

Supplementary Material: Isotope analysis of iron on structural materials of nuclear power plant using double-pulse laser ablation molecular isotopic spectrometry

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S-1. Chemical composition of structural materials

Table S-1. Chemical Composition of Utilized Specimens

Stainless steel 304 (wt%)		Inconel 690 (wt%)		Portland cement (wt%)	
Fe	70.9	Ni	60.4	CaO	64.6
Cr	18.2	Cr	31.0	SiO ₂	21.3
Ni	8.5	Fe	7.0	Al ₂ O ₃	5.6
Mn	1.8	Cu	0.5	Fe ₂ O ₃	3.4
Si	0.6	Mn	0.5	MgO	2.1
N	0.05	Cu	0.5	SO ₃	2.1
C	0.05	C	0.05	N ₂ O	0.05
S	0.01	Si	0.02		
P	0.03				

S-2. Optimized measurement condition according to matrix

The optimized measurement conditions (see Table S-2) were determined by considering the result of Figure S-1.

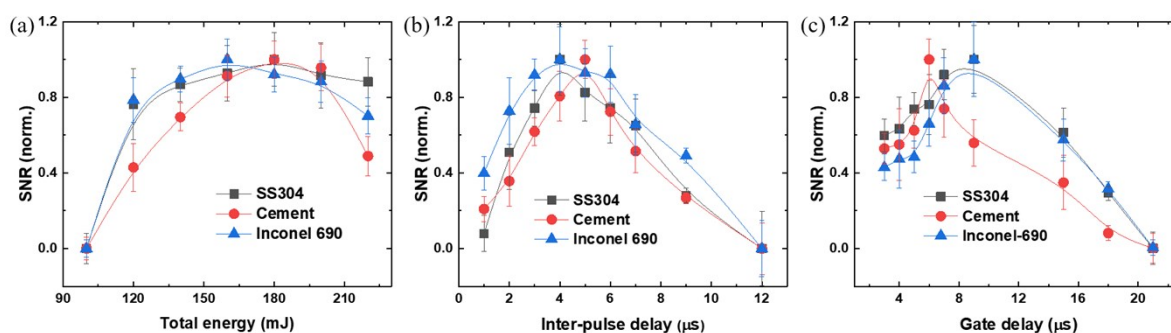


Figure S-1. Signal to noise ratio (SNR) of iron oxide emission as a function of (a) total energy, (b) inter-pulse delay, and (c) gate delay according to the matrix

Table S-2. Optimized Measurement Conditions for Surface Detection of Each matrix

	Total energy (mJ)	Inter-pulse delay (μs)	Gate delay (μs)	Gate width (μs)
SS304	180	4	4	100
Inconel	165	4	4	100
Cement	180	5	4	100

S-3. Methods of plasma characterization

Under the local thermal equilibrium (LTE) condition, plasma temperature (T) could be determined by Boltzmann plot method with below equation (1)^{S-1}.

$$\ln \left(\frac{I_{mn} \lambda_{mn}}{A_{ki} g_m} \right) = - \frac{E_m}{k_B T} + \ln \left(\frac{h c n_0(T)}{4 \pi Z(T)} \right) \quad (1)$$

I_{mn} : Line intensity of transition from upper level m to lower level n

λ_{mn} : Wavelength of the transition

A_{mn} : Spontaneous emission probability

g_m : Statistic weight of the upper level m

E_m : Energy of the upper level m

k_B : Boltzmann constant

h : Planck constants

$n_0(T)$: Number density

$Z(T)$: Partition function

Table S-3. Utilized Spectral Parameters of Iron Atomic Emission^{S-1}

λ_{mn} (nm)	E_m (cm ⁻¹)	g_m	A_{mn} (x10 ⁸ s ⁻¹)
371.9	26875	11	0.163
373.5	33695	11	0.902
374.6	27395	7	0.115
375.8	34329	7	0.634
376.4	34547	5	0.540

Plasma electron density could be obtained using Stark broadening effect of Fe I (541.4 nm) with the below equation (2)^{S-2}.

$$\Delta \lambda_S^{Fe} = 0.3612 \frac{N_e}{10^{23}} \left(\frac{T}{13000} \right)^{1.6551} \quad (2)$$

$\Delta \lambda_S^{Fe}$: Linewidth of iron atomic line (541.4 nm)

N_e : electron density [m⁻³]

References

(S-1) Rifai, K.; Laville, S.; Vidal, F.; Sabsabi, M.; Chaker, M. Quantitative analysis of metallic traces in water-based liquids by UV-IR double-pulse laser-induced breakdown spectroscopy. *J. Anal. At. Spectrom.* **2012**, 27(2), 276-283.

(S-2) Zielinska, S.; Pellerin, S.; Dzierzega, K.; Valensi, F.; Musiol, K.; Briand, F. Measurement of atomic Stark parameters of many Mn I and Fe I spectral lines using GMAW process. *J. Phys. D: Appl. Phys.* **2010**, 43(43), 434005.