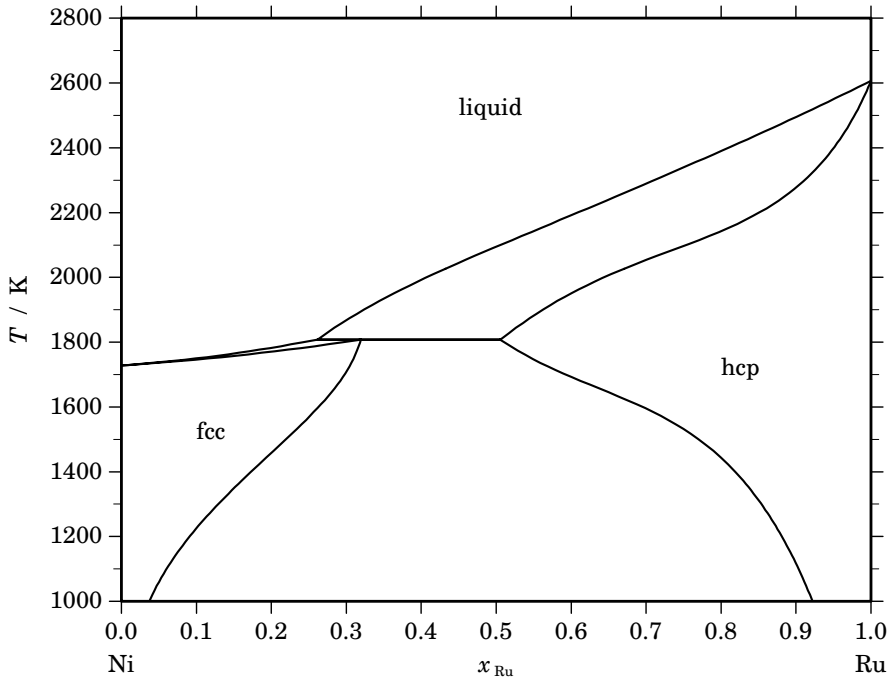

Fig. 1. Calculated phase diagram for the system Ni-Ru.

The Ni-Ru binary system contains two components interesting in the nuclear field, nickel being a major component of stainless steel structures of the vessel, and ruthenium being selected as representative of a family of non-volatile fission products. Experimental information on the phase diagram has been reported in the compilations of Hansen and Anderko [1958Han], Elliott [1965Ell] and Shunk [1969Shu]. It is based on the investigations of Raub and Menzel [1961Rau], and Kornilov and Myasnikova [1964Kor]. There is complete solubility of the components in the liquid state and a limited mutual solubility of Ni and Ru in the solid state, being maximal at the peritectic temperature. No thermodynamic data are available for the binary system. The system was assessed by Chevalier and Fischer [2001Che], and by Hallström [2004Hal]. The excess Gibbs energy of the liquid, fcc and hcp solution phases was optimised from the selected phase diagram information. A regular substitution model was used for the first two phases, and a sub-regular description for the hcp phase. The agreement with the experimental information [1961Rau, 1964Kor] is quite satisfactory.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Ni,Ru)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Ni,Ru)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Ni,Ru)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ru}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid + hcp $\rightleftharpoons$ fcc	peritectic	1807.8	0.261	0.505	0.319	−10683

Table IIIa. Integral quantities for the liquid phase at 2700 K.

x_{Ru}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G_{\mathrm{m}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{m}}^{\mathrm{E}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−6511	786	2.703	786	0.000	0.000
0.200	−9836	1398	4.161	1398	0.000	0.000
0.300	−11878	1835	5.079	1835	0.000	0.000
0.400	−13011	2097	5.596	2097	0.000	0.000
0.500	−13376	2185	5.763	2185	0.000	0.000
0.600	−13011	2097	5.596	2097	0.000	0.000
0.700	−11878	1835	5.079	1835	0.000	0.000
0.800	−9836	1398	4.161	1398	0.000	0.000
0.900	−6511	786	2.703	786	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

Reference states: Ni(liquid), Ru(liquid)

Table IIIb. Partial quantities for Ni in the liquid phase at 2700 K.

x_{Ni}	ΔG_{Ni} [J/mol]	ΔH_{Ni} [J/mol]	ΔS_{Ni} [J/(mol·K)]	$G_{\mathrm{Ni}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ni}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ni}	γ_{Ni}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2278	87	0.876	87	0.000	0.904	1.004
0.800	−4660	350	1.855	350	0.000	0.813	1.016
0.700	−7221	786	2.966	786	0.000	0.725	1.036
0.600	−10070	1398	4.247	1398	0.000	0.639	1.064
0.500	−13376	2185	5.763	2185	0.000	0.551	1.102
0.400	−17424	3146	7.619	3146	0.000	0.460	1.150
0.300	−22747	4282	10.010	4282	0.000	0.363	1.210
0.200	−30538	5592	13.382	5592	0.000	0.257	1.283
0.100	−44613	7078	19.145	7078	0.000	0.137	1.371
0.000	$-\infty$	8738	∞	8738	0.000	0.000	1.476

Reference state: Ni(liquid)

Table IIIc. Partial quantities for Ru in the liquid phase at 2700 K.

x_{Ru}	ΔG_{Ru} [J/mol]	ΔH_{Ru} [J/mol]	ΔS_{Ru} [J/(mol·K)]	$G_{\mathrm{Ru}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ru}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ru}	γ_{Ru}
0.000	$-\infty$	8738	∞	8738	0.000	0.000	1.476
0.100	−44613	7078	19.145	7078	0.000	0.137	1.371
0.200	−30538	5592	13.382	5592	0.000	0.257	1.283
0.300	−22747	4282	10.010	4282	0.000	0.363	1.210
0.400	−17424	3146	7.619	3146	0.000	0.460	1.150
0.500	−13376	2185	5.763	2185	0.000	0.551	1.102
0.600	−10070	1398	4.247	1398	0.000	0.639	1.064
0.700	−7221	786	2.966	786	0.000	0.725	1.036
0.800	−4660	350	1.855	350	0.000	0.813	1.016
0.900	−2278	87	0.876	87	0.000	0.904	1.004
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ru(liquid)

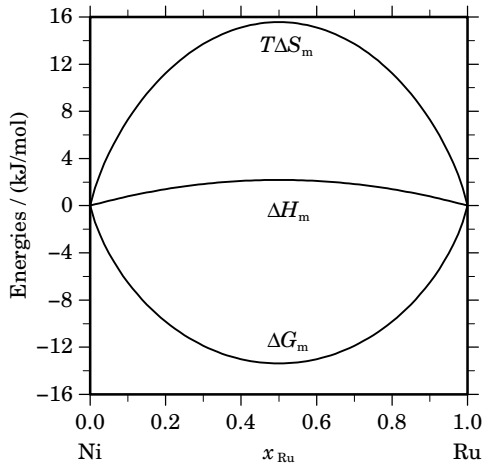

Fig. 2. Integral quantities of the liquid phase at T=2700 K.

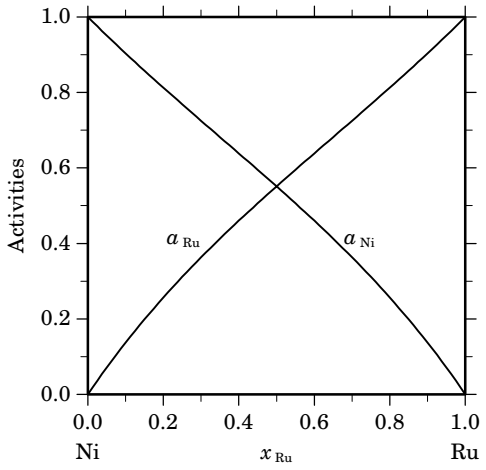

Fig. 3. Activities in the liquid phase at T=2700 K.

Table IVa. Integral quantities for the stable phases at 1700 K.

Phase	x_{Ru}	ΔG_{m} [J/mol]	ΔH_{m} [J/mol]	ΔS_{m} [J/(mol·K)]	$G_{\mathrm{m}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{m}}^{\mathrm{E}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
fcc	0.000	0	0	0.000	0	0.000	0.000
	0.100	−2763	3743	3.827	1832	1.124	−0.008
	0.200	−3629	6932	6.212	3444	2.052	−0.011
	0.298	−3801	9510	7.830	4806	2.767	−0.012
hcp	0.593	−3584	10118	8.060	5969	2.440	−0.009
	0.600	−3578	9930	7.946	5935	2.350	−0.008
	0.700	−3409	7141	6.206	5226	1.127	−0.006
	0.800	−3036	4272	4.299	4037	0.139	−0.004
	0.900	−2282	1750	2.372	2313	−0.331	−0.002
	1.000	0	0	0.000	0	0.000	0.000

Reference states: Ni(fcc), Ru(hcp)

Table IVb. Partial quantities for Ni in the stable phases at 1700 K.

Phase	x_{Ni}	ΔG_{Ni} [J/mol]	ΔH_{Ni} [J/mol]	ΔS_{Ni} [J/(mol·K)]	$G_{\mathrm{Ni}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Ni}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Ni}	γ_{Ni}
fcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1379	278	0.975	110	0.099	0.907	1.008
	0.800	−2714	1110	2.249	440	0.394	0.825	1.032
	0.702	−4019	2457	3.810	975	0.872	0.752	1.071
hcp	0.407	−4019	25335	17.267	8677	9.799	0.752	1.848
	0.400	−4091	25562	17.443	8861	9.824	0.749	1.872
	0.300	−5212	27439	19.206	11806	9.196	0.692	2.305
	0.200	−7134	26409	19.731	15615	6.349	0.604	3.018
	0.100	−12151	21616	19.863	20396	0.718	0.423	4.233
	0.000	$-\infty$	12208	∞	26259	−8.265	0.000	6.409

Reference state: Ni(fcc)

Table IVc. Partial quantities for Ru in the stable phases at 1700 K.

Phase	x_{Ru}	ΔG_{Ru} [J/mol]	ΔH_{Ru} [J/mol]	ΔS_{Ru} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Ru}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ru}}$ [J/(mol·K)]	a_{Ru}	γ_{Ru}
fcc	0.000	$-\infty$	40211	∞	19422	12.229	0.000	3.951
	0.100	−15217	34935	29.501	17329	10.356	0.341	3.408
	0.200	−7291	30219	22.065	15458	8.683	0.597	2.985
	0.298	−3284	26153	17.316	13844	7.241	0.793	2.663
hcp	0.593	−3284	−338	1.733	4109	−2.616	0.793	1.337
	0.600	−3236	−492	1.614	3985	−2.633	0.795	1.326
	0.700	−2636	−1558	0.634	2406	−2.331	0.830	1.186
	0.800	−2012	−1262	0.441	1142	−1.414	0.867	1.084
	0.900	−1185	−458	0.428	304	−0.448	0.920	1.022
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ru(hcp)

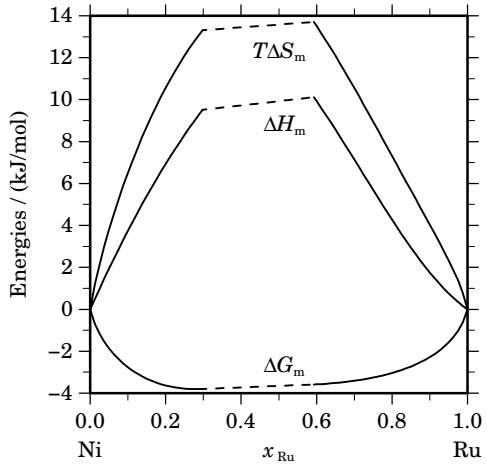

Fig. 4. Integral quantities of the stable phases at T=1700 K.

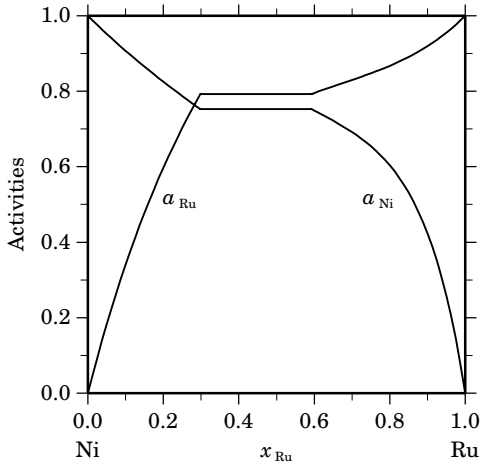

Fig. 5. Activities in the stable phases at T=1700 K.

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