Enhancement of high-alumina glass and glass-ceramics through dual modification of Zn^{2+} and its mechanism

Beibei Ren[a], Yaxin Liu[a], Jiani Yu[a], Ting Wang[ab], Hong Jiang[c], Chuang Dong[d], Chunrong Xiong[c], Na Wang[ab], Xin Huang[abe]*, Hongxun Hao[abe]*

[a] National Engineering Research Center of Industrial Crystallization Technology, Tianjin University, Tianjin 300072, China;

[b] Collaborative Innovation Center of Chemical Science and Engineering, Tianjin, 300072, China;

[c] Special Glass Key Laboratory of Hainan Province, Hainan University, Hainan 5711900, China;

[d] School of Materials Science and Engineering, Dalian Jiaotong University, Dalian 116028, China

[e] State Key Laboratory of Chemical Engineering, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China;

Corresponding Author

Email: x_huang@tju.edu.cn; hongxunhao@tju.edu.cn

Table S1 Relative area and peak position variation of Q^n in PG samples

Structural unit		Q^1	Q^2	Q^n	Q^3	Q^4
PG-2Z	Relative area/%	8.13	28.87	45.69	13.14	4.17
	Peak position/cm^{-1}	894.06	945.26	1039.90	1128.00	1177.50
PG-3Z	Relative area/%	8.37	21.91	54.14	11.81	3.77
	Peak position/cm^{-1}	885.36	946.98	1031.80	1124.70	1176.30
PG-4Z	Relative area/%	8.73	20.00	54.09	12.72	4.46
	Peak position/cm^{-1}	885.75	943.34	1032.40	1124.20	1177.10
PG-5Z	Relative area/%	10.17	19.33	51.75	13.43	5.32
	Peak position/cm^{-1}	888.75	945.86	1034.00	1125.00	1179.10

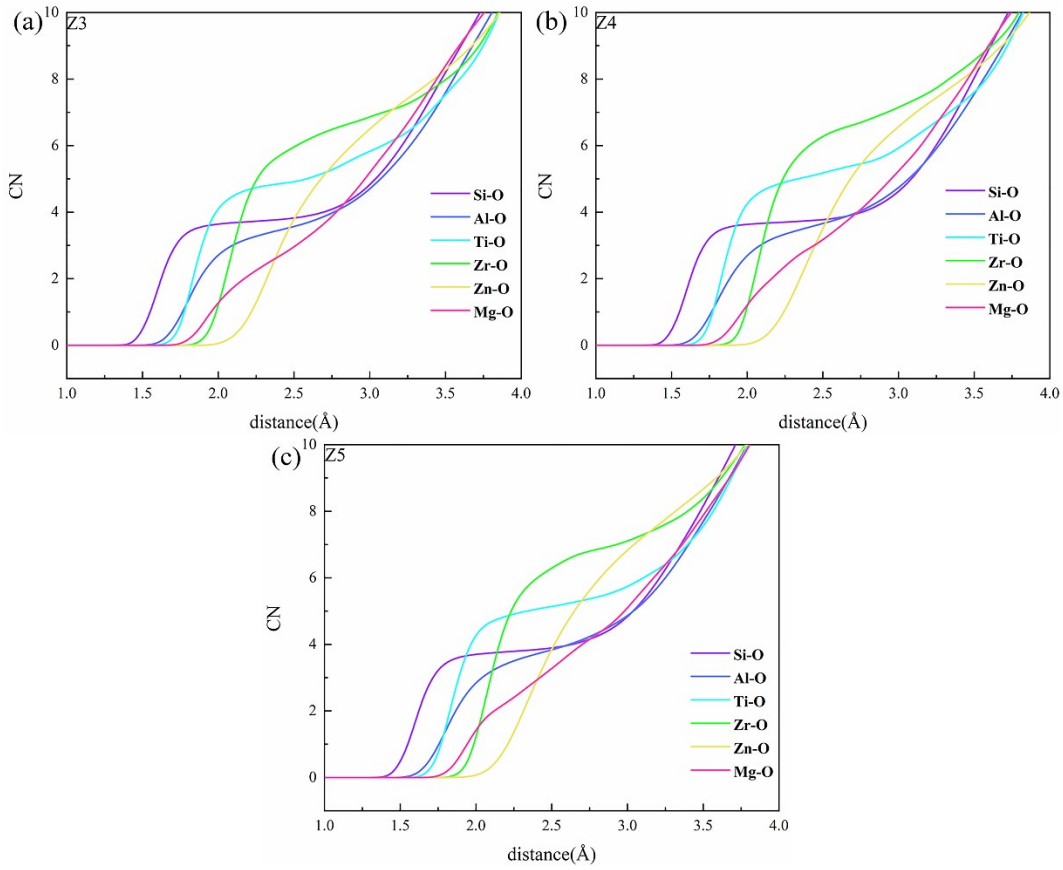

Fig. S1. Coordination number of PG samples: (a) PG-3Z Sample; (b) PG-4Z Sample; (c) PG-5Z Sample

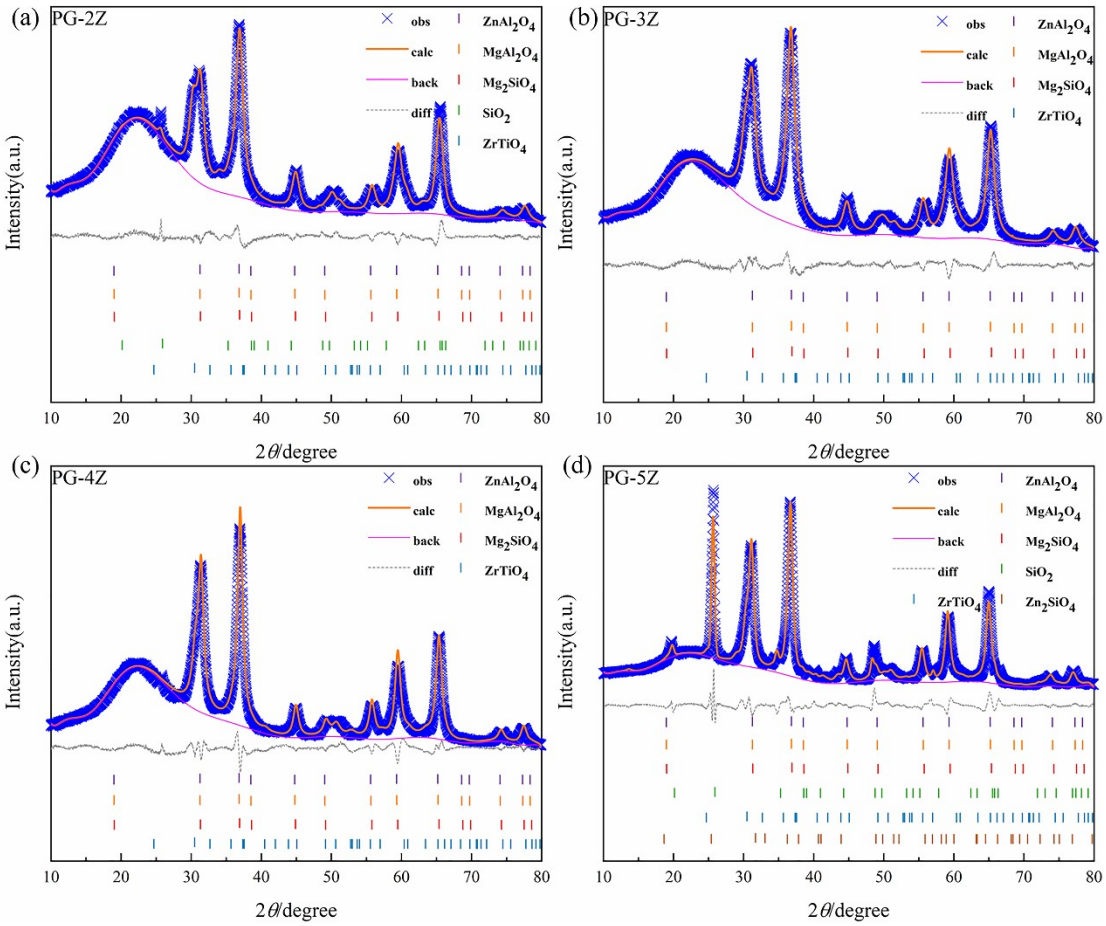

Fig.S2. Rietveld refinement of the XRD slow-sweep patterns of GC samples：(a) GC-2Z sample; (b) GC-3Z sample; (c) GC-4Z sample; (d) GC-5Z sample

Table S2 Rietveld finishing data for PG samples (crystal phase ratio and fit factor)

	crystalline phase (Proportion of total crystalline phase)				Inaccuracies	Goodness-of-fit factor
Sample	$Zn/MgAl_2O_4+Mg_2SiO_4$	$ZrTiO_4$	Zn_2SiO_4	SiO_2	wR	GOF
PG-2Z	79.80%	13.65%	/	6.55%	3.406	2.12
PG-3Z	86.70%	13.30%	/	/	3.229	1.97
PG-4Z	80.10%	19.90%	/	/	4.739	2.88
PG-5Z	58.00%	12.7%	8.70%	20.60%	4.988	2.99

Table S3 Simulation of Zn2p photoelectron spectroscopy peak splitting for two-step heat treatment samples

Sample		GC-2Z	GC-3Z	GC-4Z	GC-5Z
$2p_{1/2}$ in crystal	BE (eV)	1044.8	1044.8	1044.8	1044.7
	FWHM	1.52	1.76	1.87	1.87
	Area (%)	44.9	51.5	56.7	57.5
$2p_{1/2}$ in glass	BE (eV)	1045.7	1045.6	1045.6	1045.6
	FWHM	1.52	1.99	1.87	1.87
	Area (%)	55.1	48.5	43.3	42.5
$2p_{3/2}$ in crystal	BE (eV)	1021.9	1021.8	1021.8	1021.7
	FWHM	1.78	1.79	1.64	1.76
	Area (%)	44.7	52.7	59.1	61.2
$2p_{3/2}$ in glass	BE (eV)	1022.6	1022.6	1022.6	1022.5
	FWHM	1.87	1.87	1.76	2.11
	Area (%)	55.3	47.3	40.9	38.8

Table S4 Simulation of O1s photoelectron spectroscopy peak splitting for GC sample

Sample		GC-2Z	GC-3Z	GC-4Z	GC-5Z
BO_{Si}	BE (eV)	532.2	532.2	532.3	532.3
	FWHM	1.77	2.09	2.03	1.96
	Area (%)	54.94	56.82	58.48	59.17
BO_{Al}	BE (eV)	531.3	531.4	531.4	531.5
	FWHM	1.39	1.58	1.90	1.96
	Area (%)	30.07	30.11	30.41	31.36
NBO	BE (eV)	530.4	530.4	530.4	530.4
	FWHM	1.58	1.52	1.58	1.52
	Area (%)	14.99	13.07	11.11	9.47