

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

DATA TITLE: Analysis of ferritic Cr-Mo-V steel T91 (UNS: K90901) after oxidation at 1200 C for 2 h using synchrotron x-ray diffraction

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: Synchrotron x-ray diffraction (XRD) was used to identify oxidation products and their respective structural phases on the surface of Cr-Mo-V steel T91 (UNS: K90901) before and after oxidation at 1200 degrees Celsius for 2 h in steam and air. Tab-delimited text files are included for the patterns displayed in the high-resolution plot, listing the momentum transfer of scattering (Q), the intensity, and error values of the intensity. Text files are truncated to $Q = 8 \text{ \AA}^{-1}$ because beyond that point the pattern is only background noise.

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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
XRD_T91.png	High-resolution plot comparing XRD patterns collected at the XPD beamline for T91 before and after steam/air oxidation
XRD_T91_Air.txt	Tab-delimited text file with Q versus Intensity data used in XRD_T91.png for air-oxidized T91
XRD_T91_Control.txt	Tab-delimited text file with Q versus Intensity data used in XRD_T91.png for T91 before oxidation

XRD_T91_Steam.txt	Tab-delimited text file with Q versus Intensity data used in XRD_T91.png for steam-oxidized T91

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

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

Synchrotron x-ray power diffraction (XPD) studies were conducted at the ID-28-2 beamline at the National Synchrotron Light Source II (NSLS-II). Measurements were conducted in shallow angle beam reflection mode using a silicon-base flat panel detector. The wavelength of the incident x-rays was exactly 0.236996 Å (52.314912 keV). The specimen-to-detector distance and tilts of the detector relative to the beam were refined using a LaB₆ standard. Beamline operation was performed using xpdAcq, a Python-based package developed by the XPD beamline scientists for data collection.

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

All the raw two-dimensional XRD patterns were processed using xpdAn, a Python package developed by the XPD beamline scientists to streamline data analysis. XRD patterns were background corrected by subtracting a dark current image. Noticeable artifact regions of the detector (like the beam stop and dead pixels) were masked. The corrected and masked two-dimensional detector images were then radially integrated to obtain one-dimensional powder diffraction patterns. Identifying oxidation products was conducted using the PDF-4+ software published by the International Center for Diffraction Data (ICDD). One-dimensions XPD data was then plotted using OriginLab.

----- SOFTWARE -----

Name: xpdAcq

Version: 0.10.4

System Requirements: N/A

URL: <https://xpdacq.github.io/xpdAcq/>

Developer: Brookhaven National Laboratory, NSLS-II

Additional Notes: This software is only installed on the XPD beamline workstations

Name: xpdAn

Version: 0.8.1

System Requirements: N/A

URL: <https://xpdacq.github.io/xpdAn/>

Developer: Brookhaven National Laboratory, NSLS-II

Additional Notes: This software is only installed on the XPD beamline workstations

Name: PDF-4+

Version: 2019

System Requirements: Intel® Core™ 2 Duo processor or better; Supported Microsoft®

Operating Systems: Windows Vista® (32-bit) SP2, Windows® 7 SP1, Windows® 8, Windows® 8.1, Windows® 10; NTFS File System required; 4 GB of System Memory; Installation requires 10 GB of hard-disk space

URL: <http://www.icdd.com/pdf-4/>

Developer: International Center for Diffraction Data

Name: OriginLab 2016

Version: 64-bit

System Requirements:

Windows: Operating System: 64-bit (x64) Microsoft Windows® 7 SP1, Windows® 8, Windows® 8.1, Windows® 10; Processor: 1.6 GHz 64-bit (x64); Memory: 4 GB RAM (8 GB recommended); Hard Disk Space: 2.0 GB of free hard disk space for program installation + Help files (does not include data storage); Other hardware: USB port or DVD drive (if installing from USB stick or DVD); Browser: The Learning Center dialog requires Internet Explorer version 11.

Mac: Mac users can run Origin by using Microsoft Windows® via Boot Camp or within OS X using third-party virtual machine software.

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

Developer: OriginLab Corporation

----- LICENSING -----

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