

**The relationship between local structure and photo-Fenton catalytic ability of glasses and glass-ceramics prepared from Japanese slag**

ALI, Ahmed S <<http://orcid.org/0000-0001-9943-5220>>, NOMURA, Kiyoshi, HOMONNAY, Zoltan, KUZMANN, Erno, SCRIMSHIRE, Alex <<http://orcid.org/0000-0002-6828-3620>>, BINGHAM, Paul A <<http://orcid.org/0000-0001-6017-0798>>, KREHULA, Stjepko, RISTIĆ, Mira, MUSIĆ, Svetozar and KUBUKI, Shiro

Available from Sheffield Hallam University Research Archive (SHURA) at:

<https://shura.shu.ac.uk/25058/>

---

This document is the Accepted Version [AM]

**Citation:**

ALI, Ahmed S, NOMURA, Kiyoshi, HOMONNAY, Zoltan, KUZMANN, Erno, SCRIMSHIRE, Alex, BINGHAM, Paul A, KREHULA, Stjepko, RISTIĆ, Mira, MUSIĆ, Svetozar and KUBUKI, Shiro (2019). The relationship between local structure and photo-Fenton catalytic ability of glasses and glass-ceramics prepared from Japanese slag. *Journal of Radioanalytical and Nuclear Chemistry*. [Article]

---

**Copyright and re-use policy**

See <http://shura.shu.ac.uk/information.html>

**Table 1** Fe<sub>2</sub>O<sub>3</sub> (batch) content and bandgap energy of heat-treated slag samples calculated from DRS

Sample	Total Fe <sub>2</sub> O <sub>3</sub> content (mass % )	E <sub>g</sub> (eV)
SF11 Original	11.45 ± 0.01	2.15 ± 0.02
SF11 Melted	11.45 ± 0.01	2.09 ± 0.02
RSF14 Melted	14.40 ± 0.01	2.22 ± 0.04
SF30 Melted	30.00 ± 0.01	1.96 ± 0.01
SF50 Melted	50.00 ± 0.01	1.96 ± 0.01

**Table 2**  $^{57}\text{Fe}$ -Mössbauer parameters at room temperature of slag glass samples before and after heat treatment at 800 °C for 100 min

	Sample	assignment	A (%)	$\delta$ (mm s $^{-1}$ )	$\Delta$ (mm s $^{-1}$ )	$H_{\text{int}}$ (T)	$\Gamma$ (mm s $^{-1}$ )
Before	SF50 Melted	mag + mgh	32.2	$0.30 \pm 0.01$	$-0.02 \pm 0.02$	$48.10 \pm 0.01$	$0.42 \pm 0.03$
		mag.	34.4	$0.52 \pm 0.02$	0.00	$44.80 \pm 0.02$	$0.88 \pm 0.10$
		$\text{Fe}^{\text{III}} T_{\text{d}}$	23.6	$0.27 \pm 0.02$	$1.21 \pm 0.03$	-	$0.84 \pm 0.05$
		hem.	9.8	$0.37 \pm 0.03$	$-0.20 \pm 0.01$	$49.96 \pm 0.02$	$0.43 \pm 0.04$
	SF30 Melted	$\text{Fe}^{\text{III}} O_{\text{h}}$	100.0	$0.40 \pm 0.01$	$0.89 \pm 0.02$	-	$0.99 \pm 0.03$
	RSF14 Melted	$\text{Fe}^{\text{III}} T_{\text{d}}$	100.0	$0.31 \pm 0.01$	$1.25 \pm 0.02$	-	$0.69 \pm 0.02$
	SF11 Melted	$\text{Fe}^{\text{III}} T_{\text{d}}$	100.0	$0.33 \pm 0.01$	$1.25 \pm 0.01$	-	$0.69 \pm 0.02$
	SF11 Original	$\text{Fe}^{\text{II}} T_{\text{d}}$	85.5	$1.00 \pm 0.01$	$1.89 \pm 0.02$	-	$0.63 \pm 0.02$
		$\text{Fe}^{\text{III}} O_{\text{h}}$	14.5	$0.50 \pm 0.02$	$1.16 \pm 0.08$	-	$0.51 \pm 0.10$
After	SF50 Melted	$\text{Fe}^{\text{III}} T_{\text{d}}$	25.5	$0.31 \pm 0.03$	$1.14 \pm 0.01$	-	$0.89 \pm 0.01$
		hem.	38.1	$0.37 \pm 0.01$	$-0.18 \pm 0.04$	$51.40 \pm 0.01$	$0.34 \pm 0.03$
		mgh.	36.4	$0.37 \pm 0.01$	$-0.02 \pm 0.01$	$46.40 \pm 0.01$	$1.23 \pm 0.02$
	SF30 Melted	$\text{Fe}^{\text{III}} T_{\text{d}}$	100.0	$0.32 \pm 0.02$	$0.84 \pm 0.03$	-	$0.76 \pm 0.01$
	RSF14 Melted	$\text{Fe}^{\text{III}} T_{\text{d}}$	100.0	$0.18 \pm 0.01$	$1.34 \pm 0.01$	-	$0.78 \pm 0.01$
	SF11 Melted	$\text{Fe}^{\text{III}} O_{\text{h}}$	100.0	$0.38 \pm 0.04$	$0.92 \pm 0.01$	-	$0.63 \pm 0.01$
	SF11 Original	$\text{Fe}^{\text{II}} O_{\text{h}}$	9.8	$1.10 \pm 0.02$	$2.25 \pm 0.05$	-	$0.44 \pm 0.06$
		$\text{Fe}^{\text{III}} O_{\text{h}}$	90.2	$0.37 \pm 0.01$	$0.88 \pm 0.01$	-	$0.75 \pm 0.01$

hem.: Hematite, mag.: Magnetite, mgh.: Maghemite,  $T_{\text{d}}$ : Tetrahedra,  $O_{\text{h}}$ : Octahedra, A: Absorption area,

$\delta$ : Isomer shift,  $\Delta$ : Quadrupole splitting,  $H_{\text{int}}$ : Internal magnetic field,  $\Gamma$ : Line width.

**Table 3**  $^{57}\text{Fe}$ -Mössbauer parameters at 77 K of slag samples heat-treated at 800 °C for 100 min

sample	assignment	A (%)	$\delta$ (mm s $^{-1}$ )	$\Delta$ (mm s $^{-1}$ )	$H_{\text{int}}$ (T)	$\Gamma$ (mm s $^{-1}$ )
SF50 Melted	Fe <sup>III</sup> $T_d$	14.1	$0.40 \pm 0.02$	$1.31 \pm 0.03$	-	$0.92 \pm 0.05$
	hem.	49.0	$0.48 \pm 0.01$	$0.13 \pm 0.01$	$53.50 \pm 0.01$	$0.37 \pm 0.01$
	mgh.	36.9	$0.43 \pm 0.01$	$-0.11 \pm 0.01$	$50.40 \pm 0.08$	$0.71 \pm 0.02$
SF30 Melted	Fe <sup>III</sup> $T_d$	15.6	$0.41 \pm 0.02$	$1.50 \pm 0.03$	-	$1.05 \pm 0.05$
	Mag + mgh	27.9	$0.40 \pm 0.03$	$-0.08 \pm 0.05$	$41.90 \pm 0.40$	$1.40 \pm 0.10$
	hem.	28.1	$0.48 \pm 0.01$	$0.01 \pm 0.01$	$50.20 \pm 0.10$	$0.65 \pm 0.04$
	mag.	28.4	$0.42 \pm 0.01$	$-0.04 \pm 0.02$	$46.80 \pm 0.10$	$0.73 \pm 0.07$
RSF14 Melted	Fe <sup>III</sup> $T_d$	58.5	$0.29 \pm 0.01$	$0.96 \pm 0.01$	-	$0.46 \pm 0.01$
	Fe <sup>III</sup> $T_d$	41.5	$0.24 \pm 0.01$	$1.90 \pm 0.01$	-	$0.40 \pm 0.02$
SF11 Melted	Fe <sup>III</sup> $O_h$	50.0	$0.58 \pm 0.01$	$1.09 \pm 0.01$	-	$0.46 \pm 0.03$
	Fe <sup>III</sup> $T_d$	50.0	$0.32 \pm 0.02$	$1.21 \pm 0.02$	-	$0.50 \pm 0.03$
SF11 Original	Fe <sup>III</sup> $T_d$	100.0	$0.42 \pm 0.01$	$1.20 \pm 0.01$	-	$1.03 \pm 0.03$

hem.: Hematite, mag.: Magnetite, mgh.: Maghemite,  $T_d$ : Tetrahedra,  $O_h$ : Octahedra, A: Absorption area,

$\delta$ : Isomer shift,  $\Delta$ : Quadrupole splitting,  $H_{\text{int}}$ : Internal magnetic field,  $\Gamma$ : Line width.