

----- **GENERAL INFORMATION** -----

DATA TITLE: Raman spectroscopy of surfaces on ferritic Fe-Cr-Al-Mo alloy Kanthal APMT and Cr-Mo-V steel T91 (UNS: K90901) after oxidation at 1200 C for 2 h

PROJECT TITLE: Materials Characterization of High-Temperature Oxidation on ferritic Fe-Cr-Al-Mo alloy Kanthal APMT and Cr-Mo-V steel T91 (UNS: K90901)

DATA ABSTRACT: Comma-separated text files with Raman spectra data acquired from the surface of ferritic Fe-Cr-Al-Mo alloy Kanthal APMT and Cr-Mo-V steel T91 (UNS: K90901) after oxidation at 1200 C for 2 h in steam and air. Python Jupyter Notebook used to visualize the data is also included.

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ASSOCIATED PUBLICATIONS:

T. Copeland-Johnson, C.K.A. Nyamekye, S.K. Gill, L. Ecker, N. Bowler, E.A. Smith, R.B. Rebak, Characterization of Kanthal APMT and T91 oxidation at beyond design-basis accident temperatures, Corros. Sci. (2020).

COLLECTION INFORMATION:

Time period(s): 2017-2019

Location(s): Iowa State University, Brookhaven National Laboratory

----- FILE DIRECTORY -----

----- FILE LIST-----

File Name	Description
APMT.csv	Comma-separated file containing background corrected data for APMT
Raman Standards.csv	Comma-separated file containing standard Raman data acquired from RRUFF database.
Steam-Oxidized T91.csv	Comma-separated file containing background corrected data for steam-oxidized T91
Air-Oxidized T91.csv	Comma-separated file containing background corrected data for air-oxidized T91

Figure 5a.html	High-resolution, interactive version of Figure 5a in html format generated with the Python Bokeh library
Figure 5b.html	High-resolution, interactive version of Figure 5b in html format generated with the Python Bokeh library
Figure 5c.html	High-resolution, interactive version of Figure 5c in html format generated with the Python Bokeh library
Figure 5d.html	High-resolution, interactive version of Figure 5d in html format generated with the Python Bokeh library
Raman Spectra Viewer for Figure 5.ipynb	Viewer for generating Figures 5a.html to Figure 5d.html using Anaconda Jupyter Notebook. Notebook is already configured to use included .csv files.

----- METHODS AND MATERIALS -----

----- DATA COLLECTION METHODS -----

The specimens were placed onto a glass slide and irradiated with a $1.44 \times 10^5 \text{ W cm}^{-2}$ solid-state 532-nm diode laser producing a $2.95 \pm 0.06 \text{ }\mu\text{m}$ laser spot size on the specimen surface and analyzed with an Olympus 10× objective (0.25 numerical aperture). A 60 s acquisition time with three accumulations were used for all Raman measurements.

----- DATA PROCESSING METHODS -----

Raman spectra data was plotted using Jupyter Notebook in Anaconda. Data is normalized from 0 to 1, to allow for comparison between spectra, the minimum intensity assigned as 0 and the maximum intensity assigned as 1. Afterwards data is plotted using Bokeh library (<https://docs.bokeh.org/en/latest/>).

----- SOFTWARE -----

Name: Anaconda

Version: 64-bit

System Requirements:

Windows: Windows 7 or newer, 64-bit macOS 10.13+, or Linux, including Ubuntu, RedHat, CentOS 6+, and others

URL: <http://www.anaconda.com>

Developer: Anaconda, Inc. (Note that Anaconda is an open-source distribution for Python and R programming languages)

Additional Notes: Minimum 5 GB disk space to download and install.

----- EQUIPMENT -----

Manufacturer: HORIBA Scientific

Model: XploRA Plus Raman confocal upright microscope

Embedded Software/Firmware Name: (if applicable) N/A

Embedded Software/Firmware Version: (if applicable) N/A

Additional Notes: Raman shift signal was collected in the epi-direction using a 300 μm confocal pinhole and an 1800 g/mm grating with 3 cm^{-1} resolution.

----- LICENSING -----

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