Hydrous olivine defect reactions

List of defects

Description	Label	Kroger-Vink	Formula	Peak (cm ⁻¹)
Ti on an M site, likely M1, a Si vacancy and ferric iron	[Ti-anhyd]	$\{{\rm Ti}^{**}{}_{M1} - {\rm V}^{""}{}_{Si} - 2({\rm Fe}^{3+})^{*}{}_{M}\}$	MgTiFe ₂ SiO ₈	None
Titanium clinohumite. See, e.g., Walker et al. 2007	[Ti-2H]	{Ti** _{M1} -V"" _{Si} -2(OH)* _O }	MgTiH ₂ O ₄	3525, 3573
A Si vacancy and 4H ⁺	[Si-4H]	{V"" _{Si} -4(OH)* _O }	Mg ₂ H ₄ O ₄	3600
A Si vacancy and 4 ferric irons on M sites	[Si-anhyd]	$\{V^{""}_{Si}-4(Fe^{3+})^*_{M}\}$	Fe ₄ SiO ₈	None
A Si vacancy, 2H ⁺ , and 2 ferric irons on M sites	[Si-2H]	$\{V^{""}_{Si}-2(Fe^{3+})^*_{M}-2(OH)^*_{O}\}$	Fe ₂ H ₂ O ₄	3600
A metal vacancy, a ferric iron on an M site, and H ⁺	[tri-H]	${V''_{M}-(Fe^{3+})^*_{M}-(OH)^*_{O}}$	FeHSiO ₄	3356
A metal vacancy and 4 ferric irons on M sites	[tri-anhyd]	$\{V''_{M}-2(Fe^{3+})^{*}_{M}\}$	$MgFe_2Si_2O_8$	None

Fast diffusion in and out (decoration of pre-existing Ti defects)

Overview

$$[Ti-anhyd] + H_2 = [Ti-2H]$$

Kroger-Vink

$$\{Ti_{M1}^{**} - V_{Si}^{**} - 2(Fe_{M}^{3+})_{M}^{*}\} + H_2 = \{Ti_{M1}^{**} - V_{Si}^{**} - 2(OH)_{O}^{*}\} + 2Fe_{M}^{*}$$

Formula

 $MgTiFe_2SiO_8 + H_2 = MgTiH_2O_4 + Fe_2SiO_4$

Slow redistribution of H between Si vacancies

Overview

$$[Ti-anhyd] + [Si-4H] \rightarrow [Ti-2H] + [Si-2H]$$

Kroger-Vink

$$\{ {\rm Ti}^{**}_{\ M1} - {\rm V}^{""}_{\ Si} - 2({\rm Fe}^{3+})^{*}_{\ M} \} + \{ {\rm V}^{""}_{\ Si} - 4({\rm OH})^{*}_{\ O} \} \ \rightarrow \ \{ {\rm Ti}^{**}_{\ M1} - {\rm V}^{""}_{\ Si} - 2({\rm OH})^{*}_{\ O} \} \ + \{ {\rm V}^{""}_{\ Si} - 2({\rm Fe}^{3+})^{*}_{\ M} - 2({\rm OH})^{*}_{\ O} \} \ + \{ {\rm V}^{""}_{\ Si} - 2({\rm Fe}^{3+})^{*}_{\ M} - 2({\rm OH})^{*}_{\ O} \} \ + \{ {\rm V}^{""}_{\ Si} - 2({\rm Fe}^{3+})^{*}_{\ M} - 2({\rm OH})^{*}_{\ O} \} \ + \{ {\rm V}^{""}_{\ Si} - 2({\rm OH})^{*}_{\ O} \} \ + \{ {\rm V}^{""}_{\ OH} + 2({\rm OH})^{*}_{\ OH} + 2({\rm OH})$$

Formula

$$MgTiFe_2SiO_8 + Mg_2H_4O_4 \rightarrow MgTiH_2O_4 + Fe_2H_2O_4 + Mg_2SiO_4$$

Alternative: full dehydration of [Si]

$$2[Ti-anhyd] + [Si-4H] \rightarrow 2[Ti-2H] + [Si-anhyd]$$

Redistribution of H in Kilauea lki at 800C

Overview

$$[Si-anhyd] + 4[tri-H] \rightarrow [Si-4H] + 4[tri-anhyd]$$

Kroger-Vink

$$\{V^{""}_{Si}-4(Fe^{3+})^*_{M}\}+4\{V^{"}_{M}-(Fe^{3+})^*_{M}-(OH)^*_{O}\} \rightarrow \{V^{""}_{Si}-4(OH)^*_{O}\}+4\{V^{"}_{M}-2(Fe^{3+})^*_{M}\}$$

Formula

$$Fe_4SiO_8 + 4FeHSiO_4 + 3Mg_2SiO_4 \rightarrow Mg_2H_4O_4 + 4MgFe_2Si_2O_8$$