Fe – Ru (Iron – Ruthenium)

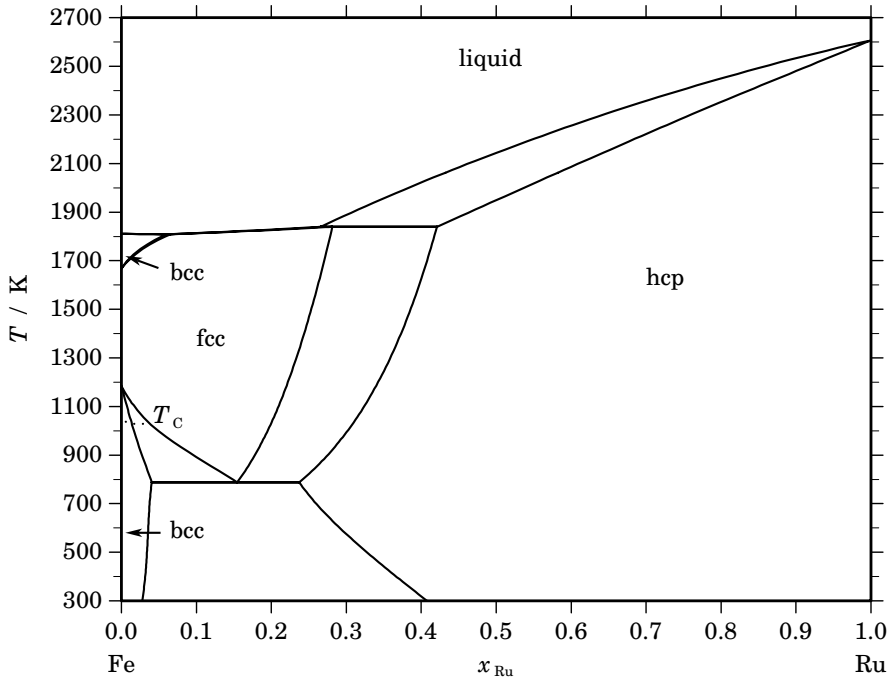

Fig. 1. Calculated phase diagram for the system Fe-Ru.

The Fe-Ru binary system contains two components interesting for the nuclear field, iron 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 several compilations of binary systems [1958Han, 1965Ell, 1969Shu]. The components are completely miscible in the liquid state. The maximal solubility of ruthenium reaches 5 at.% at 1809 K and 4.8 at.% at 773 K in iron-rich bcc terminal solid solutions, and varies from 9.3 at.% at 773 K to 29.5 at.% at 1863 K in the iron-rich fcc terminal solid solution. The solubility of iron in ruthenium-rich hcp terminal solid solutions varies from 76.5 at.% at 773 K to 64.5 at.% at 1863 K. The transition temperatures fcc/bcc have been studied by Fallot [1938Fal] and Martelly [1938Mar] using X-ray and magnetic analysis. The iron-rich side at high temperature was determined by Gibson and Hume-Rothery [1958Gib] by thermal analysis. Raub and Plate [1960Rau] determined monophasic and diphasic domains between fcc, hcp and bcc in the range from 673 K to 1473 K. The activity of iron in the fcc and hcp domains was determined by Stepakoff and Kaufman [1968Ste] from vapour pressure measurements at 1600 K. The system was assessed by Chevalier and Fischer [2004Che]. The excess Gibbs energy of the liquid, bcc, fcc and hcp solution phases was optimised based on selected experimental information for the phase diagram and thermodynamic properties. A regular substitution model was used for all solution phases. The agreement with the experimental information is satisfactory, but however the vertical shape of the fcc/hcp region [1960Rau] cannot be easily reproduced to be compatible with the peritectic determined by Obrowski [1959Obr]. This point should be re-analysed.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					LIQUID	$(Fe,Ru)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,Ru)_1$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,Ru)_1$
hcp	$A3$	Mg	$hP2$	$P6_3/mmc$	HCP_A3	$(Fe,Ru)_1$

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_{Ru}			$\Delta_{\mathrm{r}}H$ / (J/mol)
liquid + hcp $\rightleftharpoons$ fcc	peritectic	1839.4	0.266	0.421	0.281	−17178
liquid $\rightleftharpoons$ bcc + fcc	eutectic	1808.4	0.061	0.060	0.065	−14565
fcc $\rightleftharpoons$ bcc + hcp	eutectoid	788.2	0.154	0.041	0.237	−3042

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)]	$G^{\mathrm{E}}_{\mathrm{m}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{m}}$ [J/(mol·K)]	ΔC_P [J/(mol·K)]
0.000	0	0	0.000	0	0.000	0.000
0.100	−9093	−1795	2.703	−1795	0.000	0.000
0.200	−14426	−3192	4.161	−3192	0.000	0.000
0.300	−17903	−4189	5.079	−4189	0.000	0.000
0.400	−19897	−4788	5.596	−4788	0.000	0.000
0.500	−20548	−4987	5.763	−4987	0.000	0.000
0.600	−19896	−4788	5.596	−4788	0.000	0.000
0.700	−17903	−4189	5.079	−4189	0.000	0.000
0.800	−14426	−3192	4.161	−3192	0.000	0.000
0.900	−9093	−1795	2.703	−1795	0.000	0.000
1.000	0	0	0.000	0	0.000	0.000

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

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

x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	$G^{\mathrm{E}}_{\mathrm{Fe}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Fe}}$ [J/(mol·K)]	a_{Fe}	γ_{Fe}
1.000	0	0	0.000	0	0.000	1.000	1.000
0.900	−2565	−199	0.876	−199	0.000	0.892	0.991
0.800	−5807	−798	1.855	−798	0.000	0.772	0.965
0.700	−9803	−1795	2.966	−1795	0.000	0.646	0.923
0.600	−14660	−3192	4.247	−3192	0.000	0.520	0.867
0.500	−20548	−4987	5.763	−4987	0.000	0.400	0.801
0.400	−27752	−7182	7.619	−7182	0.000	0.290	0.726
0.300	−36804	−9775	10.010	−9775	0.000	0.194	0.647
0.200	−48898	−12768	13.382	−12768	0.000	0.113	0.566
0.100	−67850	−16159	19.145	−16159	0.000	0.049	0.487
0.000	$-\infty$	−19950	∞	−19950	0.000	0.000	0.411

Reference state: Fe(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)]	$G^{\mathrm{E}}_{\mathrm{Ru}}$ [J/mol]	$S^{\mathrm{E}}_{\mathrm{Ru}}$ [J/(mol·K)]	a_{Ru}	γ_{Ru}
0.000	$-\infty$	−19950	∞	−19950	0.000	0.000	0.411
0.100	−67850	−16159	19.145	−16159	0.000	0.049	0.487
0.200	−48898	−12768	13.382	−12768	0.000	0.113	0.566
0.300	−36804	−9775	10.010	−9775	0.000	0.194	0.647
0.400	−27752	−7182	7.619	−7182	0.000	0.290	0.726
0.500	−20548	−4987	5.763	−4987	0.000	0.400	0.801
0.600	−14660	−3192	4.247	−3192	0.000	0.520	0.867
0.700	−9803	−1795	2.966	−1795	0.000	0.646	0.923
0.800	−5807	−798	1.855	−798	0.000	0.772	0.965
0.900	−2565	−199	0.876	−199	0.000	0.892	0.991
1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ru(liquid)

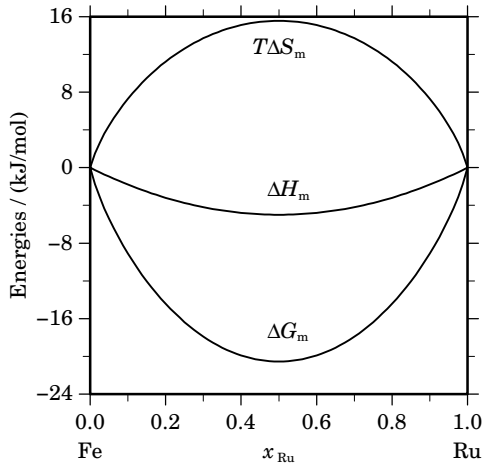

Fig. 2. Integral quantities of the liquid phase at T=2700 K.

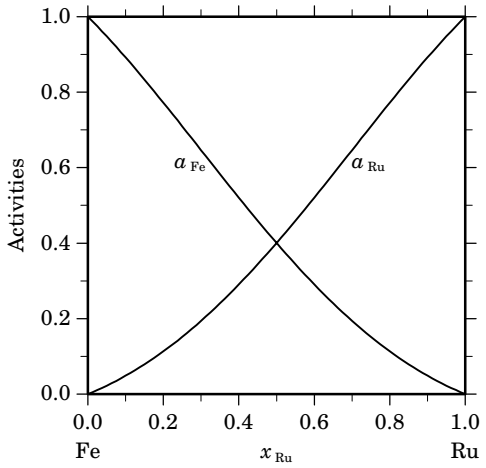

Fig. 3. Activities in the liquid phase at T=2700 K.

Table IVa. Integral quantities for the stable phases at 1600 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	−5240	−1834	2.129	−915	−0.574	0.000
	0.200	−8092	−2983	3.193	−1435	−0.968	0.000
	0.262	−9212	−3352	3.663	−1559	−1.121	0.000
hcp	0.397	−11174	−5881	3.308	−2235	−2.279	0.000
	0.400	−11213	−5886	3.329	−2260	−2.266	0.000
	0.500	−12156	−5850	3.941	−2935	−1.822	0.000
	0.600	−12143	−5437	4.191	−3190	−1.404	0.000
	0.700	−11150	−4645	4.066	−3024	−1.013	0.000
	0.800	−9094	−3475	3.512	−2437	−0.649	0.000
	0.900	−5753	−1927	2.392	−1429	−0.311	0.000
	1.000	0	0	0.000	0	0.000	0.000

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

Table IVb. Partial quantities for Fe in the stable phases at 1600 K.

Phase	x_{Fe}	ΔG_{Fe} [J/mol]	ΔH_{Fe} [J/mol]	ΔS_{Fe} [J/(mol·K)]	$G_{\mathrm{Fe}}^{\mathrm{E}}$ [J/mol]	$S_{\mathrm{Fe}}^{\mathrm{E}}$ [J/(mol·K)]	a_{Fe}	γ_{Fe}
fcc	1.000	0	0	0.000	0	0.000	1.000	1.000
	0.900	−1600	−343	0.786	−198	−0.090	0.887	0.985
	0.800	−3760	−1371	1.493	−792	−0.362	0.754	0.942
	0.738	−5406	−2356	1.906	−1361	−0.622	0.666	0.903
hcp	0.603	−5406	−5229	0.111	1330	−4.099	0.666	1.105
	0.600	−5511	−5270	0.151	1284	−4.096	0.661	1.101
	0.500	−9831	−6972	1.787	−610	−3.977	0.478	0.955
	0.400	−15114	−9053	3.788	−2924	−3.830	0.321	0.803
	0.300	−21677	−11512	6.353	−5660	−3.657	0.196	0.653
	0.200	−30227	−14349	9.924	−8816	−3.458	0.103	0.515
	0.100	−43025	−17565	15.913	−12393	−3.232	0.039	0.394
	0.000	$-\infty$	−21158	∞	−16392	−2.979	0.000	0.292

Reference state: Fe(fcc)

Table IVc. Partial quantities for Ru in the stable phases at 1600 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	$-\infty$	−21771	∞	−11134	−6.648	0.000	0.433
	0.100	−38005	−15259	14.216	−7373	−4.929	0.057	0.575
	0.200	−25419	−9433	9.991	−4008	−3.391	0.148	0.740
	0.262	−19924	−6156	8.605	−2115	−2.525	0.224	0.853
hcp	0.397	−19924	−6871	8.158	−7644	0.483	0.224	0.563
	0.400	−19765	−6809	8.097	−7575	0.479	0.226	0.566
	0.500	−14482	−4729	6.096	−5261	0.332	0.337	0.673
	0.600	−10162	−3026	4.460	−3367	0.213	0.466	0.776
	0.700	−6639	−1702	3.085	−1894	0.120	0.607	0.867
	0.800	−3810	−757	1.909	−842	0.053	0.751	0.939
	0.900	−1612	−189	0.889	−210	0.013	0.886	0.984
	1.000	0	0	0.000	0	0.000	1.000	1.000

Reference state: Ru(hcp)

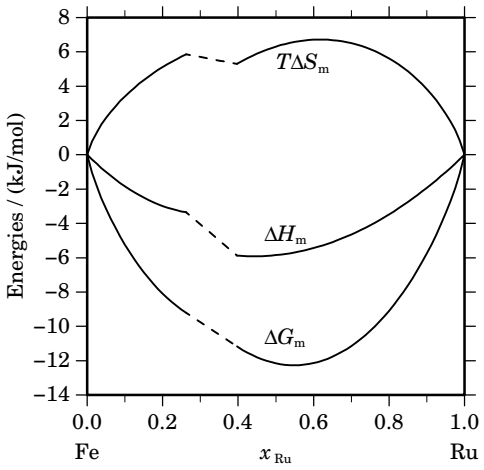

Fig. 4. Integral quantities of the stable phases at T=1600 K.

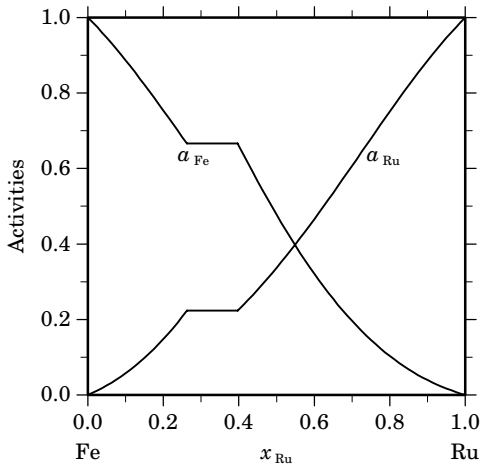

Fig. 5. Activities in the stable phases at T=1600 K.

References

[1938Fal] M. Fallot: Ann. Phys. **10** (1938) 291–332.

[1938Mar] J. Martelly: Ann. Phys. **9** (1938) 318–333.

[1958Gib] W.S. Gibson, F. Hume-Rothery: J. Iron Steel Inst. **189** (1958) 243–250.

[1958Han] M. Hansen, K. Anderko, "Constitution of Binary Alloys", McGraw-Hill, 1958.

[1959Obr] W. Obrowski: Naturwiss. **46** (1959) 624–625.

[1960Rau] E. Raub, W. Plate: Z. Metallkd. **51** (1960) 477–481.

[1965Ell] R.P. Elliott, "Constitution of Binary Alloys", 1st Suppl., McGraw-Hill, New-York, 1965.

[1968Ste] G.L. Stepakoff, L. Kaufman: Acta Metall. **16** (1968) 13–22.

[1969Shu] F.A. Shunk, "Constitution of Binary Alloys", 2nd Suppl., McGraw-Hill, New-York, 1969.

[2004Che] P.-Y. Chevalier, E. Fischer, unpublished work, 2004.