

O-Si (Oxygen-Silicon)

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The Si-O phase diagram in [Massalski2], drawn from [1990Wri], showed the equilibrium under a pressure high enough to suppress the gas phase.

[2004Sch] evaluated the Si-O system thermodynamically and proposed the phase diagram at 1 bar (Fig. 1). Figure 2 shows the detail on the Si-rich end. Only one intermediate phase, γSiO_2 (cristobalite), is stable in the temperature range shown in Fig. 1. βSiO_2 and αSiO_2 are stable from 872 to 575 °C and below 575 °C, respectively [2004Sch].

According to [1990Wri], SiO_2 exists in four polymorphic, but the highest temperature form is metastable according to [2004Sch].

Table 1 shows Si-O crystal structure data.

References

- 1990Wri:** H. Wriedt, The O-Si (Oxygen-Silicon) System, *Bull. Alloy Phase Diagrams*, 1990, **11**(1), p 43-61
2004Sch: S.M. Schnurre, J. Grobner, and R. Schmid-Fetzer, Thermodynamics and Phase Stability in the Si-O System, *J. Non-Cryst. Solids*, 2004, **336**, p 1-25

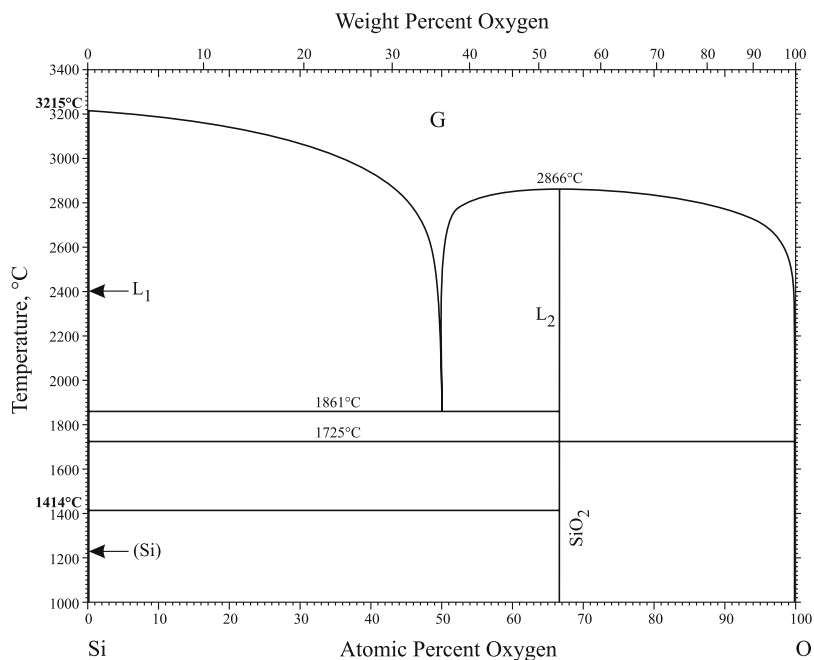


Fig. 1 Si-O phase diagram

Section III: Supplemental Literature Review

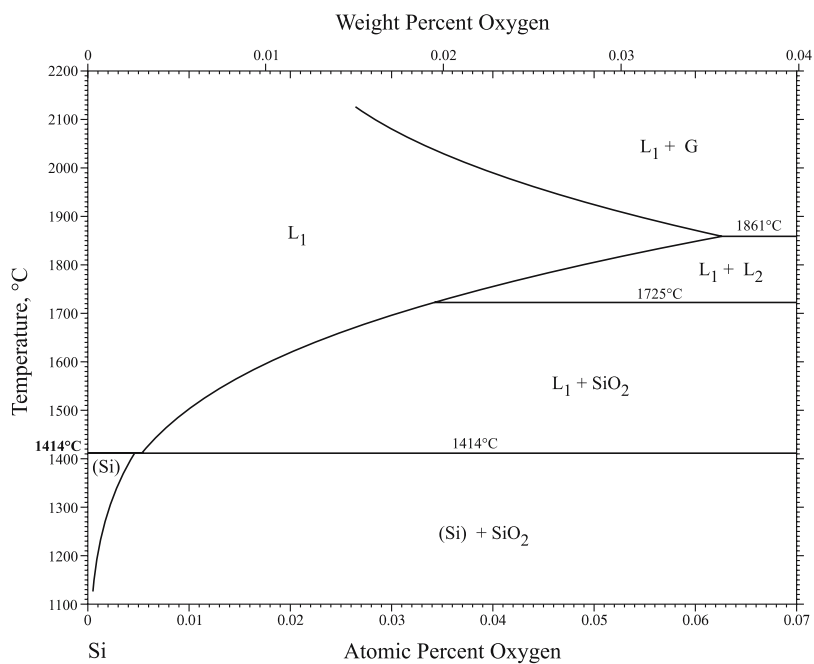


Fig. 2 Partial Si-O phase diagram around the Si-rich end

Table 1 Si-O crystal structure data

| Phase | Composition, at.% O | Pearson symbol | Space group | Struktur-bericht designation | Prototype |
|---------------------------|---------------------|----------------|--------------------------------|------------------------------|--------------|
| (Si) | 0 | <i>cF8</i> | <i>Fd$\bar{3}m$</i> | <i>A4</i> | C (diamond) |
| γ SiO ₂ | 66.7 | <i>cF104</i> | <i>Fd$\bar{3}m$</i> | ... | Cristobalite |
| β SiO ₂ | 66.7 | <i>hP9</i> | <i>P6₂66</i> | ... | High quartz |
| α SiO ₂ | 66.7 | <i>hP9</i> | <i>P3₂21</i> | ... | Low quartz |