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Data Article

Data describing characteristics of waste foundry dust (WFD), sorbent obtained before and after batch sorption tests using As(III) and Cr(VI) aqueous solutions



Sunwon Rha, Ho Young Jo*

Department of Earth and Environmental Sciences, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul 02841, Republic of Korea

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ABSTRACT

This article presents data on characteristics of waste foundry dust (WFD), sorbent obtained before and after batch sorption tests using As(III) and Cr(VI) aqueous solutions, by performing X-ray Diffraction (XRD), field-emission scanning electron microscopy (FE-SEM) coupled with energy dispersive X-ray spectroscopy (EDX), Fourier-transform infrared spectroscopy (FT-IR), and X-ray photoelectron spectroscopy (XPS) analyses. Data are related to a research article “Waste foundry dust (WFD) as a reactive material for removing As(III) and Cr(VI) from aqueous solutions” [1]. The data provide information obtained from various analytical methods to investigate mechanisms of As(III) and Cr(VI) removal from aqueous solutions by WFD, an industrial by-product. These data can be of interest to researchers studying contaminant removal mechanisms by reactive materials, in particular industrial by-products.

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* Corresponding author.

E-mail address: hyjo@korea.ac.kr (H.Y. Jo).<https://doi.org/10.1016/j.dib.2021.106921>

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Specifications Table

Subject	Environmental Science: Environmental chemistry: Environmental engineering
Specific subject area	Characterization of sorbent and sorbate
Type of data	Table, Figure
How data were acquired	X-ray diffractometer (XRD, X'Pert MPD, Philips) Field-emission scanning electron microscopy (FE-SEM, Quanta 250FEG, FEI) with energy dispersive X-ray spectroscopy (EDX) Fourier-transform infrared spectroscopy (FT-IR, Cary 630 FT-IR, Agilent) X-ray photoelectron spectroscopy (XPS, PHI 5000 VersaProbe, ULVAC PHI)
Data format	Raw and analyzed data
Parameters for data collection	The samples obtained before and after batch sorption tests under various test conditions [i.e., sorbate (As(III) and Cr(VI)) and initial solution pHs (3, 5, and 7)] were used.
Description of data collection	XRD analysis was performed using a Cu α target (1.5412 Å) at 40 kV and 30 mA in 3–65° range at a scan speed of 2°/min in 0.01° steps. FE-SEM analysis was performed in SE mode at 10 kV in a high-vacuum state after Pt coating, and EDX analysis performed at 15 kV and a rate of 10000 times. FT-IR analysis was performed in the range of 400–4000 cm ⁻¹ in ATR mode. XPS analysis was performed with monochromated Al α (1486.6 eV) at a base pressure of 2.0×10^{-7} Pa, wide scan measured as pass energy of 187.85 eV in the range of 10–1000 eV with a step size of 1.0 eV, and the narrow scan measured as pass energy of 58.70 eV for Fe 2p, As 3d, Cr 2p, and O 1s with a step size of 0.1 eV.
Data source location	Institution: Korea University City/Town/Region: Seoul Country: Korea
Data accessibility	Data are provided in Mendeley Data, http://dx.doi.org/10.17632/cfyhsy6rr5.1
Related research article	Sunwon Rha, and Ho Young Jo, Waste foundry dust (WFD) as a reactive material for removing As(III) and Cr(VI) from aqueous solutions, J. Hazard. Mater., 412(15), 2021, 125290. https://doi.org/10.1016/j.jhazmat.2021.125290

Value of the Data

- This article provides raw data from various analyses (i.e., XRD, SEM-EDS, FT-IR and XPS) on waste foundry dust (WFD) samples obtained before and after batch As(III) and Cr(VI) sorption tests, which can give insight into characterization processes of industrial by-products as reactive materials.
- Based on the data, how the WFD removes As(III) and Cr(VI) from aqueous solutions, and what species of As and Cr are formed on WFD are described, which will be useful to the researchers in the field of wastewater treatment.
- The data provide information on characteristics of sorbed or removed As and Cr obtained by using various analytical methods, which can be applied to other studies regarding the sorption mechanisms of heavy metals.

1. Data Description

Waste foundry dust (WFD), an industrial by-product can be used as a reactive material to treat wastewater [1]. Various analyses (i.e., XRD, SEM-EDX, FT-IR, and XPS) were performed on WFD samples, obtained before and after the batch sorption tests using As(III) and Cr(VI) aqueous solutions under various conditions (i.e., initial pH and reaction time) described in Table 1 for determining As(III) and Cr(VI) removal characteristics.

Table 1

Summary of the batch sorption test conditions for the samples: WFD refers as-received (i.e., unreacted) WFD sample, and A- and B- series samples refer reacted WFD samples with As(III) and Cr(VI), respectively.

Sample name	Sorption test conditions				
	Target contaminants	Contaminant concentration (mg/L)	Initial solution pH	Solid-to-liquid ratio (g/L)	Reaction time (h)
WFD	–	–	–	–	–
A31	As(III)	100	3	12.5	24
A51	As(III)	100	5	12.5	24
A71	As(III)	100	7	12.5	24
B31	Cr(VI)	100	3	12.5	48
B51	Cr(VI)	100	5	12.5	48
B71	Cr(VI)	100	7	12.5	48

Table 2

Peak positions and their possible mineral phases of the samples observed in the XRD pattern.

Observed peak position (2 theta, °)	Possible mineral phase	WFD							
		WFD	A31	A51	A71	B31	B51	B71	
19.9	Microcline		o						
20.9	Quartz	o	o	o	o	o	o	o	o
23.5	Microcline	o							o
23.8	Microcline		o		o				
24.5	Microcline		o					o	
24.8	Microcline					o		o	
25.6	Microcline	o	o	o	o	o	o	o	o
26.6	Quartz	o	o	o	o	o	o	o	o
27.5	Microcline	o	o	o	o	o	o	o	o
29.5	Microcline	o		o					o
30.1	Magnetite	o	o	o	o	o	o	o	o
30.8	Microcline	o	o	o	o	o	o	o	o
35.1	Microcline			o					
35.5	Magnetite	o	o	o	o	o	o	o	o
36.5	Quartz	o	o	o	o	o	o	o	o
38.4	Microcline	o			o				
39.5	Quartz	o	o	o	o	o	o	o	o
40.3	Quartz	o	o	o	o	o	o	o	o
41.8	Microcline	o	o	o	o	o	o	o	o
42.5	Quartz	o	o	o	o	o	o	o	o
44.8	Microcline	o				o		o	
45.8	Quartz	o	o	o	o	o	o	o	o
50.1	Quartz	o	o	o	o	o	o	o	o
50.6	Microcline	o	o	o					
51.8	Microcline				o				
54.9	Quartz	o	o	o	o	o	o	o	o
55.3	Quartz	o	o	o	o	o	o	o	o
57.2	Quartz	o		o	o	o	o	o	o
60.0	Quartz	o	o	o	o	o	o	o	o
62.6	Magnetite	o	o	o	o	o	o	o	o
64.0	Quartz	o	o	o	o	o	o	o	o

1.1. XRD data

The locations of the peaks and their possible mineral phases observed in the XRD patterns on the WFD samples are summarized in Table 2. The XRD raw data are provided in Mendeleev Data, <http://dx.doi.org/10.17632/cfyhsy6rr5.1>. XRD analysis was conducted to determine the change in the mineral phase of the samples after the batch sorption tests. Quartz (SiO₂), microcline (KAlSi₃O₈), and magnetite (Fe₃O₄) were observed for all samples [1].

Table 3

Element contents in the samples obtained by SEM-EDX analysis.

Element (wt.%)	O	Al	Si	Fe	As	Cr	Mn
WFD	19.7	1.8	5.2	26.3	n.d. ¹⁾	n.d. ¹⁾	n.d. ¹⁾
A31	35.5	0.7	17.3	10.8	2.6	n.d. ¹⁾	n.d. ¹⁾
A51	26.5	0.8	6.2	14.4	2.2	n.d. ¹⁾	n.d. ¹⁾
A71	29.2	0.6	16.5	10.9	1.7	n.d. ¹⁾	n.d. ¹⁾
B31	31.0	4.1	9.4	37.6	n.d. ¹⁾	1.1	1.1
B51	27.2	0.6	6.7	29.1	n.d. ¹⁾	0.6	n.d. ¹⁾
B71	14.1	1.5	6.6	34.9	n.d. ¹⁾	n.d. ¹⁾	0.7

¹⁾ n.d.: not detected.

1.2. SEM-EDX data

The SEM-EDX elemental mapping images of A- and B-series samples are shown in Figs. 1 and 2, respectively. Element contents of the samples according to SEM-EDX analysis on the WFD samples are summarized in Table 3. The SEM images and EDX raw data are provided in Mendeleev Data, <http://dx.doi.org/10.17632/cfyhsy6rr5.1>. Particles of various shapes and sizes were observed in the low magnification ($\times 2000$) SEM image for all samples: very small amounts of large particles ($> 10 \mu\text{m}$), which has clean surface and angular shape; large particles ($1\text{--}20 \mu\text{m}$) with small particles ($< 0.1 \mu\text{m}$) that were randomly distributed on large particles surfaces; relatively small particles ($< 10 \mu\text{m}$) with a very rough surface formed by agglomerating small particles ($< 0.5 \mu\text{m}$). As in the as-received WFD sample, the major elements detected in the samples after the batch sorption tests were Si, Al, and Fe [1]. In addition, a small amount of As and Cr were detected in A- and B-series samples, respectively (Figs. 1 and 2, and Table 3). In the B31 and B71 samples, a Mn peak was also observed at 5.9 keV in EDX spectrum, as shown in the data provided in Mendeleev Data <http://dx.doi.org/10.17632/cfyhsy6rr5.1>. Since Mn was hardly present under the experimental conditions and the $K\alpha$ peak of Mn (5.9 keV) is similar with the $K\alpha$ peak of Cr (5.4 keV), the Mn peak is likely to be the Cr peak.

1.3. FT-IR data

The FT-IR spectrum and peak position at full scale of the WFD samples are shown in Fig. 3. The FT-IR spectrum data are provided in Mendeleev Data, <http://dx.doi.org/10.17632/cfyhsy6rr5.1>. In all samples, peaks were observed at 585 (Fe-O), 773 (Si-O), 1010 (Si-O-Si), 1560 (C=C), 2115 (C=C), 2340–2372 (O=C=O), and 2650–2700 (C-H) cm^{-1} . The peaks above 1560 cm^{-1} are related to organic matters in the WFD, and peaks below 1010 cm^{-1} are related to quartz, microcline, and magnetite [1]. No changes were observed in the main functional groups of the samples before and after the batch As(III) and Cr(VI) sorption tests because As(III) and Cr(VI) sorption cannot cause a large-scale phase change (Fig. 3).

1.4. XPS data

XPS wide scan spectra of WFD samples are shown in Fig. 4. The XPS raw data are provided in Mendeleev Data, <http://dx.doi.org/10.17632/cfyhsy6rr5.1>. The XPS high-resolution spectra for C 1s are shown in Fig. 5. C 1s peaks for C-C, C-O, and C=O were observed at a binding energy of 284.8, 286.0, and 287.0 eV [2]. The XPS high-resolution spectra for Si 2p are shown in Fig. 6. Only SiO₂ peak for Si 2p was observed at 103.8 eV.

Spectral fitting parameters and relative peak areas in various chemical states for O 1s, As 3d and Cr 2p are summarized in Tables 4 and 5. Oxygen in all samples was mainly present in the

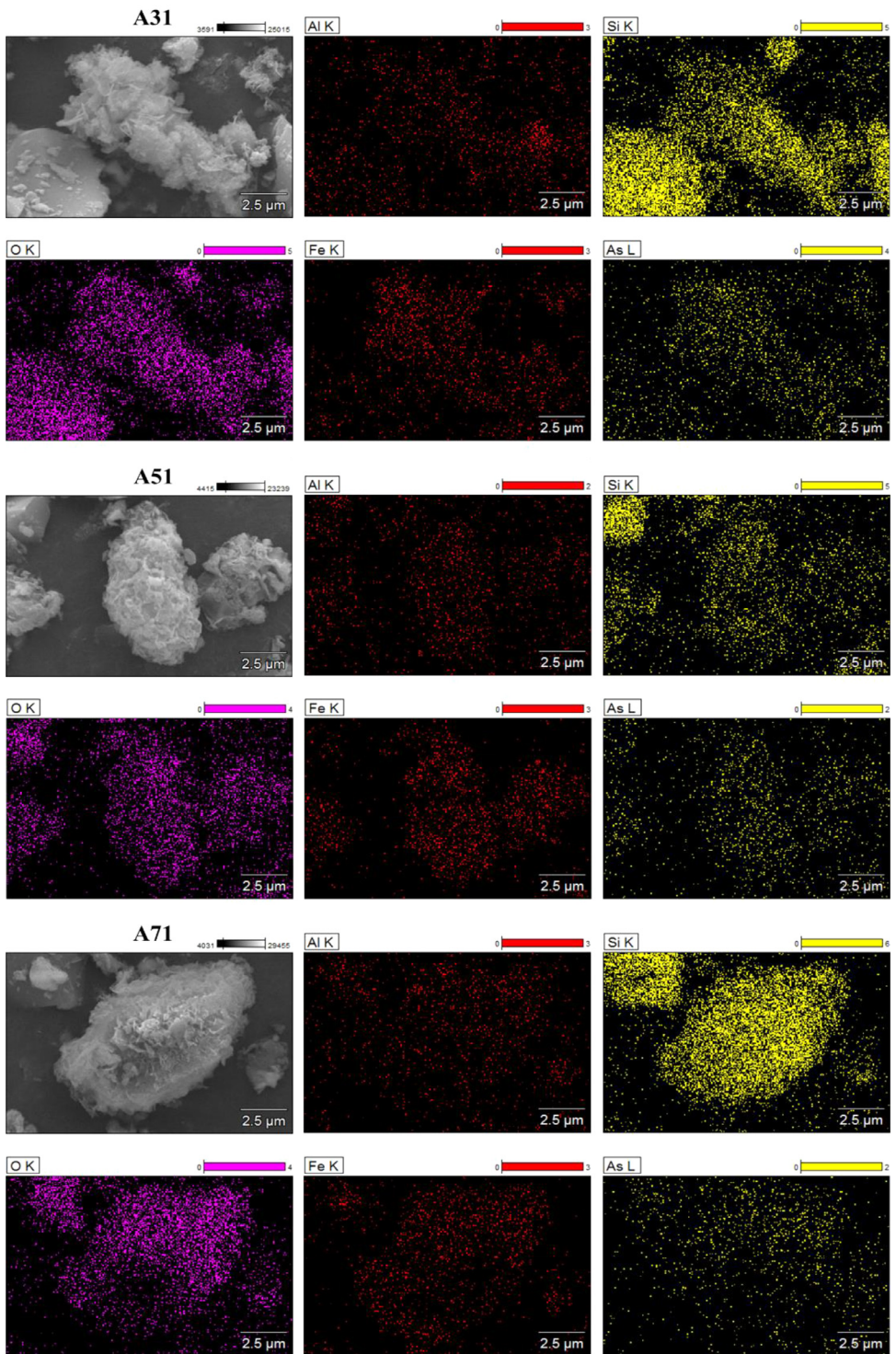


Fig. 1. SEM-EDX elemental mapping images of A-series samples.

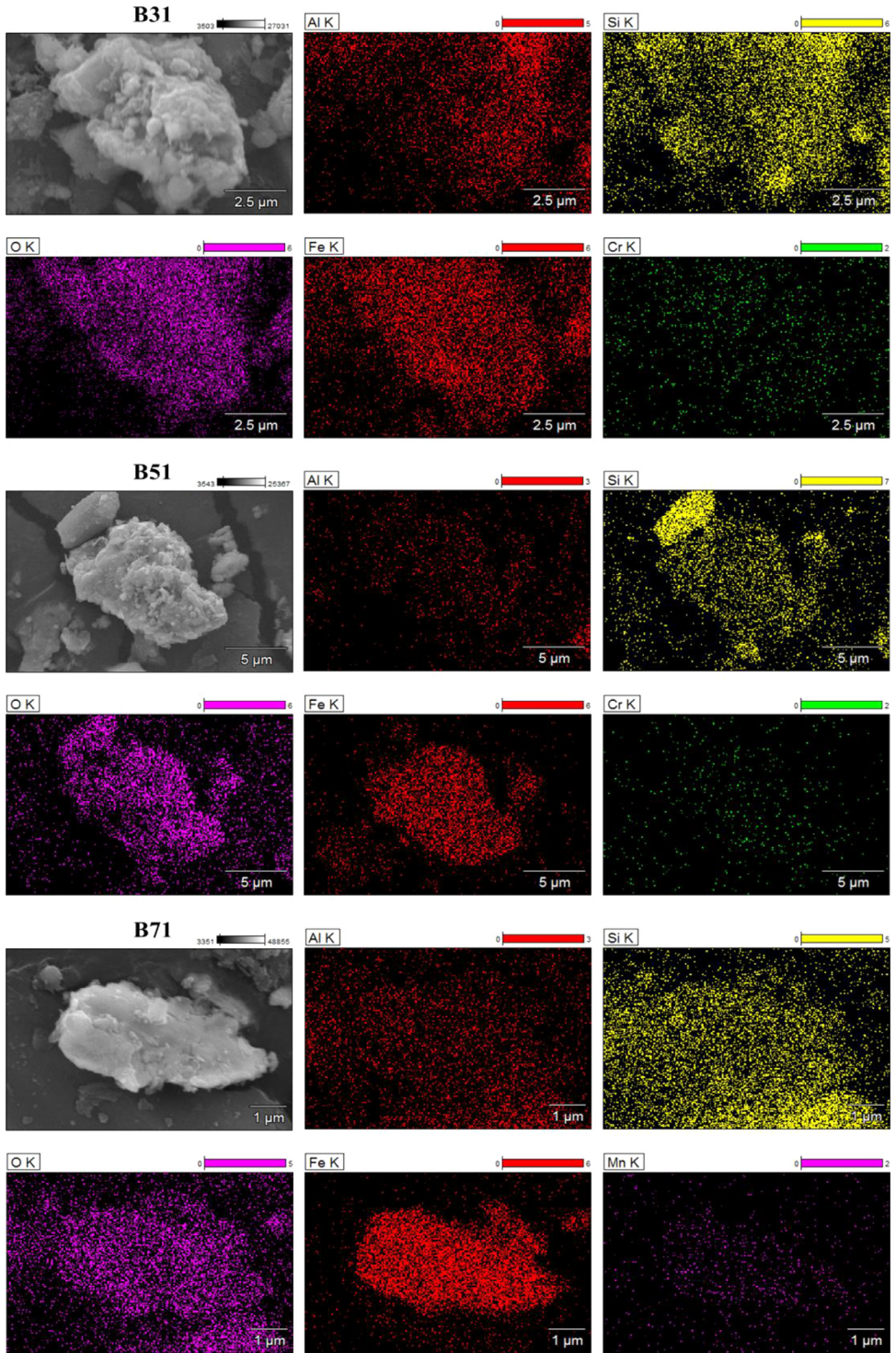


Fig. 2. SEM-EDX elemental mapping images of B-series samples.

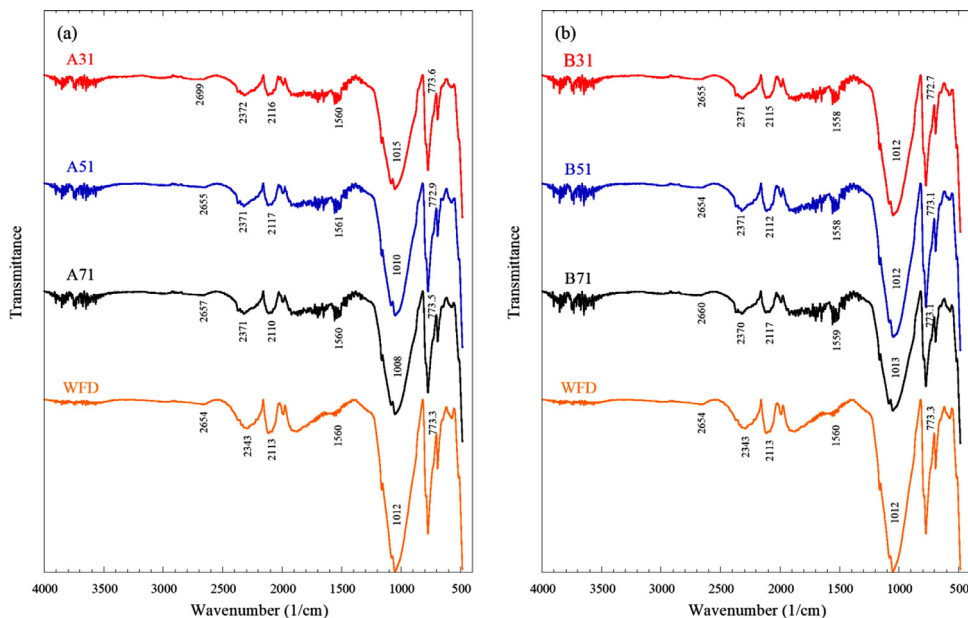


Fig. 3. FT-IR full scan spectra of (a) A-series and (b) B-series samples.

Table 4

O 1s spectral fitting parameters and relative peak areas in various chemical states.

Peak	Binding Energy (eV)	Chemical state	Peak area (%)						
			WFD	A31	A51	A71	B31	B51	B71
O 1s	530.1 ± 0.1	Fe-O ¹⁾	6.13	5.17	5.65	7.06	14.79	4.29	11.08
	531.3 ± 0.1	M-OH ¹⁾	8.58	71.89	72.96	64.87	22.66	39.32	49.28
	533.0 ± 0.1	SiO ₂ ¹⁾	85.29	22.94	21.39	28.07	62.55	56.39	39.64

¹⁾ [3]

Table 5

As 3d and Cr 2p_{3/2} spectral fitting parameters and relative peak areas in various chemical states.

Peak	Binding Energy (eV)	Chemical state	Peak area (%)						
			WFD	A31	A51	A71	B31	B51	B71
As 3d	44.9 ± 0.1	As(III) oxide ¹⁾	n.d. ³⁾	37.61	29.99	29.77	–	–	–
	45.8 ± 0.1	As(V) oxide ¹⁾	n.d. ³⁾	62.39	70.01	70.23	–	–	–
Cr 2p _{3/2}	577.3 ± 0.1	Cr(III) hydroxide ²⁾	n.d. ³⁾	–	–	–	56.33	44.55	60.87
	579.0 ± 0.1	Cr(VI) mixed species ²⁾	n.d. ³⁾	–	–	–	43.67	55.45	39.13

¹⁾ [3,4]

²⁾ [3,5]

³⁾ n.d.: not detected.

form of SiO₂, Fe-O, and M-OH (Table 4) [3]. The peak area of SiO₂, calculated in O 1s spectra was proportional to the total intensity of Si 2p spectra (Fig. 6). The ratio of SiO₂ peak area was the highest at 85.3% in the as-received WFD, and about 22.7–63.9% lower in the WFD samples obtained after the sorption tests. On the contrary, the ratio of M-OH peak area was the lowest at 8.6% in as-received WFD, and 14.1–64.4% higher in the sample after the sorption tests. The As 3d spectra were fitted with As(III) oxide at 44.9 eV of binding energy and As(V) oxide at 45.8 eV

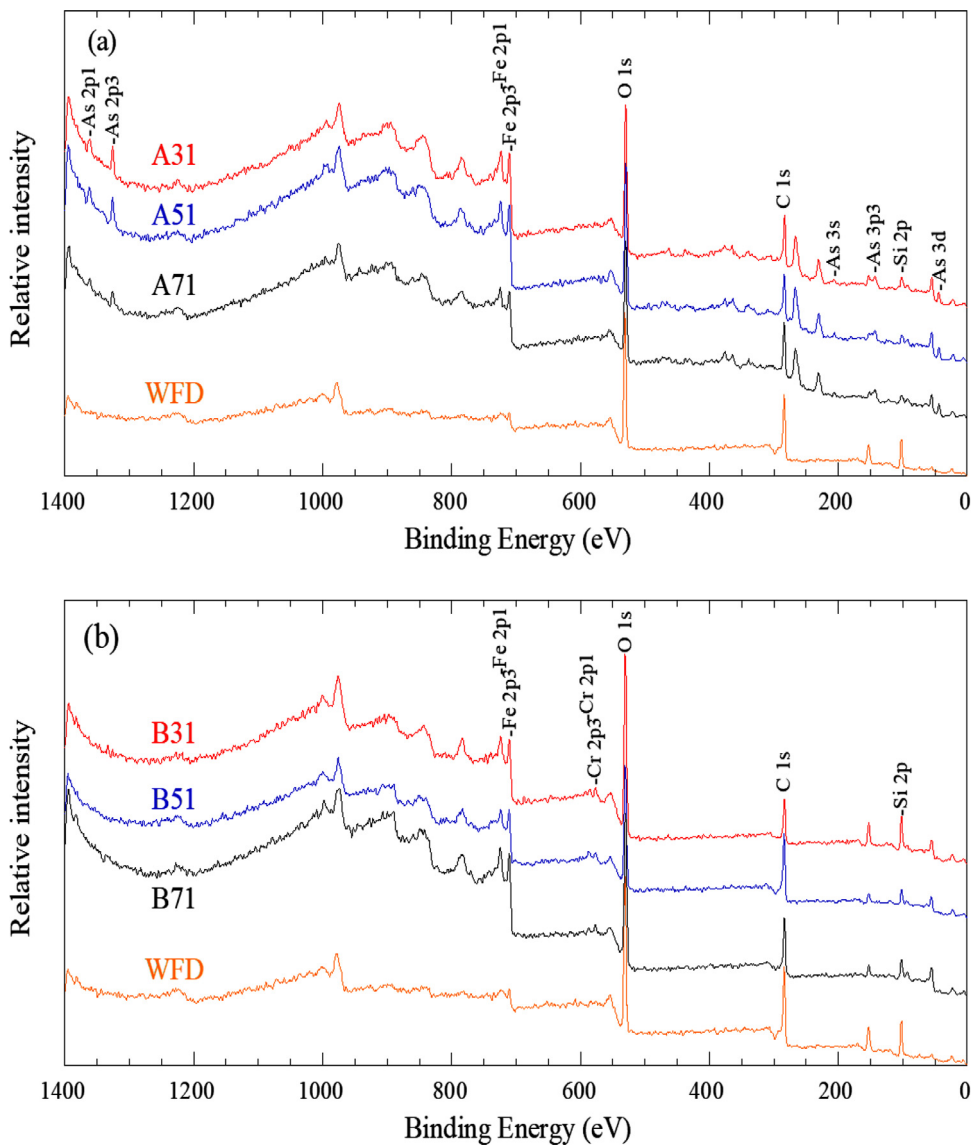


Fig. 4. XPS wide scan spectra of (a) A-series and (b) B-series samples.

of binding energy (Table 5) [3,4]. The ratio of As(V) peak area was 62.4–70.2%, which was higher than that of As(III), and increased with increasing initial solution pH for the batch sorption tests. The Cr $2p_{3/2}$ spectra were fitted with Cr(III) hydroxide at 557.3 eV and Cr(VI) mixed species at 579.0 eV [3,5]. The ratio of Cr(III) peak area was 44.6–60.9%, showing no tendency depending on the initial solution pH.

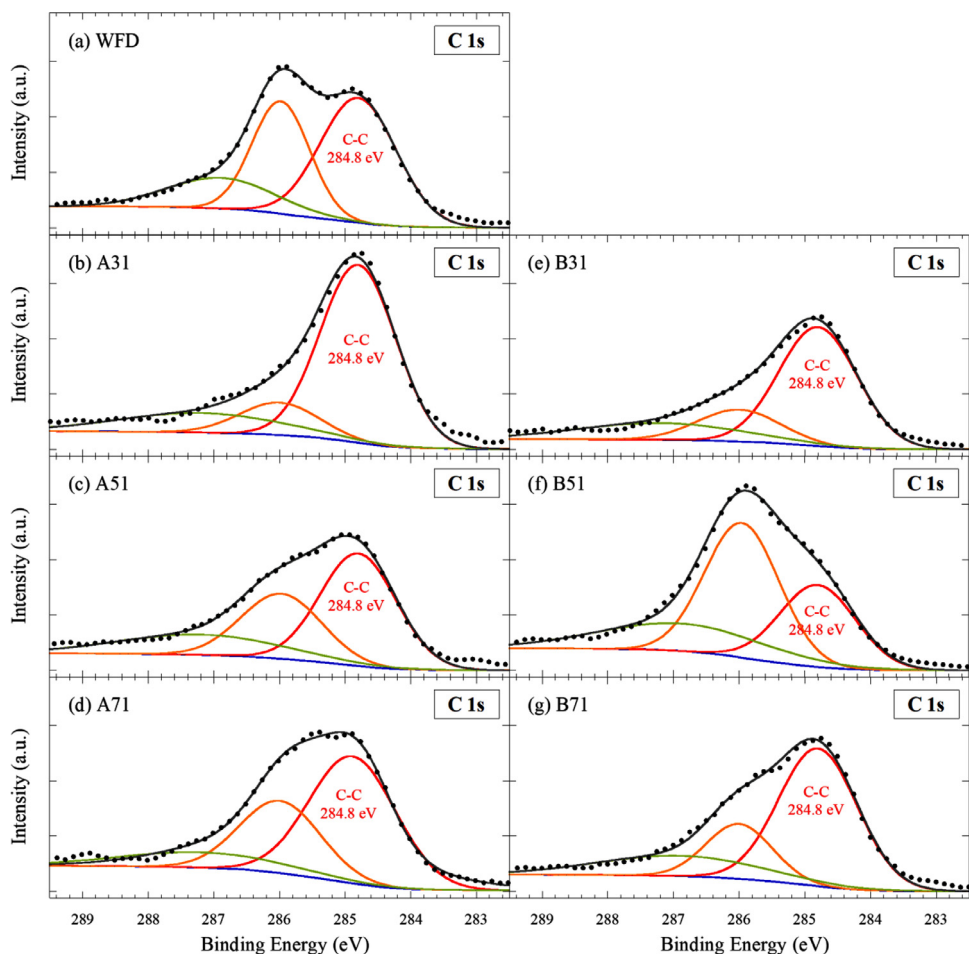


Fig. 5. High-resolution C 1s XPS spectra of the samples.

2. Experimental Design, Materials and Methods

2.1. Materials and sample preparation

WFD used in this article was obtained from a foundry plant in South Korea. Detailed WFD characterization was described in [1]. Before the analysis and sorption tests, WFD was dried at 40 °C for 48 h and stored in a vacuum desiccator. For the batch sorption tests, analytical grade NaAsO₂ (Sigma-Aldrich Co.) and Na₂CrO₄•4H₂O (Junsei Chemical Co., Ltd.) were used for preparing 100 mg/L concentration of As(III) and Cr(VI) stock solutions. 0.1 and 0.01 M HNO₃ (Sigma-Aldrich Co.) solutions were used to adjust the stock solution pH to 3, 5 and 7. The batch sorption tests for As(III) and Cr(VI) were conducted under following conditions: initial concentration of 100 mg/L; initial solution pHs of 3, 5, and 7; solid-to-liquid ratio of 12.5 g/L; solution volume of 400 mL; and reaction time of 24 h for As(III) and 48 h for Cr(VI) (Table 1). After the batch sorption tests, the solutions were centrifuged for 10 min at 5000 rpm using a tabletop centrifuge (VS-5500i, Vision Scientific Co., Ltd.) to separate liquid and solid phases. The solid

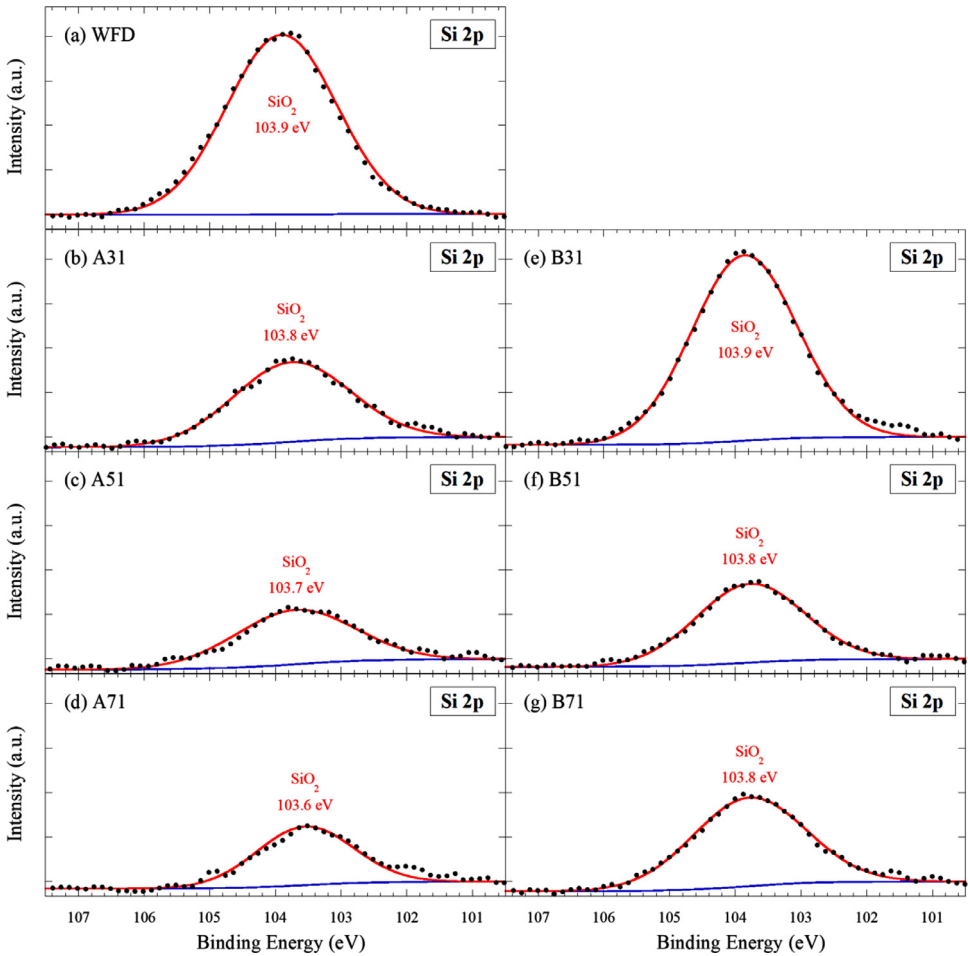


Fig. 6. High-resolution Si 2p XPS spectra of the samples.

samples were dried at 40 °C for 48 h in a vacuum desiccator and stored in a vacuum desiccator for characterization.

2.2. Methods

The as-received WFD sample and WFD samples obtained after the batch sorption tests using As(III) and Cr(VI) aqueous solutions were characterized with various analytical methods. XRD analysis was conducted with an X-ray diffractometer (XRD, X'Pert MPD, Philips) using a Cu α target (1.5412 Å) at 40 kV and 30 mA, and the XRD spectra were obtained in the range of 3–65 ° 2θ at a scan speed of 2 °/min with a step size of 0.01 °.

SEM-EDX analysis was conducted with a field-emission scanning electron microscopy (FE-SEM, Quanta 250FEG, FEI) and energy dispersive X-ray spectroscopy (EDX). The samples were distributed on carbon tape and coated with Pt. FE-SEM analysis was performed in SE mode at 10 kV in a high-vacuum state at various magnifications. EDX analysis was performed at 15 kV at

a magnification of 30000, image resolution of 1024 by 682 (0.01 μm of pixel size), and elemental mapping resolution of 256 by 170 (0.03 μm of pixel size).

FT-IR analysis was conducted with a Fourier-transform infrared spectroscopy (FT-IR, Cary 630 FT-IR, Agilent) in the range of 400–4000 cm^{-1} in ATR mode. XPS analysis was conducted with an X-ray photoelectron spectroscopy (XPS, PHI 5000 VersaProbe, ULVAC PHI) with monochromated Al $K\alpha$ (1486.6 eV) and anode (25 W at 15 kV) at a base pressure of 2.0×10^{-7} Pa and using dual neutralizer (Ar ion and electrons). For a wide scan, pass energy set 187.85 eV in the range of 10–1000 eV with a step size of 1.0 eV, and for a narrow scan, pass energy set 58.70 eV for C 1s (280–290 eV), O 1s (526–543 eV), Si 2p (96–113 eV), Fe 2p (701–741 eV), As 3d (40–52 eV), and Cr 2p (572–584 eV) region with a step size of 0.1 eV. The charge correction of the XPS spectra was performed using the C-C peak of adventitious carbon contamination at a binding energy of 284.8 eV. The XPS spectra for elements were fitted using a peak analyzer of the OriginPro 9 (1991–2012 OriginLab Corporation) program.

Ethics Statement

The authors declare that this article has not been published and has not been submitted elsewhere for publication. The authors have agreed to the submission.

CRedit Author Statement

Sunwon Rha: Methodology, Formal analysis, Investigation, Writing - Original draft preparation, Visualization; **Ho Young Jo:** Conceptualization, Resources, Writing - Review and Editing, Project administration, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that have influenced or could be perceived as affecting the work reported in this paper.

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References

- [1] S. Rha, H.Y. Jo, Waste foundry dust (WFD) as a reactive material for removing As(III) and Cr(VI) from aqueous solutions, *J. Hazard. Mater.* 412 (2021) 125290, doi:10.1016/j.jhazmat.2021.125290.
- [2] S. Zhang, X.Y. Li, J.P. Chen, An XPS study for mechanisms of arsenate adsorption onto a magnetite-doped activated carbon fiber, *J. Colloid Interf. Sci.* 343 (2010) 232–238, doi:10.1016/j.jcis.2009.11.001.
- [3] M.C. Biesinger, X-ray Photoelectron Spectroscopy (XPS) Reference Pages. www.xpsfitting.com, 2009–2018.
- [4] H.W. Nesbitt, M. Reinke, Properties of As and S at NiAs, NiS, and Fe1-xS surfaces, and reactivity of niccolite in air and water, *Am. Mineral.* 84 (1999) 639–649, doi:10.2138/am-1999-0417.
- [5] M.C. Biesinger, B.P. Payne, A.P. Grosvenor, L.W. Lau, A.R. Gerson, R.S.C. Smart, Resolving surface chemical states in XPS analysis of first row transition metals, oxides and hydroxides: Cr, Mn, Fe, Co and Ni, *Appl. Surf. Sci.* 257 (2011) 2717–2730, doi:10.1016/j.apsusc.2010.10.051.