

Supplemental information for Classification of Zirconium-Rich Engineered and Natural Nano Particles using Single Particle ICP-TOFMS

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Table S1. ICP-TOFMS instrument parameters

ICP Parameters	
Nebulizer gas	0.68 L min ⁻¹
Auxillary gas	1.48 L min ⁻¹
Cool gas	13 L min ⁻¹
RF power	1550 W
Sampling depth	4.9 mm
Torch/Injector	iCAP Q Quartz torch with 2.5 mm quartz injector
Skimmer/sampler cone	iCAP Q Nickel Samples (X Series) with Skimmer (with insert)
Mass Spectrometer Parameters	
Extraction Lens	-180 V
CCT mass	222 V
CCT Bias	-1.7 V
Deflection entry	-29.8 V
Deflection exit	35 V
CCT H ₂ flow rate	3.8 mL min ⁻¹
Notch filter (m/z)	19, 31.5, 37, 39.5
Time resolution	1.19 ms
Number of mass spectra averaged per time point	99

Table S2: Element names, measured Isotopes, sensitivities and critical masses obtained from spICP-TOFMS measurements

Element Name	Isotopes Used	Sensitivity (TofCts/g)	$X_{C,sp}^{mass}$ (g)
Mg	$^{24}\text{Mg}+^{25}\text{Mg}$	2.70E+15	2.89E-15
Al	^{27}Al	8.93E+15	9.00E-16
Ti	^{46}Ti or ^{48}Ti	5.39E+16	1.37E-16
Mn	^{55}Mn	1.18E+17	7.14E-17
Fe	^{56}Fe	1.17E+17	1.57E-16
Y	^{89}Y	3.01E+17	2.07E-17
Zr	^{90}Zr	1.70E+17	2.65E-17
Nb	^{93}Nb	2.97E+17	2.39E-17
Cs	^{133}Cs	3.45E+17	2.21E-17
La	^{139}La	5.47E+17	1.03E-17
Ce	^{140}Ce	5.35E+17	1.06E-17
Ho	^{165}Ho	2.76E+17	1.92E-17
Hf	$^{177}\text{Hf}+^{178}\text{Hf}+^{179}\text{Hf}+^{180}\text{Hf}$	2.67E+17	1.49E-17
Ta	^{181}Ta	5.22E+17	1.04E-17
Pb	$^{206}\text{Pb}+^{207}\text{Pb}+^{208}\text{Pb}$	3.00E+17	1.84E-17
Bi	^{209}Bi	2.55E+17	1.87E-17
Th	^{232}Th	2.55E+17	1.76E-17
U	^{238}U	2.83E+17	1.68E-17

Table S3: Mass fractions of each element in Zr-eng and Zr-nat particles. Mass fractions are calculated based on the total mass of each element present in Zr-eng and Zr-nat particles by spICP-TOFMS.

Elements	Zr-eng	Zr-nat
Mg	na	$0.2 \pm 0.1\%$
Al	na	$3.1 \pm 0.3\%$
Ti	na	$0.1 \pm 0.1\%$
Mn	na	$0.010 \pm 0.001\%$
Fe	na	$18 \pm 2\%$
Y	na	$0.8 \pm 0.4\%$
Zr	$98.2 \pm 0.1\%$	$73 \pm 2\%$
Sn	na	$0.03 \pm 0.01\%$
La	na	$0.36 \pm 0.02\%$
Ce	na	$0.70 \pm 0.09\%$
Ho	na	$0.03 \pm 0.02\%$
Hf	$1.8 \pm 0.1\%$	$0.78 \pm 0.02\%$
Ta	na	$0.06 \pm 0.05\%$
Pb	na	$0.030 \pm 0.003\%$
Th	na	$3.4 \pm 0.1\%$
U	na	$0.22 \pm 0.07\%$

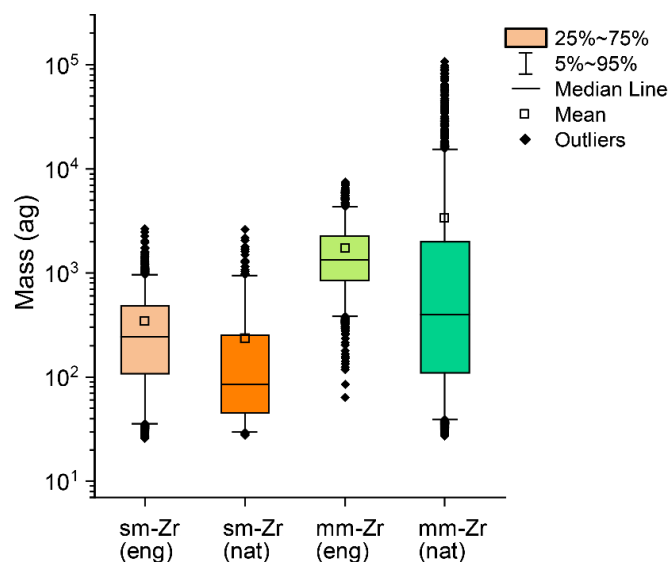


Figure S1: Boxplots showing mass distribution of Zr and Hf in single element (sm) and multi-element (mm) Zr-eng and Zr-nat particles.



Figure S2: Correlation matrix of mass amounts of each element in Zr-nat particles. Correlation matrix is generated using Streamlit webapp based on Pearson correlation coefficient.

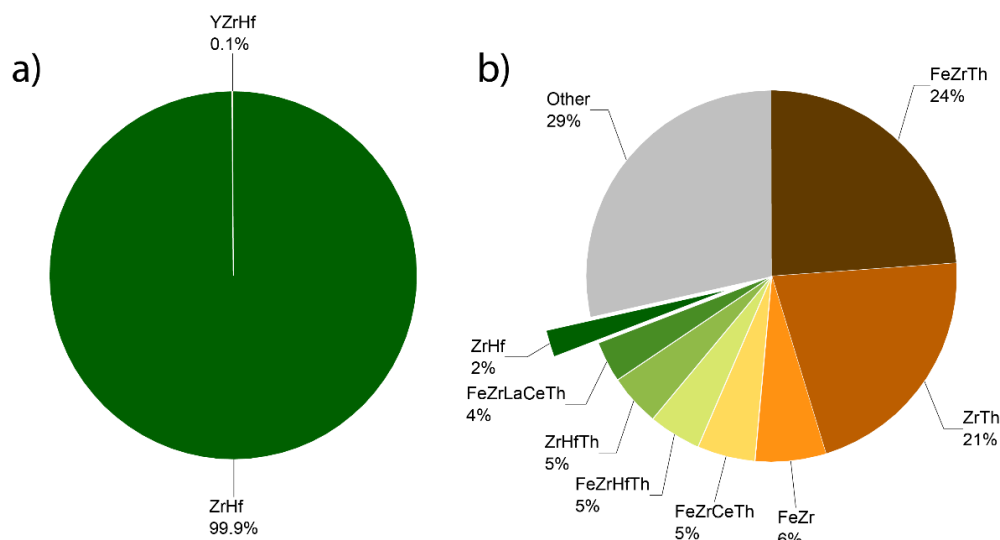


Figure S3: Pie charts of the multi-elemental signature measured by spICP-TOFMS for a) Zr-eng and b) Zr-nat particles. Only particles with recorded and multi-metal zirconium (mm-Zr) signatures are included in the pie charts.