Radiation damage from long term alpha particle bombardment of silicates - a microfocus XRD and Fe K-edge XANES study

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Supplementary Information

First Shell EXAFS Fit Results (*k* = 6) (corresponding to Figure 2 & Figure 5)

Grunerite EXAFS fit results: Line 1

Sample	(μm)	Path	CN	$S0^2$	σ^2	R	r-factor
Grunerite	0	Fe-O	6	1	0.032	2.093	0.028
Grunerite	6	Fe-O	6	1	0.031	2.067	0.026
Grunerite	12	Fe-O	6	1	0.031	2.067	0.031
Grunerite	18	Fe-O	6	1	0.033	2.08	0.04
Grunerite	24	Fe-O	6	1	0.032	2.073	0.034
Grunerite	30	Fe-O	6	1	0.032	2.066	0.033
Grunerite	36	Fe-O	6	1	0.032	2.064	0.034
Grunerite	42	Fe-O	6	1	0.032	2.062	0.031
Halo	48	Fe-O	6	1	0.032	2.081	0.029
Halo	54	Fe-O	6	1	0.029	2.203	0.039
Halo	60	Fe-O	6	1	0.029	2.203	0.039
Halo	66	Fe-O	6	1	0.029	2.138	0.026
Halo	72	Fe-O	6	1	0.029	2.206	0.013
Halo	78	Fe-O	6	1	0.029	2.188	0.013
Halo	84	Fe-O	6	1	0.027	2.206	0.016
Halo	90	Fe-O	6	1	0.027	2.188	0.015
Halo	96	Fe-O	6	1	0.026	2.157	0.023
Halo	102	Fe-O	6	1	0.027	2.178	0.021
Halo	108	Fe-O	6	1	0.027	2.119	0.015
Monazite	114	Fe-O	6	1	0.027	2.102	0.018
Monazite	120	Fe-O	6	1	0.027	2.069	0.024

Figure SI-1. EXAFS signal (blue lines) and corresponding fits (red dashed lines) from three representative regions across a radiohalo within a crystal of grunerite. 'μm' denotes microns along a traverse by the microfocus X-ray beam. 'CN' denotes coordination number, 'σ^2' denotes the Debye-Waller factor. 'R' denotes the interatomic distance, the 'r-factor' denotes the 'goodness of fit'. Note the very small shifts in the positions of the EXAFS oscillations. Data is noisy beyond k = 6, thus only a first shell fit was possible. Parameters were identical across each fit, therefore representative comparisons across fits will be valid, despite the relatively high r-factors resulting from low data resolution.

Almandine EXAFS fit results: Line 1

Sample	(μm)	Path	CN	$S0^2$	σ^2	R	r-factor
Garnet	6	Fe-O	6	1	0.023	2.231	0.011
Garnet	12	Fe-O	6	1	0.023	2.229	0.009
Garnet	18	Fe-O	6	1	0.023	2.233	0.011
Garnet	24	Fe-O	6	1	0.023	2.224	0.012
Garnet	30	Fe-O	6	1	0.023	2.227	0.01
Garnet	36	Fe-O	6	1	0.023	2.226	0.008
Garnet	42	Fe-O	6	1	0.023	2.228	0.012
Halo	48	Fe-O	6	1	0.025	2.23	0.013
Halo	54	Fe-O	6	1	0.022	2.204	0.022
Halo	60	Fe-O	6	1	0.012	2.159	0.014
Monazite	66	Fe-O	6	1	0.012	2.211	0.025
Monazite	72	Fe-O	6	1	0.013	2.232	0.023
Monazite	78	Fe-O	6	1	0.009	2.187	0.008
Monazite	84	Fe-O	6	1	0.013	2.246	0.009
Monazite	90	Fe-O	6	1	0.011	2.184	0.02
Monazite	96	Fe-O	6	1	0.01	2.119	0.017
Monazite	102	Fe-O	6	1	0.015	2.175	0.011

Almandine EXAFS fit results: Line 2

Sample	(μm)	Path	CN	$S0^2$	σ^2	R	r-factor
Garnet	6	Fe-O	6	1	0.023	2.228	0.009
Garnet	12	Fe-O	6	1	0.023	2.236	0.012
Garnet	18	Fe-O	6	1	0.023	2.218	0.01
Garnet	24	Fe-O	6	1	0.024	2.239	0.012
Garnet	30	Fe-O	6	1	0.021	2.237	0.011
Garnet	36	Fe-O	6	1	0.024	2.236	0.014
Garnet	42	Fe-O	6	1	0.024	2.233	0.014
Halo	48	Fe-O	6	1	0.025	2.243	0.019
Halo	54	Fe-O	6	1	0.021	2.206	0.024
Halo	60	Fe-O	6	1	0.018	2.204	0.008
Monazite	66	Fe-O	6	1	0.019	2.132	0.019
Monazite	72	Fe-O	6	1	0.016	2.108	0.02
Monazite	78	Fe-O	6	1	0.019	2.139	0.015
Monazite	84	Fe-O	6	1	0.018	2.102	0.019
Monazite	90	Fe-O	6	1	0.025	2.256	0.034
Monazite	96	Fe-O	6	1	0.018	2.132	0.021
Monazite	102	Fe-O	6	1	0.024	2.02	0.009

Figure SI-2. EXAFS signal (blue lines) and corresponding fits (red dashed lines) from three representative regions across a radiohalo within a crystal of garnet. 'μm' denotes microns along a traverse by the microfocus X-ray beam. 'CN' denotes coordination number, 'σ^2' denotes the Debye-Waller factor. 'R' denotes the interatomic distance, the 'r-factor' denotes the 'goodness of fit'. Note the very small shifts in the positions of the EXAFS oscillations. Data is noisy beyond k = 6, thus only a first shell fit was possible. Parameters were identical across each fit, therefore representative comparisons across fits will be valid, despite the relatively high r-factors resulting from low data resolution.