----- GENERAL INFORMATION -----

DATA TITLE: Comparison of results from Raman and EDS/SEM analysis of ferritic Cr-Mo-V steel T91 (UNS: K90901) cross-sectioned after oxidation at 1200 C for 2 hrs in air 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: Raman images acquired from a cross-sectioned segment of ferritic Cr-Mo-V steel T91 (UNS: K90901) after oxidation in air at 1200 C for 2 h. Raman data was collected using a WITec alpha 300R micro-imaging Raman microscope. Results provide evidence to the presence of Fe_(3-x)Cr_xO₄.

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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
GlotchData.csv	Comma-separated text file containing raw data for
	spectrum featuring Raman shift that indicates the
	presence of $Fe_{(3-x)}Cr_xO_4$. Data acquired from
	Timothy Glotch Group at Stony Brook University.
Figure 7c.html	High-resolution, interactive version of Figure 7c in
	html format generated with the Python Bokeh
	library.
Raman Spectra Viewer for Figure	Viewer for generating Figures 7c.html to Figure
7c.ipynb	7c.html using Anaconda Jupyter Notebook.

	Notebook is already configured to use included .csv
	files.
Raman_T91_Air_Filter Scale.png	Intensity scale for Raman shift 677 cm ⁻¹ filter image
	in Raman_T91_Air_Filter@677.png
Raman_T91_Air_Filter@677.png	Raman filter image showing the distribution of
	Raman shift located at 677 cm ⁻¹ in the site of
	interest shown in Raman_T91_Air_Image.png
Raman_T91_Air_Filter@CCD-41cts.txt	Tab-delimited text file of Raman spectra signifying
	the minimum intensity, -41 counts (cts), at which the
	Raman shift 677 cm ⁻¹ was detected in
	Raman_T91_Air_Filter@677.png
Raman_T91_Air_Filter@CCD173cts.txt	Tab-delimited text file of Raman spectra
	corresponding to the maximum intensity, 173
	counts (cts), at which the Raman shift 677 cm ⁻¹ was
	detected in Raman_T91_Air_Filter@677.png
Raman_T91_Air_Filter_Metadata.txt	Metadata for acquisition parameters used to
	acquire the Raman image in
	Raman_T91_Air_Filter@677.png
Raman_T91_Air_Image.png	Optical microscope image of a site of interest
	captured from a cross-sectioned segment of T91
	after oxidation in air for 2 hrs
Raman_T91_Air_Image_Metadata.txt	Metadata for acquisition parameters used to
	acquire the optical microscope image in
	Raman_T91_Air_Image.png

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

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

The Raman image was captured with a WITec alpha 300R microscope. The WITec alpha microscope was equipped with dual lasers operating at 532 and 785 nm, the former was used for Raman imaging. A 100 g/mm grating was utilized. The WITec alpha microscope was capable of a ~1 μ m spatial resolution, illustrating the distribution of Raman active compounds in areas up to 2500 μ m². Raman spectra were collected under an integration time of 0.23 or 1 s.

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

Raman filter images, scan data, and metadata files were exported from WITec Control 4 software suite. Raman spectra data was plotted using Jupyter Notebook in Anaconda. Data was normalized from 0 to 1, to allow for comparison between spectra, the minimum intensity assigned as 0 and the maximum intensity assigned as 1.

----- SOFTWARE ------

Name: WITec Control Version: 4 System Requirements: N/A URL: <u>https://www.witec-instruments.com/</u> Developer: WITec Wissenschaftliche Instrumente und Technologie GmbH

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: WITec Model: Alpha 300R Embedded Software/Firmware Name: (if applicable) N/A Embedded Software/Firmware Version: (if applicable) N/A

Manufacturer: JEOL Model: 7600F Embedded Software/Firmware Name: (if applicable) N/A Embedded Software/Firmware Version: (if applicable) N/A Additional Notes: Equipped with Oxford Instruments EDS 80 mm² X-Max silicon drift detector (129 eV resolution) operated through the INCA software suite.

----- LICENSING ------

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