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# ToF-SIMS spectral analysis of pristine and neutron irradiated single crystal tungsten

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ABSTRACT

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) has many promising features in studying materials including high spatial resolution and high mass accuracy of elements, molecules, and isotopes. Its ability to resolve isotopes is especially attractive in studying transmutation products of single crystal tungsten (SCW) post neutron irradiation. Tungsten (W) is a contender of plasma facing materials (PFMs) due to its high thermal and radiological stability. PFMs to be used in the construction of fusion vessels are subject to high temperature and neutron irradiation, resulting in changes to materials including transmutation, which ultimately impact material mechanical and thermal properties. We used IONTOF TOF.SIMS V instrument equipped with a 30 keV $Bi_3^+$ primary ion beam to study pristine SCW and irradiated SCW speciemens. Scanning electron microscope coupled with focused ion beam (SEM-FIB) was used to reduce the dosage of neutron irradiated tungsten and prepare for specimens for SIMS analysis. Static ToF-SIMS spectra were obtained, and transmutation product peak identification was presented in this work. Identified molecules and molecular fragments were compared against isotope theoretical mass to charge ratios of tungsten, rhenium, osmium, and other relevant products. Our results show that ToF-SIMS provides a viable means to study transmutation products of W post neutron irradiation. Such applications are suitable to investigate transmutation effects on materials that are being considered and developed for fusion pilot plants.

Specifications Table

| | |
|---|---|
| **Subject** | 6. Surface and interface modification by directed energy deposition |
| **Specific subject area** | Single crystal tungsten surface analysis |
| **Type of data** | Table<br>Figure |
| **How data were acquired** | Mass spectrometry<br>Instruments: Time-of-flight secondary ion Mass spectrometry<br>Make and model and of the instruments used: IONTOF TOF.SIMS V |
| **Data format** | Raw<br>Analyzed |
| **Parameters for data collection** | Compilation of scans with 30 keV $Bi_3^+$ metal ion gun rastered over the field of view of 150 × 150 μm$^2$ area. |
| **Description of data collection** | Static ToF-SIMS spectra were obtained using an IONTOF TOF.SIMS V equipped with a 30 keV $Bi_3^+$ metal ion gun. |
| **Data source location** | The raster size for the pristine single crystal tungsten region of interest was 150 × 150 μm$^2$. The raster size for the irraidated single crystal tungsten region of interest was 100 × 100 μm$^2$. The number of scans per depth profile scans were 450 for unirradiated SCW and 602 for irradiated W18. Peak identifications are based on mass formula with a mass deviation of less than 65 ppm.<br>Institution: Oak Ridge National Laboratory<br>City/Town/Region: Oak Ridge, TN<br>Country: United States of America |
| **Data accessibility** | Available via Dr. Xiao-Ying Yu's GitHub site, git@code.ornl.gov:nsrd_au/data_pub_sharing.githttps://github.com/Gparke4/Data-ToF-SIMS-spectral-analysis-of-pristine-and-neutron-irradiated-single-crystal-tungsten |
| **Related research article** | None |

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## 1. Value of the data

- Tungsten (W) and its alloys have attracted interest as the leading potential plasma facing material (PFM) candidate due to its ability to endure extreme conditions of exposure of severe thermal loads, high-neutron-energy bombardments, and neutron fluences in a fusion power plant [1–3]. Neutron exposure induces transmutation of W and related structural changes and consequently mechanical property degradation like hardening and brittleness. Reported transmutation products for pure W include rhenium (Re), tantalum (Ta), osmium (Os), and hafnium (Hf).
- Transmutation is known to affect W and alloys, available mass spectrometry data that characterize such isotopes are scarce. Bulk mass spectrometry, such as inductively coupled plasma mass spectrometry or thermal ionization mass spectrometry, does not have sufficient mass resolving power to identify products such as $^{182}$W, $^{183}$W, and transmutation products such as Re or Os as well as their isotopes that are close in mass.
- Time-of-flight secondary ion mass spectrometry (ToF-SIMS) offers high mass resolution, mass accuracy, and spatial resolution for metal and alloy studies [4,5]. It offers superior detection selectivity and sensitivity of elemental and isotopic analysis in metals. We study and compare the ToF-SIMS spectral analysis of the pristine and neutron irradiated single-crystal tungsten (SCW) specimens in this work. The tungsten coupons were irradiated in the High Flux Isotope Reactor (HFIR) facility as part of the fusion materials research at ORNL.
- This data set provides the first observations of irradiated SCW in comparison with pristine unirradiated SCW. The irradiated SCW post neutron irradiation shows a significant amount of transmutation products from the SEM-FIB liftout. We provide the first data set that can be used as reference data of SCW to support the development of PFM for the fusion materials research community.

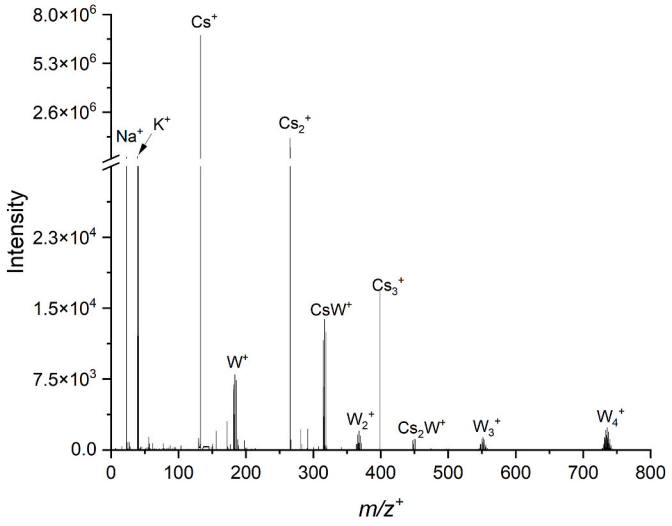


**Fig. 1.** ToF-SIMS spectral plot of the unirradiated single crystal tungsten specimen, SCW, in the $m/z^+$ range of 0–800 in the positive ion mode. Spectral results were reconstructed from scans 47 to 450 to reduce possible surface oxidation and contamination.

## 2. Data Description

We focus on reporting the elemental and isotopic composition of relevance to SCW and its transmutation products after irradiation. Collected ToF-SIMS spectra have the mass range of 0–800 Da. We highlighted the mass range of 150–225 Da, because this region is of interest for W and its transmutation products, such as Re and Os. Fig. 1 shows the ToF-SIMS spectra of unirradiated SCW in the positive mode. Similarly, Fig. 2 shows the spectra of the un-shielded, irradiated SCW, designated as W18, in the positive mode. Figs. 3 and 4 depict the sectional SIMS spectra of the pristine and irradiated SCW coupons, respectively, showing a closer look of the isotopes of W and W clusters for SCW as well as transmutation products and corresponding isotopes in the same mass regions.

Table 1 shows possible peak identifications of pure SCW, designated as SCW, in the positive mode. The unirradiated SCW spectra showed observation of pristine tungsten signals and the accompanying clusters of $W_2^+$, and $W_3^+$ respectively. Using sputtered Cs, the analyte (M) can cluster together creating observable $CsM^+$ ions [6–8], potentially providing a means to detect $M^+$ or $W^+$ in a quantitative manner. Using the $CsM^+$ method, we can view $CsW^+$ with high intensity signal. This serves as the control basis for future measurements. Table 2 displays possible peak identifications for the unshielded, irradiated W18 sample in the positive mode. Many transmutation products are observed throughout this collected spectra. Some representative observed transmutation products are $Re^+$, $Os^+$, $ReO^+$, and $OsO^+$ among others, in agreement with literature findings [9,10]. The $CsM^+$ molecules, showing as $CsW^+$, are observed among other products. Neutron bombardment has a major impact on the composition of the SIMS spectra for the irradiated SCW. We highlight ions, such as Hf, Ta, Re, and Os, due to the importance in the transmutation of W. Although $^{181}$W was

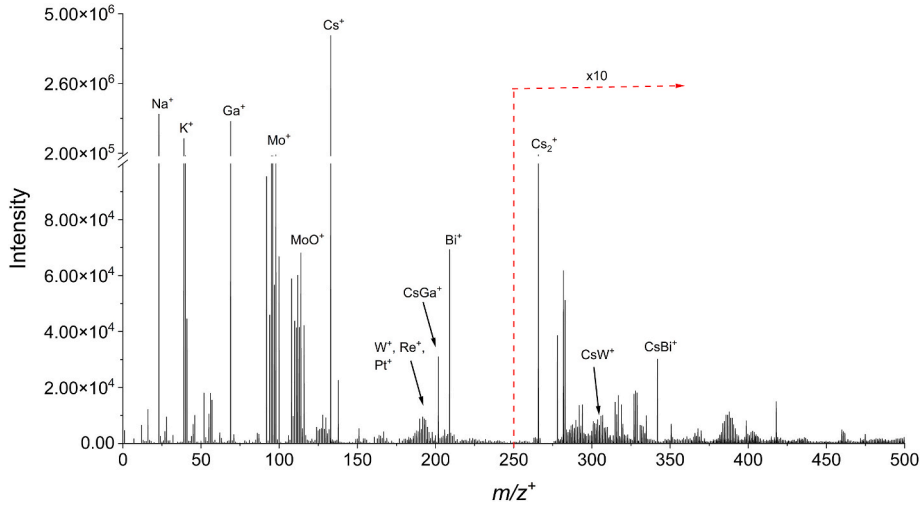


**Fig. 2.** Static ToF-SIMS spectral plot of the unshielded irradiated single crystal tungsten specimen, W18, in the $m/z^+$ range of 0–500 in the positive ion mode. Spectral results were reconstructed from scans 200 to 600.

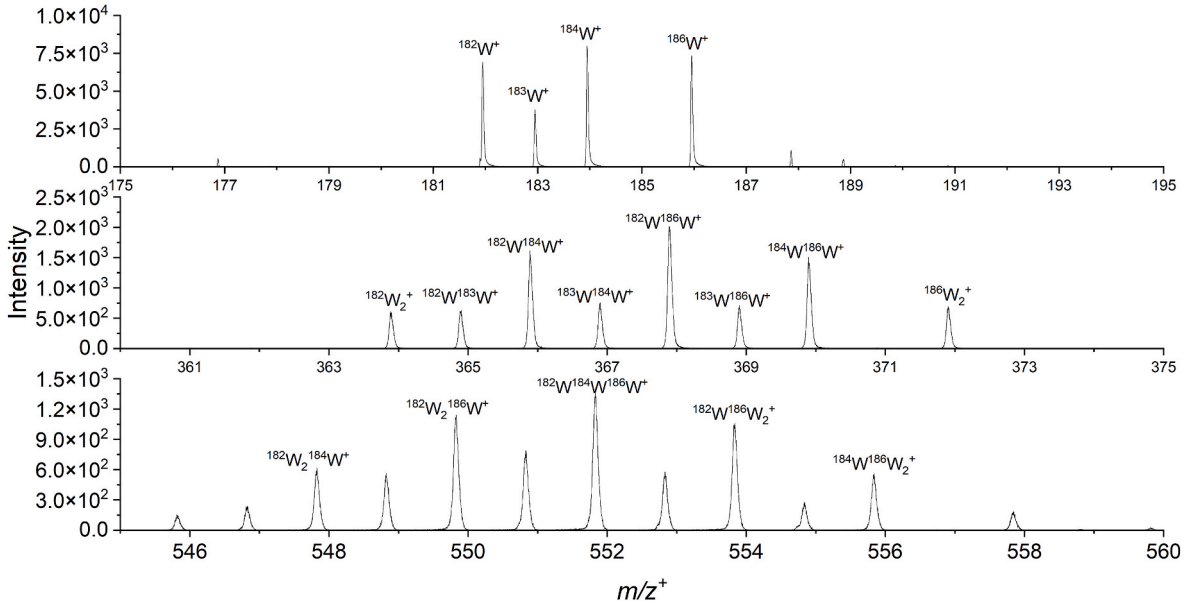


**Fig. 3.** ToF-SIMS spectral plots of single crystal tungsten of different mass sections corresponding to $W_1$, $W_2$, and $W_3$ in the positive ion mode, with identified W isotopes.

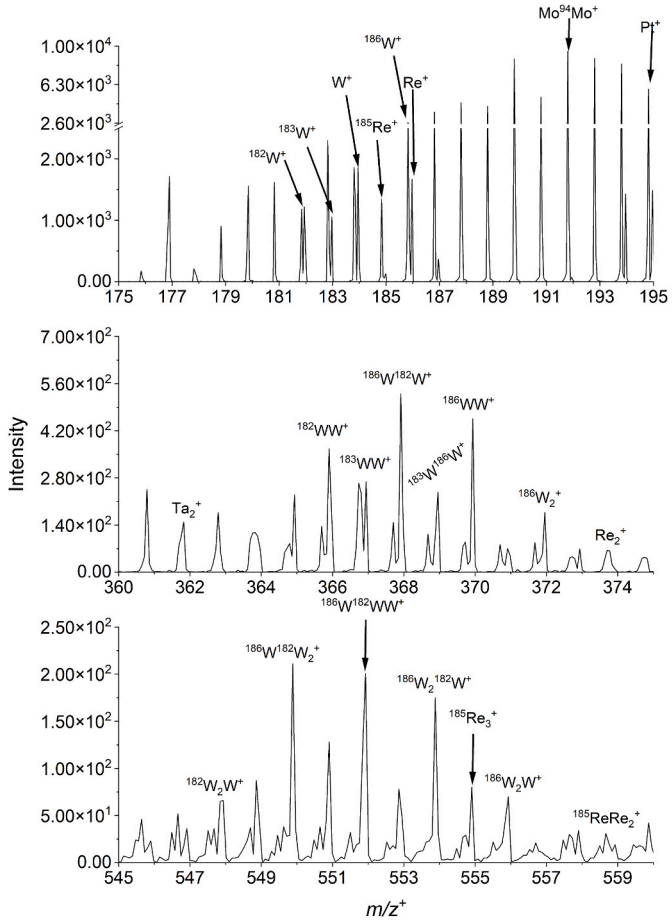


**Fig. 4.** ToF-SIMS spectral plots of the unshielded, irradiated single crystal tungsten W18 specimen of different mass sections corresponding to $W_1$, $W_2$, and $W_3$ in the positive ion mode, with identified isotopes.

reported as a possible transmutation product of W post neutron irradiation in HFIR using atom probe tomography, [11] the identification of this peak is not unambiguous due to low ion count and poor mass deviation. Supplementary Table S1–S2 show ToF-SIMS acquisition conditions used for the pristine and irradiated SCW specimens, respectively.

## 3. Experimental Design, materials and methods

The W18 sample was irradiated at a temperature of 700 °C. The neutron fluence was consistently maintained at a level of 2.2–3.5x$10^{25}$ n/$m^2$ (equivalent to 0.6–0.7 dpa). All samples have a purity exceeding 99.99 wt% in W prior to irradiation. W18 was prepared by using the FIB to lift out a small specimen from the irradiated sample in a SEM. Two liftout samples were prepared, both were in tens of micrometers, i.e., 20 μm × 10 μm × 10 μm. One of them was Pt welded onto a clean silicon (Si) wafer and the other to a TEM grid placed on a Si wafer. Depth profiling was performed on the liftout samples in the positive and negative mode consecutively. The positive data are reported here as isotopes of W are better detected in the positive ion mode.

ToF-SIMS depth profile spectra were obtained using an IONTOF TOF-SIMS V equipped with a 30 keV $Bi_3^+$ metal ion gun. The analysis area was approximately 100–150 $\mu m^2$ for the irradiated W18 liftout, and the FIB liftout was smaller than the analysis area. The electron flood gun was used to minimize surface charging for each sample. The figures shown here have identifications of molecules matching software (IONTOF *SurfaceSpectra v7*) suggested mass formula with a mass deviation of less than 65 ppm. The SIMS mass accuracy is defined as $\Delta M = 10^6 \times (m/z_{obs} - m/z_{the})/m/z_{the}$ (expressed in ppm), where $m/z_{obs}$ and $m/z_{the}$ refer to the observed and theoretical mass to charge ratio of a specific peak in the negative or positive ion mode [12]. Depth profiling was performed using 1 keV and 2 keV $Cs^+$ sputter beam for W18 and SCW samples, respectively. The sputtered areas were 500 × 500 $\mu m^2$ for the un-irradiated SCW and 400 × 400 $\mu m^2$ for the irradiated W18 liftout, respectively. The presented ToF-SIMS spectra herein were reconstructed from the depth profiling scans to reduce interferences of surface oxidation of W. A region of interest (ROI) was used to analyze the irradiated W18 sample as the actual tungsten liftout was small within the sputtered area nominally 100 × 100 $\mu m^2$ or 150 × 150 $\mu m^2$. Using the ROI results in lower ion counts. The analysis volume for each sample is 2.07 × $10^4$ $\mu m^3$ and 9.20 × $10^3$ $\mu m^3$ for unirradiated SCW and irradiated W18, respectively, based on the correlative atomic force measurements of the crater depth and the assumption of anisotropic profiling.

**Table 1**
Peak identification of isotopes and clusters of the pristine single crystal tungsten in the positive ion mode from this work.

| $m/z^{+}_{theo.}$ | $m/z^{+}_{obs.}$ | ΔM, ppm | Species | Assignment |
|---|---|---|---|---|
| 179.9467 | 179.9473 | 3.3343 | $^{180}W$ | Tungsten isotope 180 |
| 181.9477 | 181.9544 | 37.0608 | $^{182}W^{+}$ | Tungsten isotope 182 |
| 182.9497 | 182.9565 | 37.1677 | $^{183}W^{+}$ | Tungsten isotope 183 |
| 183.9504 | 183.9574 | 38.0991 | $W^{+}$ | Tungsten 184 |
| 185.9538 | 185.9610 | 38.8108 | $^{186}W^{+}$ | Tungsten isotope 186 |
| 314.8531 | 314.8447 | 26.7242 | $Cs\ ^{182}W^{+}$ | Tungsten isotope 182 and Cesium cluster |
| 315.8551 | 315.8468 | 26.2243 | $Cs\ ^{183}W^{+}$ | Tungsten isotope 183 and Cesium cluster |
| 316.8558 | 316.8476 | 25.9889 | $CsW^{+}$ | Tungsten 184 and Cesium cluster |
| 318.8593 | 318.8508 | 26.4941 | $Cs\ ^{186}W^{+}$ | Tungsten isotope 186 and Cesium cluster |
| 363.8959 | 363.8973 | 4.0365 | $^{182}W_2^{+}$ | Tungsten isotope 182 cluster |
| 364.8979 | 364.8992 | 3.5807 | $^{183}W^{182}W^{+}$ | Tungsten isotope 182 and 183 cluster |
| 365.8999 | 365.8997 | 0.6241 | $^{183}W_2^{+}$ | Tungsten isotope 183 cluster |
| 366.9006 | 366.9017 | 2.8730 | $^{183}WW^{+}$ | Tungsten isotope 182 and 184 cluster |
| 367.9013 | 367.9033 | 5.3138 | $W_2^{+}$ | Tungsten 184 cluster |
| 368.9040 | 368.9057 | 4.4236 | $^{186}W^{183}W^{+}$ | Tungsten isotope 186 and 183 cluster |
| 369.9047 | 369.9064 | 4.3904 | $^{186}WW^{+}$ | Tungsten isotope 186 and 184 cluster |
| 371.9082 | 371.9096 | 3.7954 | $^{186}W_2^{+}$ | Tungsten isotope 186 cluster |
| 496.8013 | 496.7850 | 32.9321 | $Cs^{182}W_2^{+}$ | Tungsten isotope 182 and Cesium cluster |
| 497.8033 | 497.7794 | 48.0827 | $Cs^{183}W^{182}W^{+}$ | Tungsten isotope 183, 182andCesium cluster |
| 498.8040 | 498.8046 | 1.0947 | $Cs^{182}WW^{+}$ | Tungsten isotope 182, 184 and Cesium cluster |
| 499.8061 | 499.7857 | 40.7977 | $Cs^{183}WW^{+}$ | Tungsten isotope 183, 184 and Cesium cluster |
| 500.8068 | 500.8087 | 3.8080 | $CsW_2^{+}$ | Tungsten 184 and Cesium cluster |
| 501.8095 | 501.8134 | 7.7065 | $Cs^{186}W^{183}W^{+}$ | Tungsten isotope 183, 186 and Cesium cluster |
| 502.8102 | 502.8126 | 4.7647 | $Cs^{186}WW^{+}$ | Tungsten isotope 184, 186 and Cesium cluster |
| 504.8136 | 504.8159 | 4.4924 | $Cs^{186}W_2^{+}$ | Tungsten isotope 186 and Cesium cluster |
| 545.8441 | 545.8227 | 39.1855 | $^{182}W_3^{+}$ | Tungsten isotope 182 triplelet cluster |
| 546.8461 | 546.8256 | 37.4082 | $^{183}W^{182}W_2^{+}$ | Tungsten isotope 182 and 183 cluster |
| 547.8468 | 547.8259 | 38.1928 | $W^{182}W_2^{+}$ | Tungsten isotope 182 and 184 cluster |
| 548.8488 | 548.8270 | 39.7093 | $W^{183}W^{182}W^{+}$ | Tungsten isotope 182, 183, and 184 cluster |
| 549.8495 | 549.8284 | 38.3997 | $W_2^{182}W^{+}$ | Tungsten isotope 182 and 184 cluster |
| 550.8515 | 550.8300 | 39.1138 | $W_2^{183}W^{+}$ | Tungsten isotope 183 and 184 cluster |
| 551.8522 | 551.8313 | 38.0140 | $W_3^{+}$ | Tungsten isotope 184 cluster |
| 552.8550 | 552.8323 | 41.0364 | $^{186}W^{183}WW^{+}$ | Tungsten isotope 183. 184, and 186 cluster |
| 553.8557 | 553.8342 | 38.7863 | $^{186}WW_2^{+}$ | Tungsten isotope 184 and 186 cluster |
| 554.8584 | 554.8348 | 42.4783 | $^{186}W_2^{183}W^{+}$ | Tungsten isotope 183 and 186 cluster |
| 555.8591 | 555.8371 | 39.6194 | $^{186}W_2W^{+}$ | Tungsten isotope 184 and 186 cluster |
| 557.8625 | 557.8401 | 40.2012 | $^{186}W_3^{+}$ | Tungsten isotope 186 cluster |

Footnotes.
$m/z^{+}_{theo.}$: theoretical mass to charge ratio in the positive ion mode.
$m/z^{+}_{obs.}$: observed mass to charge ratio in the positive ion mode.
ΔM: $\Delta M = 10^6 \times (m/z^{+}_{obs.} - m/z^{+}_{theo.})/m/z^{+}_{theo.}$ (expressed in ppm) [12].

**Table 2**
Peak identification of isotopes and clusters of the unshielded, irradiated single crystal tungsten in the positive ion mode from this work.

| $m/z^{+}_{theo.}$ | $m/z^{+}_{obs.}$ | ΔM | Species | Assignment |
|---|---|---|---|---|
| 179.9460 | 179.9459 | 0.4884 | $Hf^{+}$ | Hafnium 180 |
| 180.9474 | 180.9533 | 32.2815 | $Ta^{+}$ | Tantalum 181 |
| 181.9477 | 181.9464 | 7.0707 | $^{182}W^{+}$ | Tungsten isotope 182 |
| 182.9497 | 182.9480 | 9.2526 | $^{183}W^{+}$ | Tungsten isotope 183 |
| 183.9504 | 183.9478 | 14.2348 | $W^{+}$ | Tungsten 186 |
| 184.9524 | 184.9500 | 12.8795 | $^{185}Re^{+}$ | Rhenium isotope 185 |
| 185.9538 | 185.9494 | 23.9162 | $^{186}W^{+}$ | Tungsten isotope 186 |
| 186.9552 | 186.9579 | 14.3986 | $Re^{+}$ | Rhenium 187 |
| 187.9553 | 187.9524 | 15.1571 | $^{188}Os^{+}$ | Osmium isotope 188 |
| 188.9576 | 188.9608 | 17.0546 | $^{189}Os^{+}$ | Osmium isotope 189 |
| 191.9609 | 191.9684 | 39.0661 | $Os^{+}$ | Osmium 192 |
| 365.8999 | 365.9224 | 61.5335 | $^{183}W_2^{+}$ | Tungsten isotope 183 cluster |
| 366.9006 | 366.9218 | 57.6461 | $W^{183}W^{+}$ | Tungsten 184 and isotope 183 cluster |
| 368.9040 | 368.9165 | 33.7779 | $^{186}W^{183}W^{+}$ | Tungsten isotope 186 and 183 cluster |
| 369.9047 | 369.9275 | 61.5205 | $^{186}WW^{+}$ | Tungsten isotope 186 and 184 cluster |
| 371.9082 | 371.9284 | 54.4100 | $^{186}W_2^{+}$ | Tungsten 186 cluster |
| 373.9091 | 373.9272 | 48.3571 | $Os^{182}W^{+}$ | Osmium 192 and Tungsten 182 cluster |
| 375.9119 | 375.9298 | 47.8466 | $OsW^{+}$ | Osmium 192 and Tungsten 184 cluster |
| 377.9153 | 377.9228 | 19.9463 | $Os^{186}W^{+}$ | Osmium 192 and Tungsten isoptope 186 cluster |
| 378.9167 | 378.9288 | 31.9680 | $ReOs^{+}$ | Rhenium 187 and Osmium 192 cluster |
| 381.9200 | 381.9313 | 29.7009 | $RePt^{+}$ | Rhenium 187 and Platinum 195 cluster |
| 382.9201 | 382.9246 | 11.6185 | $Re^{196}Pt^{+}$ | Rhenium isotope 195 and Platinum 195 cluster |
| 383.9230 | 383.9309 | 20.6694 | $Ir^{191}Ir^{+}$ | Irridium isotope 191and 193 cluster |
| 385.9253 | 385.9315 | 16.0416 | $Ir_2^{+}$ | Irridium 193 cluster |

Footnotes.
$m/z^{+}_{theo.}$: theoretical mass to charge ratio in the positive ion mode.
$m/z^{+}_{obs.}$: observed mass to charge ratio in the positive ion mode.
ΔM: $\Delta M = 10^6 \times (m/z^{+}_{obs.} - m/z^{+}_{theo.})/m/z^{+}_{theo.}$ (expressed in ppm) [12].

The peak identification procedure followed a multi-step process. The mass matching function calculates different combinations of periodic table elements to mass match a selected peak and it provides a mass deviation and match score. These combinations range from organics to inorganics. Using the "peak search" function within *SurfaceSpectra*, with parameters of SNR 3.0, max background 0.8, and minimum counts 25, a peak list was generated giving the best mass matching formula for the given $m/z$ value under each specific sample. Isotopic ratios for each of the assigned peaks was considered before assignment. Peak assignment was further verified by literature search pertaining to these molecules.

SIMS spectral plotting was done using OriginPro 2023, where the data was extracted from the calibrated SIMS files and converted to ASCII files with bin equal to 1 to show raw data. Data files are made accessible to the public. Calibration points for each of the samples were selected to be the same. Calibration peaks include $Na^{+}$, $K^{+}$, $W^{+}$, $CsW^{+}$ and $W_2^{+}$ in the positive ion mode. In addition to mass accuracy, the peak identification of SCW was compared with known ratios of isotopes of W in natural abundance and a good agreement was reached. Other isotopes of the transmutation products, such as Re and Os, are compared with known isotope theoretical values during peak assignment.

The transmutation reaction initiated during the fusion neutron irradiation cause formation of transmutation elements, such as Re, Os, and Ta, in the W-based PFMs. We report the first SIMS spectral detection of elements and isotopes related to SCW, including Hf, Ta, W, Re, and Os due to the importance in the transmutation of W as a PFM candidate in fusion applications [13]. Such SIMS mass spectral data are valuable as references of pure W without neutron irradiation. Additionally, these spectral results are useful to study the neutron irradiation effect on W,

particularly in the identification of transmutation products with decent mass resolution and accuracy using SIMS. Speciation information like this is important in understanding the transmutation effects on PFMs and other structural materials and the implications on the mechanical properties and integrity of fusion materials.

## CRediT authorship contribution statement

**Gabriel D. Parker:** Writing – review & editing, Writing – original draft, Investigation, Formal analysis, Data curation. **Tobias K. Misicko:** Writing – review & editing, Writing – original draft, Investigation, Formal analysis. **Tanguy Teriler:** Writing – review & editing, Methodology, Data curation. **Yang Xiao:** Writing – review & editing. **Xiao-Ying Yu:** Writing – review & editing, Writing – original draft, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

## Ethics Statement

The authors confirm that they have read and followed the ethical requirements for publication in Data in Brief and confirm that the current work does not involve human subjects, animal experiments, or any data collected from social media platforms.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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## Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.rsurfi.2025.100577.

## Data availability

Data will be made available on request. Also available in github, https://github.com/Gparke4/Data-ToF-SIMS-spectral-analysis-of-pristine-and-neutron-irradiated-single-crystal-tungsten

Tungsten Data (Original data) (IEEE Data Portal)

## References

[1] Linsmeier, C., Rieth, M., Aktaa, J., Chikada, T., Hoffmann, A., Hoffmann, J., Houben, A., Kurishita, H., Jin, X., Li, M., Litnovsky, A., Matsuo, S., von Müller, A., Nikolic, V., Palacios, T., Pippan, R., Qu, D., Reiser, J., Riesch, J., Shikama, T., Stieglitz, R., Weber, T., Wurster, S., You, J.H., Zhou, Z., 2017. Development of advanced high heat flux and plasma-facing materials. Nucl. Fusion 57, 092007.

[2] Howard, L., Parker, G.D., Yu, X.-Y., 2024. Progress and challenges of additive manufacturing of tungsten and alloys as plasma-facing materials. Materials 17, 2104.

[3] Rieth, M., Doerner, R., Hasegawa, A., Ueda, Y., Wirtz, M., 2019. Behavior of tungsten under irradiation and plasma interaction. J. Nucl. Mater. 519, 334–368.

[4] Balamurugan, A., Dash, S., Tyagi, A.K., 2014. Mass spectral analysis and quantification of secondary ion mass spectrometry data. Int. J. Mass Spectrom. 386, 56–60.

[5] Shen, Y., Howard, L., Yu, X.-Y., 2024. Secondary ion mass spectral imaging of metals and alloys. Materials 17, 528.

[6] Gao, Y., 1988. A new secondary ion mass spectrometry technique for III-V semiconductor compounds using the molecular ions $CsM^+$. J. Appl. Phys. 64, 3760–3762.

[7] Saha, B., Chakraborty, P., 2013. $MCs_n^+$-SIMS: an innovative approach for direct compositional analysis of materials without standards. Energy Proc. 41, 80–109.

[8] Gnaser, H., Oechsner, H., 1991. SIMS depth profile analysis using $MCs^+$ molecular ions. Fresen. J. Anal. Chem. 341, 54–56.

[9] Gilbert, M.R., Sublet, J.C., 2011. Neutron-induced transmutation effects in W and W-alloys in a fusion environment. Nucl. Fusion 51, 043005.

[10] Zhao, Q., Zhang, Z., Huang, M., Ouyang, X., 2019. Effects of transmutation elements in tungsten. Comput. Mater. Sci. 162, 133–139.

[11] Inoue, K., Yamashita, T., Nogami, S., Hasegawa, A., Toyama, T., Nagai, Y., 2023. Direct observation of voids decorated with transmuted rhenium atoms in neutron-irradiated tungsten by correlative use of TEM and APT. Materialia 32, 101963.

[12] Yu, X.-Y., Yang, C., Gao, J., Xiong, J., Sui, X., Zhong, L., Zhang, Y., Son, J., 2023. Molecular detection of per- and polyfluoroalkyl substances in water using time-of-flight secondary ion mass spectrometry. Front. Chem. 11.

[13] Katoh, Y., Snead, L.L., Garrison, L.M., Hu, X., Koyanagi, T., Parish, C.M., Edmondson, P.D., Fukuda, M., Hwang, T., Tanaka, T., Hasegawa, A., 2019. Response of unalloyed tungsten to mixed spectrum neutrons. J. Nucl. Mater. 520, 193–207.