Fe – S (Iron – Sulphur)

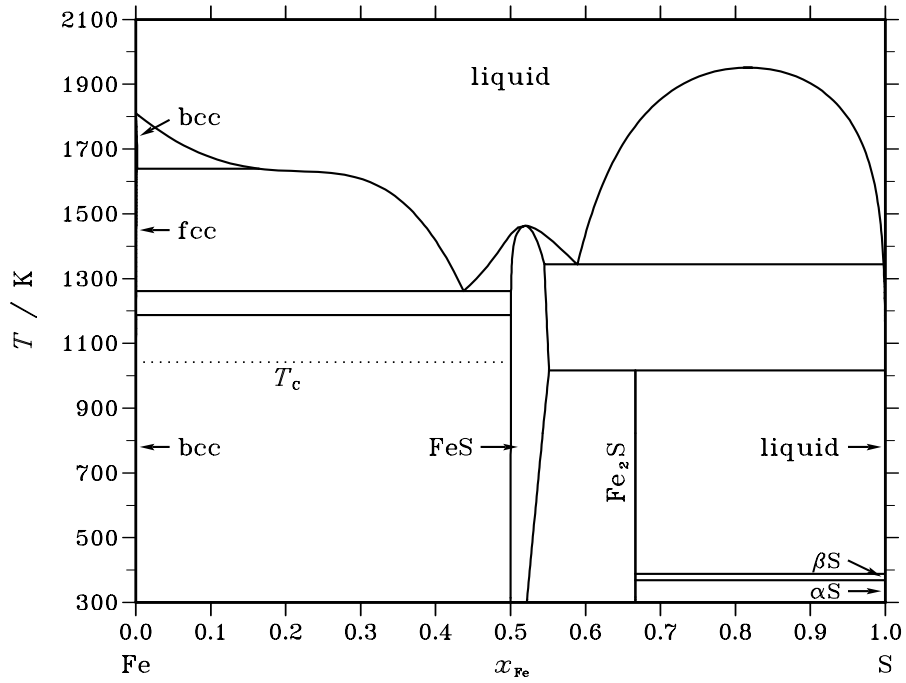

Fig. 1. Calculated phase diagram for the system Fe-S.

The Fe-S system is characterized by a low melting eutectic at 1262 K which may cause trouble in steels unless Mn is added to form solid MnS. The solubility of S in solid iron is low but the liquid can dissolve more than 50 mole-% S. At equiatomic composition there are several compounds but the high temperature form, pyrrhotite, is the only one included in the assessment. It melts congruently at 1463 K and has a rather broad solubility range because the sulfur content can vary due to vacancies on the iron lattice. The 2 polymorphs of FeS_2, marcasite and pyrite, are represented simply by a single stoichiometric compound.
At higher sulfur compositions solid or liquid sulphur or sulfur gas become stable. The calculated phase diagram is without the gas phase and shows a closed miscibility gap on the high sulfur side.
The original assessment [81Fer] has been updated [92Sun] due to later modifications of the liquid model.

Table I. Phases, structures and models.

Phase	Struktur-bericht	Prototype	Pearson symbol	Space group	SGTE name	Model
liquid					IONIC_LIQUID	$Fe_p^{2+}(S^{2-},S,\Box)_q$
bcc	$A2$	W	$cI2$	$Im\overline{3}m$	BCC_A2	$(Fe,S)_1$
fcc	$A1$	Cu	$cF4$	$Fm\overline{3}m$	FCC_A1	$(Fe,S)_1$
αFeS	···	···	···	···	···	$(Fe,\Box)_1S_1$
βFeS	···	···	$hP24$	$P\overline{6}2c$	···	$(Fe,\Box)_1S_1$
γFeS	$B8_1$	NiAs	$hP12$	$P6_3/mmc$	PYRRHOTITE	$(Fe,\Box)_1S_1$
αFeS_2	$C18$	αFeS_2 (marcasite)	$oP6$	$Pnnm$	MARCASITE	Fe_1S_2
βFeS_2	$C2$	βFeS_2 (pyrite)	$cP12$	$Pa\overline{3}$	PYRITE	Fe_1S_2
αS	$A16$	αS	$oF128$	$Fddd$	FC_ORTHO	S_1
βS	···	βS	$mP48$	$P2_1/a$	MONOCLINIC	S_1

Table II. Invariant reactions.

Reaction	Type	T / K	Compositions / x_S			$\Delta_r H$ / (J/mol)
liquid $\rightleftharpoons$ liquid′ + liquid″	critical	1951.7	0.811	0.811	0.811	0
bcc $\rightleftharpoons$ fcc + liquid′	metatectic	1639.2	0.002	0.001	0.164	−734
liquid $\rightleftharpoons$ FeS	congruent	1463.0	0.519	0.519		−13540
liquid′ $\rightleftharpoons$ FeS + liquid″	monotectic	1343.7	0.589	0.545	0.997	−16419
liquid′ $\rightleftharpoons$ fcc + FeS	eutectic	1261.9	0.437	0.000	0.501	−14414
fcc + FeS $\rightleftharpoons$ bcc	peritectoid	1187.5	0.000	0.501	0.000	−970
FeS + liquid″ $\rightleftharpoons$ FeS_2	peritectic	1016.1	0.551	1.000	0.667	−20823
liquid″ $\rightleftharpoons$ FeS_2 + βS	degenerate	388.3	1.000	0.667	1.000	−1721
FeS_2 + βS $\rightleftharpoons$ αS	degenerate	368.3	0.667	1.000	1.000	−401

Table III. Standard reaction quantities at 298.15 K for the compounds per mole of atoms.

Compound	x_S	$\Delta_f G^\circ$ / (J/mol)	$\Delta_f H^\circ$ / (J/mol)	$\Delta_f S^\circ$ / (J/(mol·K))	$\Delta_f C_P^\circ$ / (J/(mol·K))
FeS	0.500	−51473	−48992	8.322	−1.127
FeS_2	0.667	−52359	−56233	12.994	−1.390

References

[81Fer] A. Fernandez Guillermet, M. Hillert, B. Jansson, B. Sundman: Metall. Trans. B **12B** (1981) 745–754.

[92Sun] B. Sundman, unpublished work, 1992.