Supporting Information: Assessment of Martensitic Transformation Paths Based on Transformation Potential Calculations

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In addition to the technical paper[17] and the data set citation,[16] supporting information is provided in this document. The citation numbering is atypical to avoid dissimilar numbers between this supporting information document and the dataset citation.

There are three sections in this supporting information document:

1. README.txt file adaption
2. Lattice parameters and transformation values
3. Additional stress states

README.txt FILE adaption

Per discussion with the editors, the README.txt file from the dataset citation[16] has been transcribed to this supporting information document, with some modification in style to conform to the supporting information document style. The dataset citation contains the referenced files and programs.

This file (README.txt) describes the data set "Data Set: Assessment of Martensitic Transformation Paths Based on Transformation Potential Calculations". While readable as a plain text, this file uses Markdown formatting.

Questions regarding this data set may be directed to Adam Creuziger (adam.creuziger@nist.gov)

Sections
- NIST License
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- File and Directory Descriptions
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NIST License

NIST Disclaimers

Certain commercial equipment, instruments, or materials are identified in this dataset in order to specify the experimental and computational procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and

Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

File and Directory Descriptions

This data set is composed of the following:

File or Directory	Description
README.txt	File you are currently reading, describing the general structure of the data set.
JupyterNotebooks/	Directory containing Jupyter notebooks, and associated output files.
AsProcessed/	Directory containing Matlab scripts, and associated input and output files for measurement of the crystallographic texture of the as-received sample.
RD24pct/	Directory containing Matlab scripts, and associated input and output files for measurement of the crystallographic texture of the sample deformed to 24% engineering strain along the rolling direction.
CompositeFigures	Directory containing Inkscape (https://inkscape.org/) files and associated output files.
Table1.xlsx	File containing data for Table 1 in the technical paper. These values are copied from the “ExpTextureValues.txt” files and the phase fractions referenced in the text.

Citations in AvailableWork.ipynb
To clarify the source of values used in this data set, comments have been added to the AvailableWork.ipynb Jupyter notebook. These references are reproduced below with the same numbering.

- [1] A. Creuziger & T. Foecke, Acta Materialia, Vol 58, pgs 85-91, 2010. [1]
- [2] CTM code, provided by Thomas Shield (shield@aem.umn.edu). [2]
- [3] V. Randle "Measurement of Grain Boundary Geometry" CRC Press 1993.[3]
- [4] M. Humbert et. al., Materials Science and Engineering: A, Vol 454-455, pgs 508-517, 2007. [4]
- [5] C. F. Jatczak, J. A. Larson, S. W. Shin. "Retained austenite and its measurements by X-ray diffraction; an information manual (SAE SP453)." Society of Automotive Engineers, 1980.[5]
- [6] S. Kundu & H. K. D. H. Bhadeshia, Scripta Materialia, Vol 55, pgs 779-781, 2006.[6]
- [7] H. K. D. H. Bhadeshia, "Worked examples in the Geometry of Crystals" 2nd Ed, Insitute of Metals, 1987, http://www.phase-trans.msm.cam.ac.uk/2001/geometry2/Geometry.pdf [7]
- [8] S. Kundu & H. K. D. H. Bhadeshia, Scripta Materialia, Vol 57, pgs 869-872, 2007. [8]

Programs Used

The following application programs and versions were used in this data set:
- Matlab R2015a [9]
- Mtex 5.0.beta.2 -- with fixes https://github.com/Mtex-toolbox/Mtex/issues/237 [10]
- Anaconda 1.8.1 [11]
- Jupyter Notebook 4.2.3 [12]
- Python 2.7.12

- PF (Peak Fit) [13]
- Inkscape 0.91, 0.92

The Matlab scripts assume that you have successfully installed the Matlab package Mtex.

Citations for Programs:
- [9] MATLAB. Natick, MA: MathWorks Inc [Online]. Available: https://www.mathworks.com/product/Matlab.html
- [10] R. Hielscher and H. Schaeben, “A novel pole figure inversion method: specification of the Mtex algorithm,” Journal of Applied Crystallography, vol. 41, no. 6, pp. 1024–1037, Dec. 2008. (http://mtex-toolbox.github.io/)
- [11] Anaconda Software Distribution. Continuum Analytics, 2016 [Online]. Available: https://continuum.io
- [12] F. Perez and B. E. Granger, “IPython: A System for Interactive Scientific Computing,” Computing in Science Engineering, vol. 9, no. 3, pp. 21–29, May 2007.
- [13] T. Gnäupel-Herold, PF. NIST NCNR [Online]. Available: https://www.ncnr.nist.gov/instruments/bt8/BT8DataAnalysis.htm

Additional Python packages

The environment snapshot (CondaEnvironment.yml) and requirements files (requirements.txt) listing the python packages used in the jupyter notebook scripts are included in the JupyterNotebooks/ directory. Citations for these additional packages are listed below.

Citations for additional packages used in jupyter notebooks:

- [14] J. D. Hunter, “Matplotlib: A 2D graphics environment,” Computing In Science & Engineering, vol. 9, no. 3, pp. 90–95, 2007. [14]
- [15] S. van der Walt, S. C. Colbert, and G. Varoquaux, “The NumPy Array: A Structure for Efficient Numerical Computation,” Computing in Science Engineering, vol. 13, no. 2, pp. 22–30, Mar. 2011. [15]

File Format Descriptions

File Extension (Description)	How it was created
.txt (Plain Text)| Generated with a plain text editor (Atom, Textedit)
.bt8 (NCNR BT8 Data)	Raw data recorded at NCNR BT8 https://www.ncnr.nist.gov/instruments/bt8/. Read by and analyzed by program "PF".
.sum (Pole Figure Sum File)| Generated by PF. This file contains a single line header, and then four columns of whitespace delimited data.
.ipynb (Jupyter/Ipython Notebook)| Generated in a Jupyter Notebook environment
.png (Portable Network Graphics)| Image file generated by Inkscape
.pdf (Portable Document Format)	Document file generated by a Jupyter Notebook
.eps (Encapsulated PostScript)	Image file generated by a Jupyter Notebook
.m (Matlab Code)| Written using Matlab

.tif (Tagged Image File Format) | Image file generated by Matlab
.svg (Scalable Vector Graphics)| Image file generated by Inkscape
.xlsx (Excel Workbook) | Spreadsheet generated by Microsoft Excel

The programs and files should be platform independent. However, this claim has not been verified. The dataset was created on Mac OS 10.12.5 and 10.13.6. As such the line endings likely use the line feed (LF) rather than combined carriage return and line feed (CR+LF).

Miscellaneous Comments

- A naming scheme internal to NIST has been developed by the authors to track individual batches of materials (batch ID) and samples (sample ID) in our research group. The batch and sample IDs listed below uniquely identify a material that comes from the same coil/batch. These batch IDs may be referred to in subsequent publications and may be used to determine if the material described is the same or a different material of the same type.

- Internal sample names for the samples and material are:
  - B160506-AAC-002: Batch ID for 201 stainless steel
  - S161130-WAP-001: Sample ID for as-received texture measurement
  - S170501-WAP-004: Sample ID for 24% engineering strain along RD texture measurement
  - S170911-AAC-001: Sample ID for lattice parameter measurement (see below)

- The program CTM (version 0.0.2) was used to calculate the austenite (gamma) - twinned martensite (alpha prime) interface vectors via the crystallographic theory of martensite (CTM). This program was written by Thomas Shield at the University of Minnesota - Twin Cities. Please contact him (shield@aem.umn.edu) if you would like a copy of this program.

- Inkscape was used to assemble several individual images into a single figure. It was not possible to export vector graphic files from Matlab without significant artifacts (see https://www.mathworks.com/matlabcentral/answers/290313-why-is-vector-graphics-chopped-into-pieces).

- The Matlab script "ColorMap8.m" was created to plot all ODFs on the same color scale. This color map clearly partitions the ODF into values greater than 1 and less than 1, corresponding to the value of a uniform (random) texture distribution. A grayscale map is used for multiples of a uniform (random) distribution less than 1 and color maps are used for multiples of a uniform (random) distribution equal to or greater than 1. This offers a clear demarcation between regions that have a higher texture volume fraction than uniform and regions that have a lower texture volume fraction than uniform.

- Several of the Jupyter notebooks have additional cells that include information beyond what was included in the paper. These are alternative ways to display the data that the authors chose not to include in the paper. They are included as they may be of use to other researchers.

- Lattice parameters for the gamma, alpha prime and epsilon phases were measured at the Spallation Neutron Source (SNS), beamline BL-7 Engineering Materials Diffractometer (Vulcan). As this data was preliminary, the results were not included in the technical paper. However, the lattice parameters were used to calculate a separate set of austenite (gamma) - twinned martensite (alpha prime) interface vectors with the CTM program to compare with the [1] and phenomenological theory of martensite calculations [7],[8]. All values were comparable, but the exact values have been retained in this dataset for additional study.

- A portion of this research used resources at the Spallation Neutron Source a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory.

How to Cite

The data set contents should be cited as [To be updated]:

A. Creuziger, W. Poling, T. Gnaupel-Herold "Data Set: Assessment of Martensitic Transformation Paths Based on Transformation Potential Calculations", (Publisher), (Publication Year), (DOI) [16]

This data set is a companion to the following technical paper [To be updated]:

A. Creuziger, W. Poling, T. Gnaupel-Herold "Assessment of Martensitic Transformation Paths Based on Transformation Potential Calculations" submitted to Steel Research International. [17]

The technical paper describes the motivation and background for this data set, as well as analysis and key insights that were made from this data set.

Citation Guidance

If you are utilizing the results or insights of this work, please cite the technical paper. If you are utilizing parts of the programs or other documentation provided in the data set, please cite the data set.

Lattice parameters and transformation values

The technical paper[17] includes the shear and plane vectors for each transformation. Many sources will provide other mathematical representations of the transformation, either by unit cell, stretch tensor, or scalar values of the transformation such as shear and dilatation. Table S1 compiles several of these different metrics for comparison and reference. Values are reported beyond the relevant significant figures to facilitate comparison.

Stretch tensor calculations from: [1]

$$\alpha = \frac{2a_{\alpha'}}{\sqrt{2}a_{\gamma}} \tag{S1}$$

$$\gamma = \frac{c_{\alpha\prime}}{a_\gamma} \quad \text{(S2)}$$

Page 67 of Bhadeshia [7] provides scalar calculations of shear and dilatation, based on the shear plane ($\boldsymbol{m}$) and shear direction ($\mathbf{b}$) of the transformation:

$$\text{dilatation} = \mathbf{b} \cdot \boldsymbol{m} \quad \text{(S3)}$$

$$\text{shear} = \sqrt{(\parallel \mathbf{b} \parallel^2 - \text{dilatation}^2)} \quad \text{(S4)}$$

Table S1: Lattice parameters and transformation values

Source	Creuziger & Foecke[1]	SNS Vulcan Data	Kundu and Bhadeshia[6] and Bhadeshia[7]	Bhadeshia[7]
Equation number of the shear and plane vectors from[17]				
	(2)			(3)
Lattice Parameters				
a (γ) [nm]	0.35594	0.35927	0.3589	
a (α’) [nm]	0.28657	0.28711	0.2873	
c (α’)	0.28786	0.28794	= a (BCC)	
a (ε)		0.25286		
c (ε)		0.41483		
Stretch Tensor values for α’ phase				
alpha	1.138594	1.130154		
gamma	0.808732	0.801455		
Scalar values of the transformation				
α’ phase				
Dilatation	0.048407	0.023658	0.025361	
Shear	0.212367	0.219102	0.220727	
ε phase				
Dilatation				0.0
Shear				0.350224
Notes				
	lattice spacing calculated from Jatzack [5] with the composition Fe+C with 0.001 mass fraction C	See footnote 1 below.	Described as the "Standard Variant", in appendix 2 [7].	Calculated from Bhadeshia[7], pages 26, 27, 47. The transformation assumes no or negligible diliation.

1 These are preliminary values from a GSAS Rietveld fit of the same batch of 201 stainless steel measured at the VULCAN beamline of the Spallation Neutron Source at Oak Ridge National Lab. The sample rolling direction axis was loaded to a stress of 575 MPa, and data were recorded with a diffraction vector aligned with the same normal direction. These lattice values have a

slight contraction due to Poisson effects and plastic deformation. These values were not used in the paper, but included for reference and to show similarity to other values.

Additional stress states

Additional stress states, as used in previously,[1] are included in Figure S1 and Figure S2 for the $\gamma \rightarrow \alpha'$ and $\gamma \rightarrow \varepsilon$ respective martensite transformations. Note that the color range was extended to permit other stress states and is not the same as in the technical paper.[17] However, the color range is shared between Figure S1 and Figure S2 for comparison. Both plots are ϕ_2=45° cross sections and use the austenite crystal reference frame.

In discussions with Z. Wang and A. M. Beese about their recently submitted paper,[18] an observation about the shear stress tensors was jointly made. In the prior paper by the authors,[1] the following stress tensor (RDS or RD-S) was used:

$$\mathrm{RDS}^{[1]} = \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{-1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \text{(S5)}$$

However, Z. Wang and A. M. Beese used the following tensor, which more accurately matches their experimental arrangement:

$$\mathrm{RDS}^{[18]} = \begin{bmatrix} 0 & \frac{1}{\sqrt{3}} & 0 \\ \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \text{(S6)}$$

The effective stress (as calculated via equation 8 of [1]) is the same between these tensors, and are otherwise equivalent representations, if a 45° rotation of the stress axes is taken into account. As such, the transformation potential plots also differ by a 45° rotation. In the Bunge Euler angle convention used in both works, this will be a 45° shift in ϕ_1.

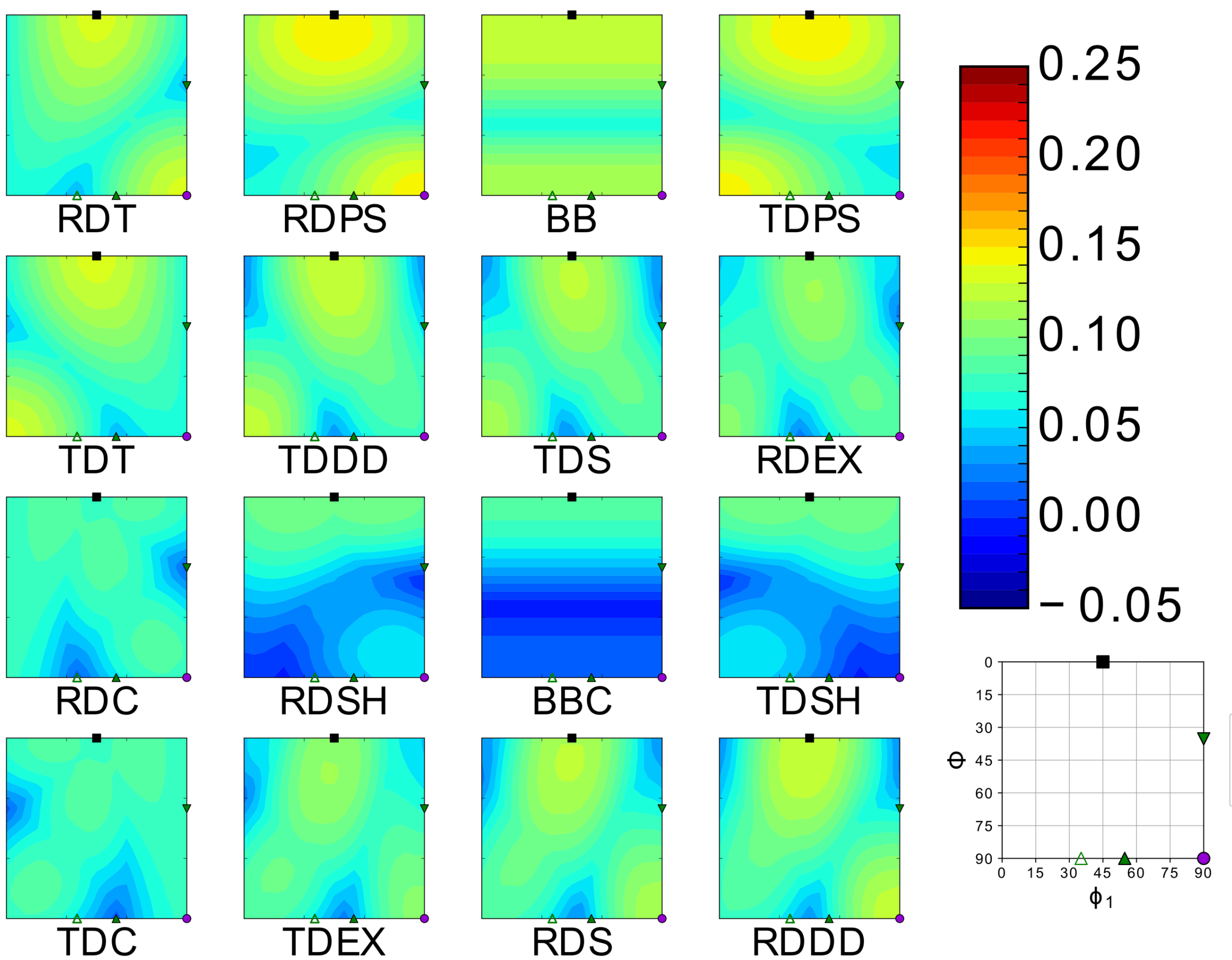

Figure S1: Maximum transformation potentials for $\gamma \rightarrow \alpha'$ martensite transformation as a function of orientation (reproduced from[1]). The additional stress states are described in Table 1 of [1]. The units on the transformation potential are $\frac{J}{m^3}$. Marks for specific orientations are superimposed on each of the plots, with a key inset.

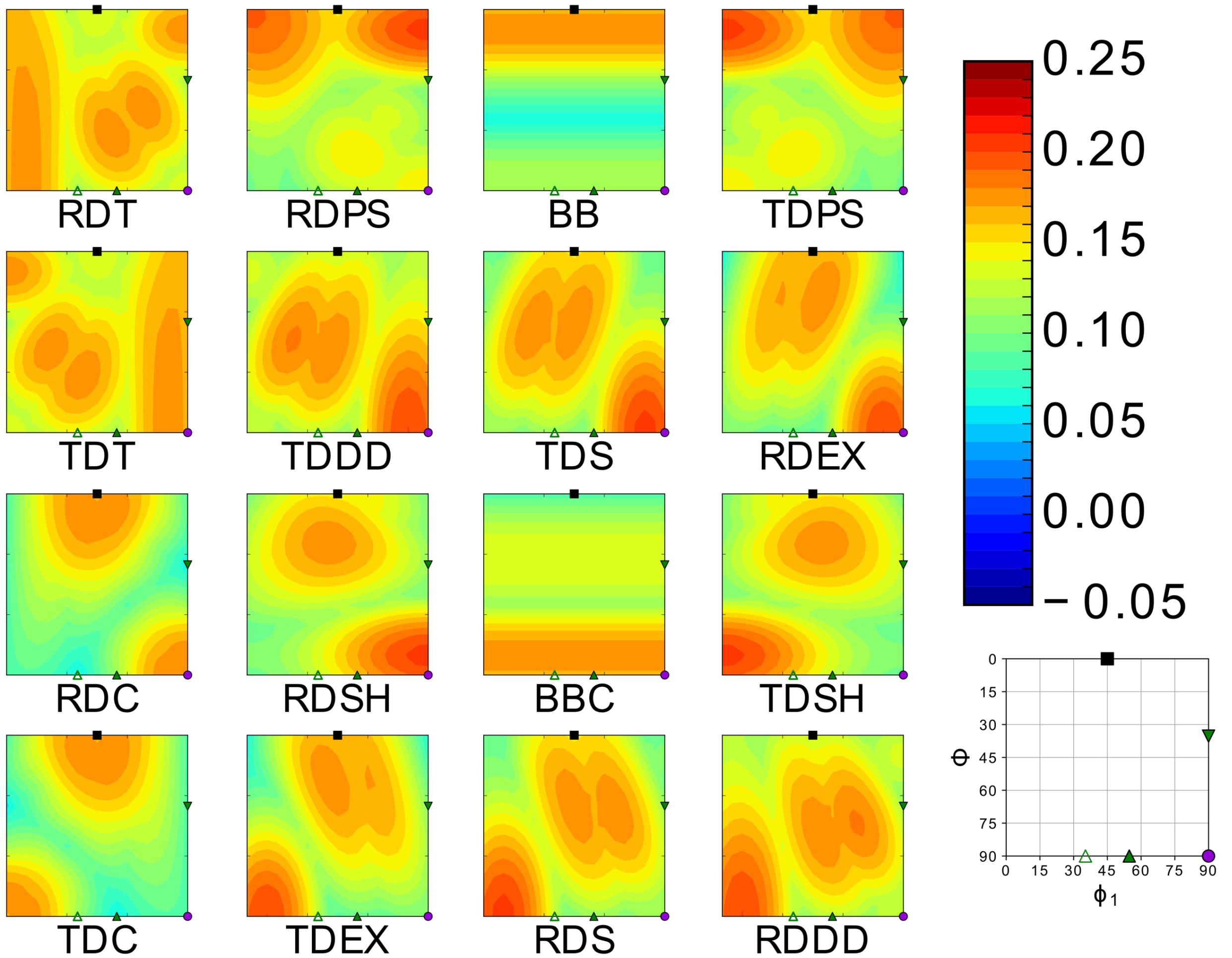

Figure S2: Maximum transformation potentials as a function of orientation for $\gamma \rightarrow \varepsilon$ martensite transformation. The additional stress states are described in Table 1 of [1]. The units on the transformation potential are $\frac{J}{m^3}$. Marks for specific orientations are superimposed on each of the plots, with a key inset.

References

[1] A. Creuziger, T. Foecke, *Acta Mater.* **2010** *58* 85–91.
[2] T.W. Shield, *CTM*, University of Minnesota - Twin Cities, **2005**.
[3] V. Randle, *The Measurement of Grain Boundary Geometry*, CRC Press, New York, **1993**.
[4] M. Humbert, B. Petit, B. Bolle, N. Gey, *Mater. Sci. Eng. A* **2007** *454–455* 508–517.
[5] C.F. Jatczak, J.A. Larson, S.W. Shin, *SAE SP-453 Retained Austenite and Its Measurements by X-Ray Diffraction: An Information Manual*, Society of Automotive Engineers, Warrendale, PA, **1980**.
[6] S. Kundu, H.K.D.H. Bhadeshia, *Scr. Mater.* **2006** *55* 779–781.
[7] H.K.D.H. Bhadeshia, *Worked Examples in the Geometry of Crystals*, Institute of Metals, London, **1987**.
[8] S. Kundu, H.K.D.H. Bhadeshia, *Scr. Mater.* **2007** *57* 869–872.
[9] *MATLAB*, MathWorks Inc, Natick, MA

[10] R. Hielscher, H. Schaeben, *J. Appl. Crystallogr.* **2008** *41* 1024–1037.
[11] *Anaconda Software Distribution*, Continuum Analytics, **2016**.
[12] F. Perez, B.E. Granger, *Comput. Sci. Eng.* **2007** *9* 21–29.
[13] T. Gnäupel-Herold, *PF*, NIST NCNR,
[14] J.D. Hunter, *Comput. Sci. Eng.* **2007** *9* 90–95.
[15] S. van der Walt, S.C. Colbert, G. Varoquaux, *Comput. Sci. Eng.* **2011** *13* 22–30.
[16] A. Creuziger, W. Poling, T. Gnäupel-Herold, NIST Public Data Repository. https://doi.org/10.18434/T4/1503156
[17] A. Creuziger, W. Poling, T. Gnaeupel-Herold, *Steel Res. Int.* ***2019*** *90* https://doi.org/10.1002/srin.201800370
[18] Z. Wang, A.M. Beese, *Mat. Sci. Eng. A* 2019 *743* 811-823.