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Fe-S-Ta (Iron-Sulfur-Tantalum)

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The previous review of this system by [1988Rag] presented a tentative partial isothermal section at 900 °C for Fe-rich alloys. Recently, [2004Wad] determined an isothermal section for this system at 950 °C, which depicts three ternary compounds.

Table 1 Fe-S-Ta crystal structure and lattice parameter data

Phase	Composition, at.%	Pearson symbol	Space group	Lattice parameter, nm
$Fe_{0.33}TaS_2$ (τ_1)	10.0 Fe 30 Ta 60 S	*hP*20	$P6_322$	a = 0.57383 c = 1.22392
$(Fe,Ta)_5S_8$ (τ_2)	23.1-30.8 Fe 15.4-7.7 Ta ~61.5 S	*hP*?	$P\bar{3}m1$	a = 0.33536 c = 0.58140
$Fe_2Ta_9S_6$ (τ_3)	11.8 Fe 52.9 Ta 35.3 S	*hP*34	$P\bar{6}2m$	a = 1.0266 c = 0.6583

Binary Systems

The Fe-S phase diagram [1982Kub] depicts two intermediate phases. The monosulfide $Fe_{1-x}S$ (NiAs-type hexagonal) is stable at Fe-deficient (S-rich) compositions and has a range of 50-55 at.% S. Cubic FeS_2 (pyrite) forms peritectically at 743 °C and undergoes a transition to the orthorhombic form (marcasite) at 425 °C. The Fe-Ta phase diagram [1993Swa] has two intermediate phases: Fe_2Ta ($C14$, $MgZn_2$-type hexagonal) and FeTa (μ) ($D8_5$, Fe_7W_6-type rhombohedral). The S-Ta phase diagram is not known. The intermediate phases, TaS_2, $Ta_{1+x}S_2$, Ta_3S_2, and Ta_6S, are shown as stable at 950 °C by [2004Wad].

Ternary Phases

There are three ternary compounds in this system: $Fe_{0.33}TaS_2$ (τ_1), $(Fe,Ta)_5S_8$ (τ_2), and $Fe_2Ta_9S_6$ (τ_3) [1986Har, 2004Wad]. $(Fe,Ta)_5S_8$ can be written as $Fe_{0.25}(Ta_{0.5}Fe_{0.5})S_2$ to indicate that it is a TaS_2-related structure with two-thirds of the Fe atoms substituting for Ta on the regular sites and one-third inserted interstitially be-

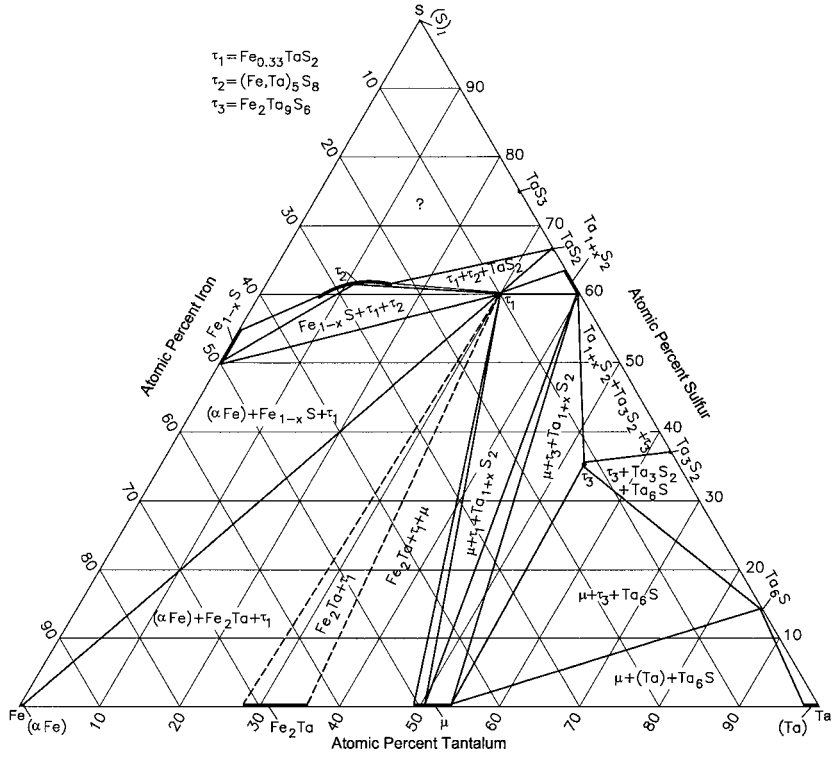

Fig. 1 Fe-S-Ta tentative isothermal section at 950 °C [2004Wad]. Narrow two-phase regions around tie-triangles are omitted

tween layers in the S-Ta-S stacking [2004Wad]. Table 1 lists the structural details of these compounds.

Isothermal Section

With starting materials of 99.9% Fe, 99.9% Ta, 99.9999% S, FeS, and TaS_2, [2004Wad] prepared powder mixtures of 13 compositions. The compacted powders were annealed at 950 °C for 5-14 days and quenched. The phase equilibria were studied by x-ray powder and single-crystal diffraction. The isothermal section constructed by [2004Wad] is redrawn in Fig. 1. The three ternary compounds τ_1, τ_2, and τ_3 are present. $(Fe,Ta)_5S_8$ (τ_2) shows a small homogeneity range. The range shown for the binary phase $Ta_{1+x}S_2$ in Fig. 1 probably includes several variants of that phase.

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