Automated Pair Distribution Function Analysis for Assessing Reaction Progress

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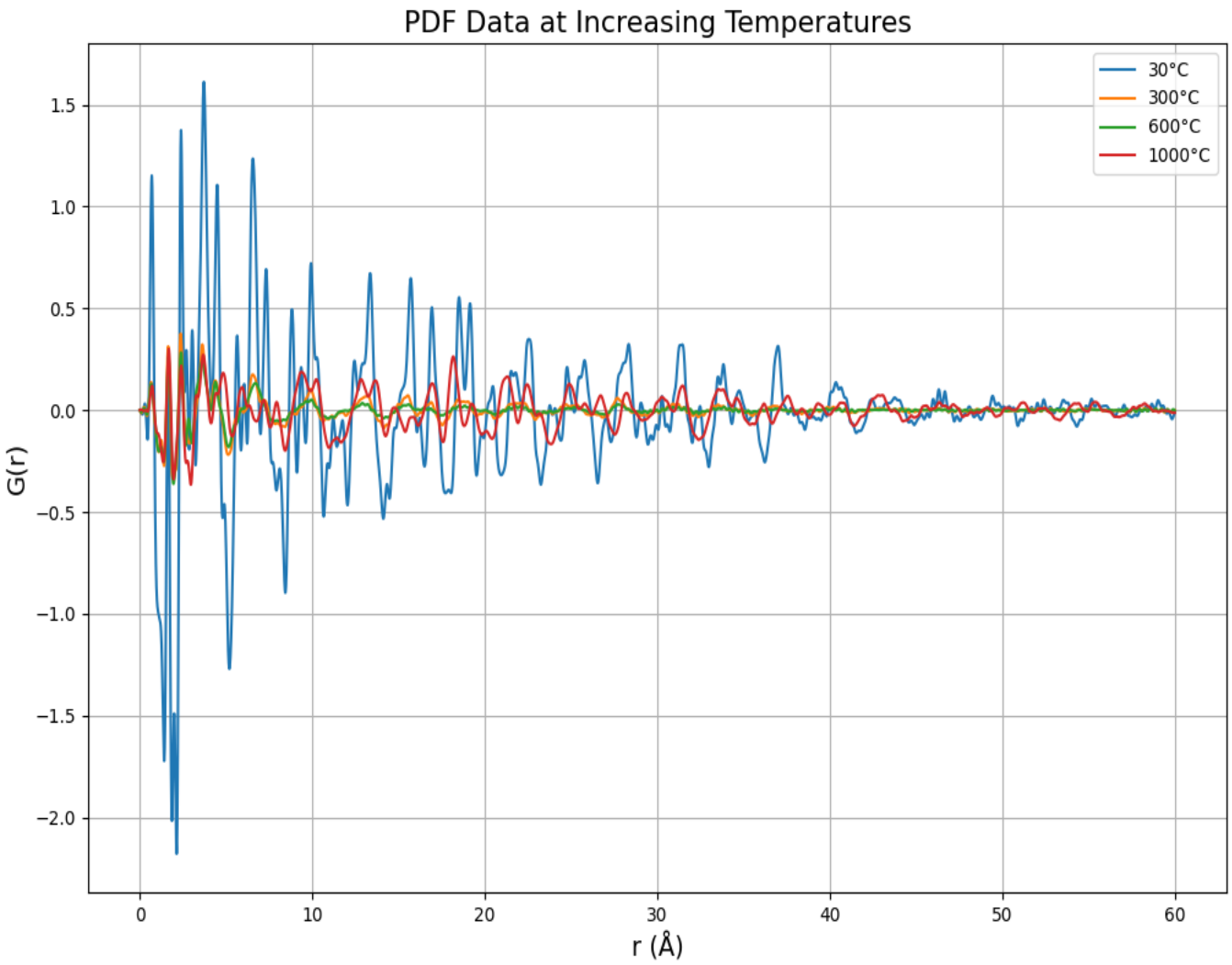
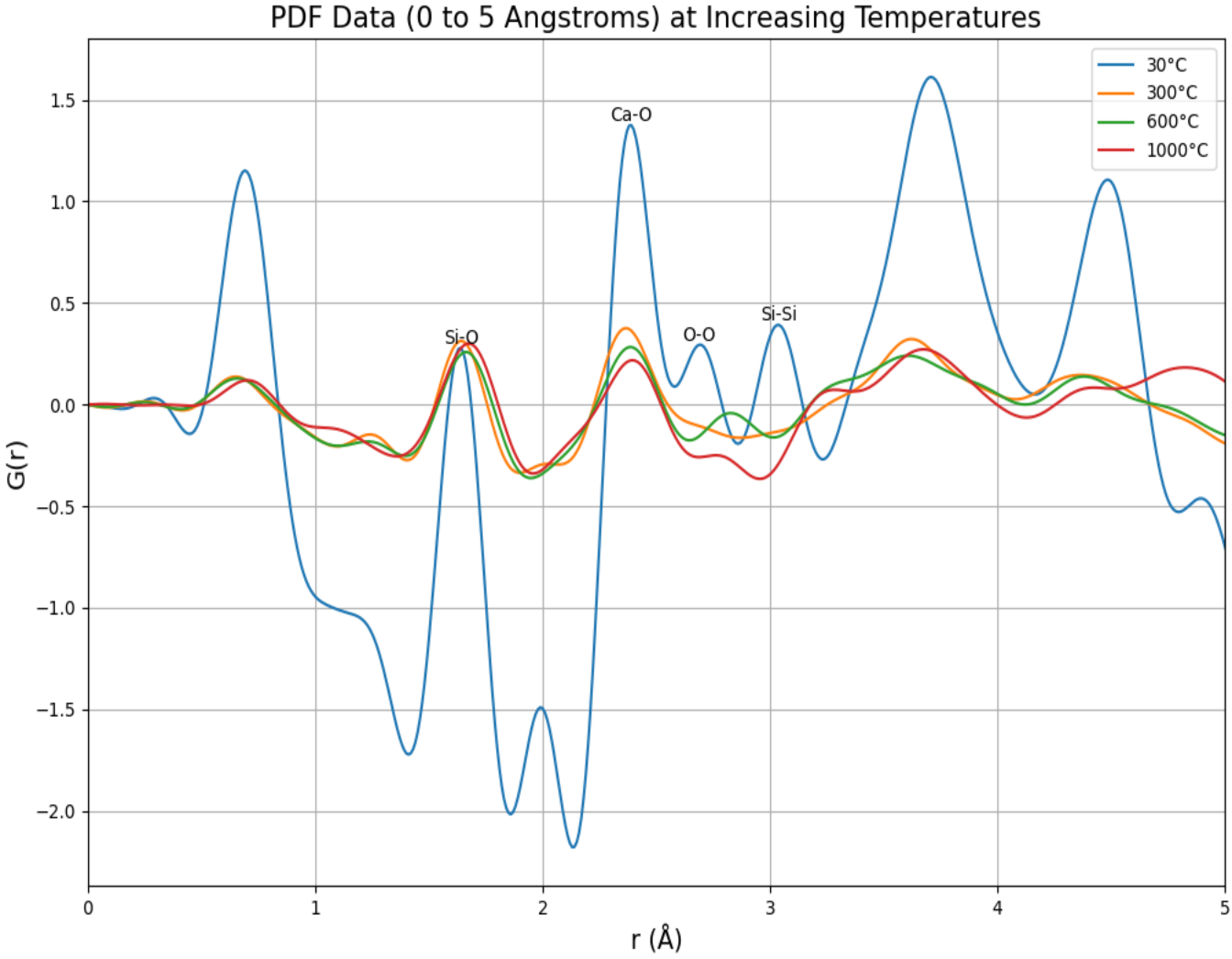
Section 1: PDF Curve Plotting

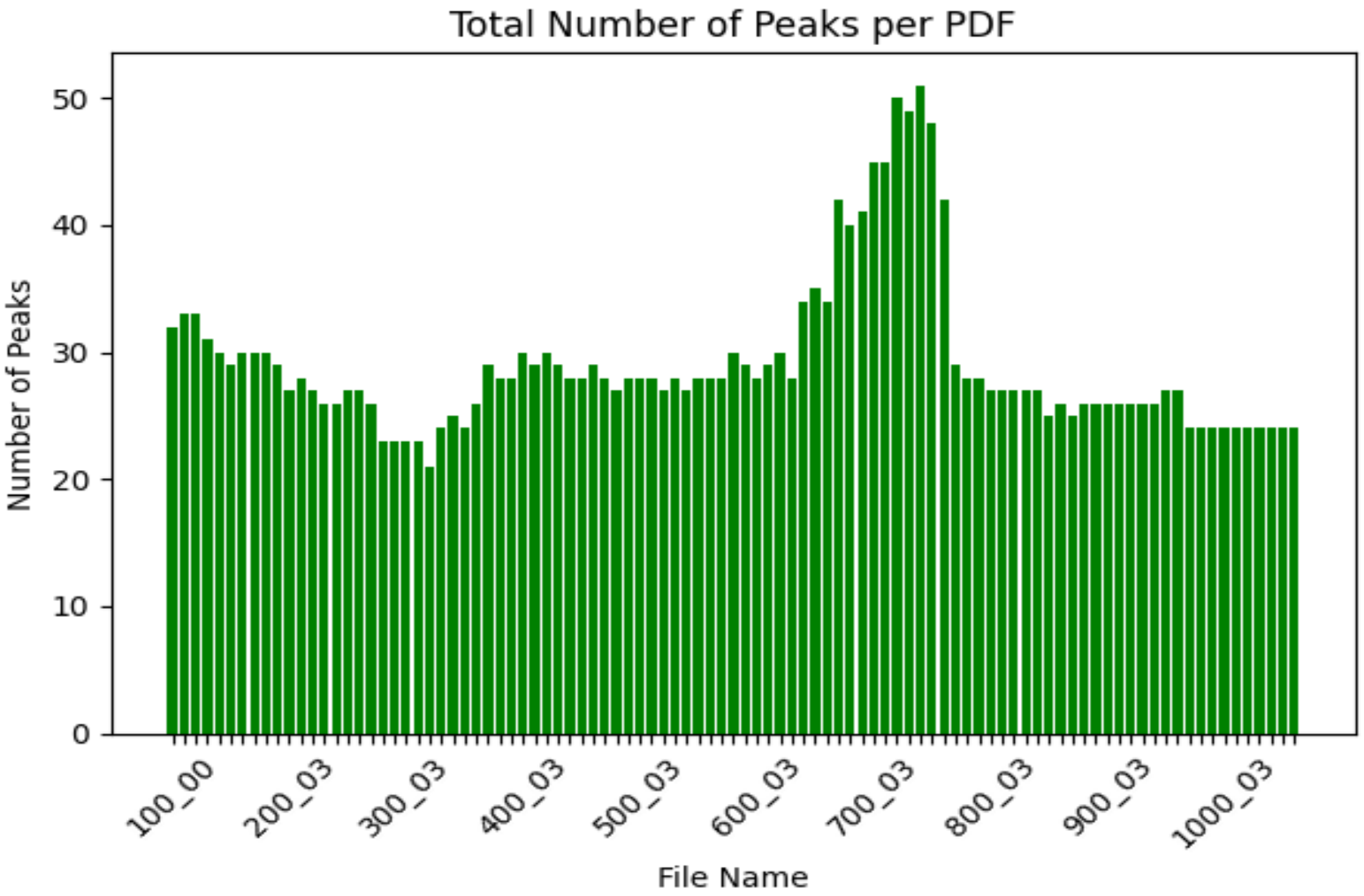
This section visualizes the PDF data.




PDF Data (0 to 5 Angstroms) at Increasing Temperatures
30°C
300°C
600°C
1000°C
Ca-O
Si-O
O-O
Si-Si
G(r)
r (Å)
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
1
2
3
4
5

Section 2: Visualizing Total Number of Peaks Over Time

This section visualizes phase changes by counting the total number of peaks in PDF files across temperatures.



Section 3: Quantifying Peak Positions

This table shows select peak positions, in Angstroms, tracked across PDFs recorded at various temperatures. Full results of tracked peak postions are shown in tracked_peak_matrix.txt.

Tracked Peak Positions for Selected PDF Peaks

	Peak 1	Peak 2	Peak 3	Peak 4	Peak 5	Peak 6	Peak 7	Peak 8
30°C	1.64	2.39	2.69	3.04	nan	3.71	4.49	nan
100°C	1.63	2.38	nan	nan	nan	3.68	4.49	nan
200°C	1.64	2.37	nan	nan	nan	3.64	4.39	nan
300°C	1.64	2.37	nan	nan	nan	3.62	4.36	nan
400°C	1.65	2.37	nan	nan	nan	3.61	4.35	nan
500°C	1.66	2.38	nan	nan	nan	3.61	4.36	nan
600°C	1.66	2.39	nan	nan	nan	3.6	4.38	nan
700°C	1.66	2.39	nan	nan	nan	3.62	4.38	nan
800°C	1.67	2.39	nan	nan	nan	3.64	4.39	4.78
900°C	1.68	2.39	nan	nan	3.29	3.65	4.41	4.82

Section 4: Peak Integration

This table lists relative differences between reference peak integrals (denoted 0) at a given temperature and peak integrals calculated at higher temperatures. These values are indicative of changes that occur to atomic coordination numbers as the structure of C-S-H changes.

Relative Changes to Atomic Coordination Numbers with Temperature

	Peak 1 (~1.63Å)	Peak 2 (~2.38Å)	Peak 3 (~3.68Å)	Peak 4 (~4.49Å)
100°C	0.0	0.0	0.0	0.0
200°C	0.0	0.4	1.8	1.6
300°C	0.0	3.7	0.4	3.2
400°C	0.0	0.3	2.1	3.9
500°C	0.0	0.5	2.0	4.4
600°C	0.0	1.8	2.2	5.4
700°C	0.0	2.8	2.0	6.8
800°C	0.0	1.7	2.7	10.2
900°C	0.0	2.0	3.4	10.4