

Li-Si (Lithium-Silicon)

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The Li-Si phase diagram in [Massalski2] was adopted from [1990Oka] (Fig. 1 excluding the LiSi phase). [1995Bra] assessed this system thermodynamically. The existence of four intermetallic compounds ($\text{Li}_{12}\text{Si}_5$, $\text{Li}_{13}\text{Si}_4$, Li_7Si_3 , and $\text{Li}_{12}\text{Si}_7$) was assumed, as in [1990Oka]. The existence of LiSi has not been reported in [1990Oka] and [1995Bra] although the other alkali monosilicides (NaSi, KSi, RbSi, and CsSi) were known to exist.

[2003Ste] observed the formation of LiSi at pressures of 1–2.5 GPa and at temperatures between 500 and 700 °C. LiSi is a stable phase, but its formation has not been

observed due to slow kinetics. LiSi decomposes on heating at 470 °C, as shown in Fig. 1.

Li-Si crystal structure data are shown in Table 1.

References

1990Oka: H. Okamoto, The Li-Si (Lithium-Silicon) System, *Bull. Alloy Phase Diagrams*, 1990, **11**(3), p 306-312

1995Bra: M.H. Braga, L.F. Malheiros, and I. Ansara, Thermodynamic Assessment of the Li-Si System, *J. Phase Equilib.*, 1995, **16**(4), p 324-329

Table 1 Li-Si crystal structure data

Phase	Composition, at.% Si	Pearson symbol	Space group	Strukturbericht designation	Prototype
(βLi)	0	<i>cI2</i>	<i>Im</i> $\bar{3}m$	<i>A2</i>	W
$\text{Li}_{22}\text{Si}_5$	18.5	<i>cF432</i>	<i>F23</i>	...	$\text{Li}_{22}\text{Pb}_5$
$\text{Li}_{13}\text{Si}_4$	23.5	<i>oP24</i>	<i>Pbam</i>
Li_7Si_3	30	<i>hR7</i>	<i>R</i> $\bar{3}m$
$\text{Li}_{12}\text{Si}_7$	36.8	<i>oP152</i>	<i>Pnma</i>
LiSi	50	<i>tI*</i>	<i>I4</i> $_1/a$
(Si)	100	<i>cF8</i>	<i>Fd</i> $\bar{3}m$	<i>A4</i>	C (diamond)

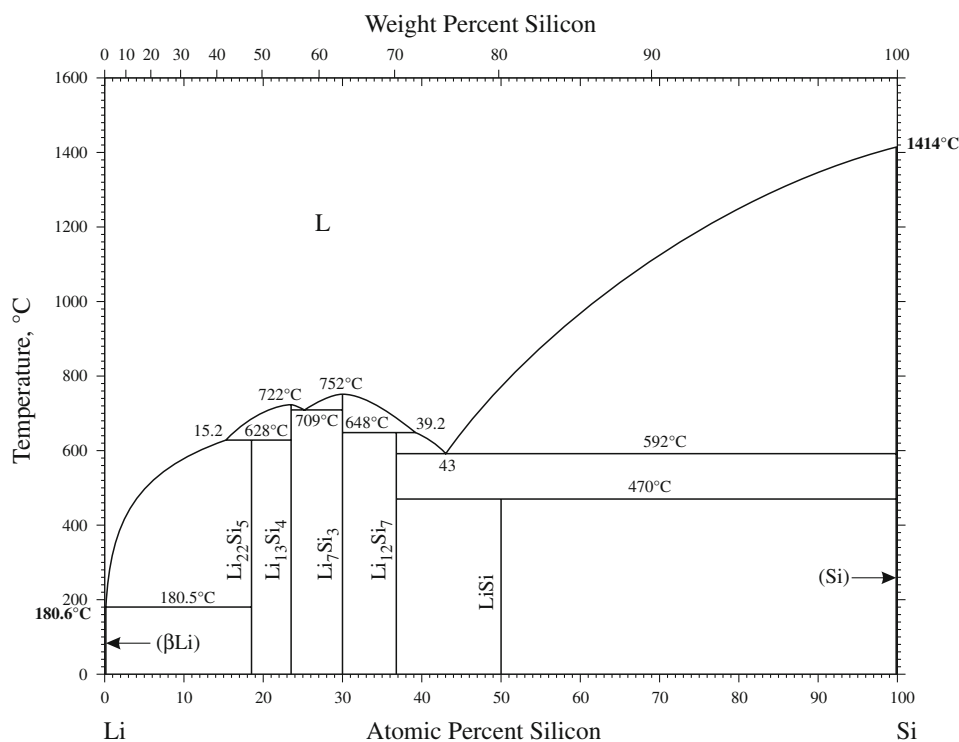


Fig. 1 Li-Si phase diagram

2003Ste: L.A. Stearns, J. Gryko, J. Diefenbacher, G.K. Ramachandran, and P.F. McMillan, Lithium Monosilicide (LiSi), a Low-dimensional Silicon-based Material Prepared by

High Pressure Synthesis: NMR and Vibrational Spectroscopy and Electrical Properties Characterization, *J. Solid State Chem.*, 2003, **173**, p 251-258