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Al-Nb-Si (Aluminum-Niobium-Silicon)

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Recently, [2004Sha] presented a thermodynamic assessment of this system and computed a liquidus projection and two isothermal sections at 1400 and 1000 °C. The available experimental data on the isothermal sections show good agreement with the computed sections.

Binary Systems

The Al-Nb phase diagram [Massalski2] has three intermediate phases: $NbAl_3$ ($D0_{22}$, $TiAl_3$-type tetragonal), Nb_2Al (30-42 at.% Al; $D8_b$, σCrFe-type tetragonal), and Nb_3Al (18.6-25 at.% Al; $A15$, Cr_3Si-type cubic). The Al-Si system is of the simple eutectic type, with the eutectic temperature at 577 °C and the composition at 12.2 at.% Si. The Nb-Si phase diagram [1993Sch, 1995Sch] has the following intermediate phases. Nb_3Si (Ti_3P-type tetragonal), βNb_5Si_3 ($D8_m$, W_5Si_3-type tetragonal), αNb_5Si_3 ($D8_1$, Cr_5Si_3-type tetragonal), and $NbSi_2$ ($C40$, $CrSi_2$-type hexagonal).

Ternary Phases

Two ternary phases have been identified in this system [1961Bru]. $Al_2Nb_3Si_5$ (denoted τ_1 here) has the $C54$, $TiSi_2$-

Table 1 Al-Nb-Si crystal structure and lattice parameter data

Phase	Composition, at.%	Pearson symbol	Space group	Prototype	Lattice parameter, nm
$Al_2Nb_3Si_5$ (τ_1)	~20 Al ~30 Nb ~50 Si	*oF*24	*Fddd*	$TiSi_2$	a = 0.8403 b = 0.4901 c = 0.8794
$Al_3Nb_{10}Si_3$ (τ_2)	~18.75 Al ~62.5 Nb ~18.75 Si	*tI*32	*I*4/*mcm*	W_5Si_3	a = 1.016 c = 0.508

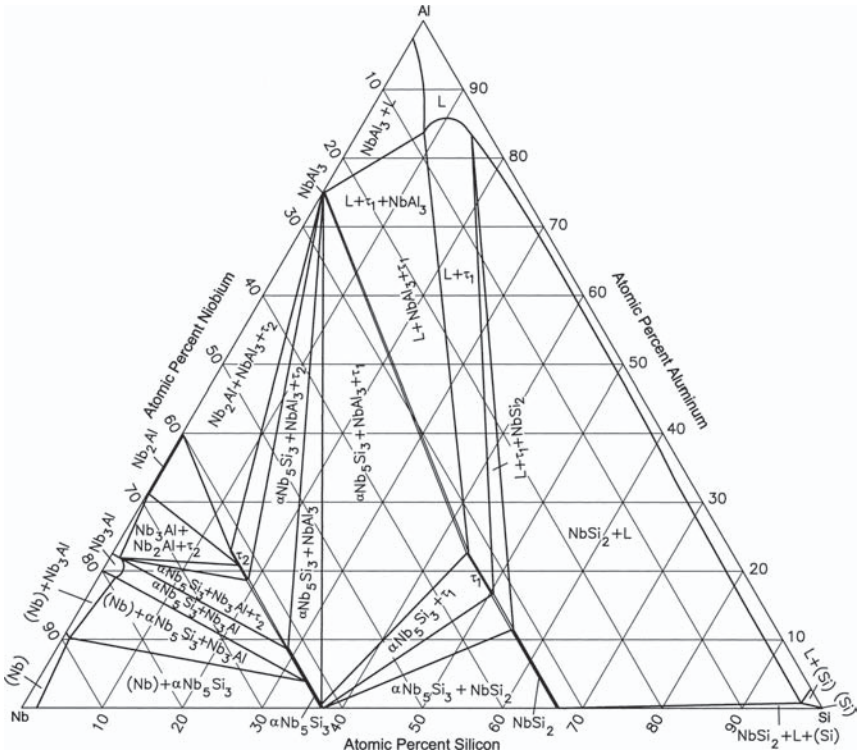

Fig. 1 Al-Nb-Si computed isothermal section at 1400 °C [2004Sha]

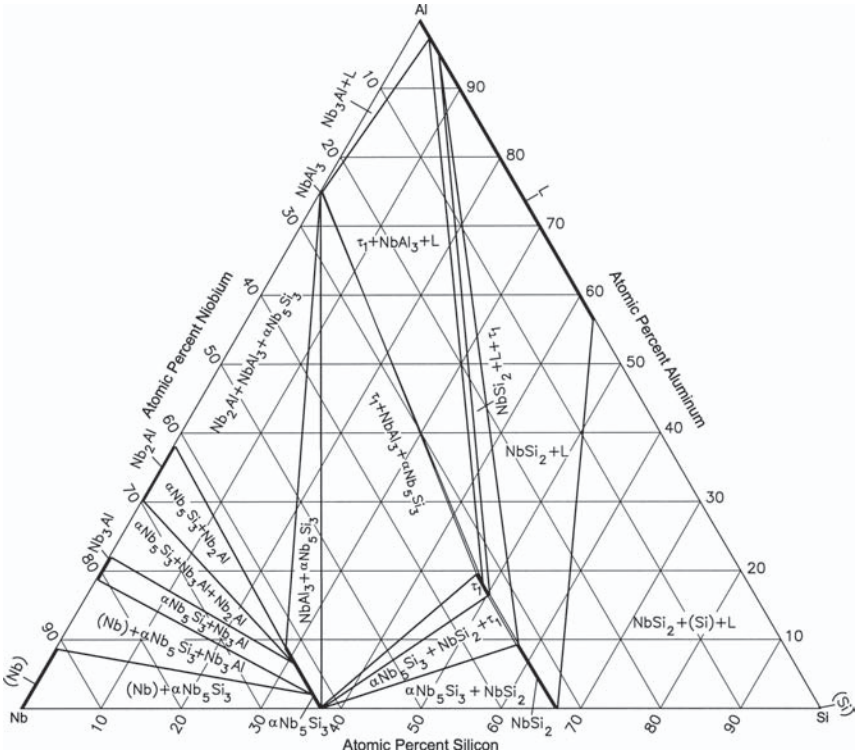

Fig. 2 Al-Nb-Si computed isothermal section at 1000 °C [2004Sha]

type orthorhombic structure, with a small homogeneity range at constant Nb content. The other compound $Al_3Nb_{10}Si_3$ (denoted τ_2 here and β by [2004Sha]) has the $D8_m$-type tetragonal structure of βNb_5Si_3. It is apparently stabilized by Al substituting for Si. It is stable at 1400 °C as a ternary phase, even though the decomposition temperature of βNb_5Si_3 in the binary system is 1650 °C. τ_2 was not found at 1000 °C by [2003Zha].

Isothermal Sections

The experimental investigations of this system are [1961Bru] (a composite isothermal section at 1400 °C for Nb-rich alloys and at 500 °C for Nb-poor alloys), [1973All] (partial isothermal sections for Nb-poor alloys at 1500 and 1300 °C), [1984Pan] (partial isothermal section at 1500 °C for Nb-rich alloys), [2001Mur] (isothermal section valid between 1600-1200 °C), and [2003Zha] (isothermal section at 1000 °C). For the isothermal sections of [1961Bru], [1973All], and [1984Pan], see [1995Vil]. [2001Mur] used powders of 99.9% Al, 99.8% Nb, and 99.9% Si to prepare samples by compacting and sintering in the temperature range of 1200-1600 °C for 0.3-0.6 ks. They confirmed the presence of the two ternary compounds τ_1 and τ_2 and drew a tentative isothermal section valid for the above temperature range. Crystallographic data for these two ternary phases are given in Table 1. Using a diffusion-multiple approach, [2003Zha] constructed an isothermal section at 1000 °C, which depicts the ternary phase τ_1. The Al-stabilized βNb_5Si_3-based ternary phase (τ_2) was not found at this temperature. Tie-lines form between αNb_5Si_3 and $NbAl_3$, confirming the results of [1984Pan] and [2001Mur]. The Al solubility in αNb_5Si_3 is ~8 at.%, with the Al atoms substituting for Si.

[2004Sha] developed a thermodynamic description of this system using the CALPHAD approach. For the Al-Nb and Al-Si systems, the earlier descriptions from the literature were used. The Nb-Si system was reoptimized by [2004Sha], using a term for the excess entropy of mixing of the liquid phase. The computed isothermal sections at 1400 and 1000 °C are redrawn in Fig. 1 and 2. [2004Sha] found good agreement with the experimental data of [1961Bru], [2001Mur], and [2003Zha]. [2004Sha] computed a liquidus projection, which depicts that τ_1 and αNb_5Si_3 form peritectically in the ternary region. There are no experimental data to compare with the computed projection.

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