

This DATSETNAMereadme.pdf file was generated on 2022-02-21 by Stefan Karlsson

GENERAL INFORMATION

1. Title of Dataset: Alkali Ion diffusion and Structure of Chemically Strengthened TiO₂ Doped Soda-Lime Silicate Glass

2. Author Information

A. Principal Investigator Contact Information

Name: Stefan Karlsson
Institution: RISE Research Institutes of Sweden
Address: RISE Glass, Vejdes plats 3, SE-352 52 Växjö, Sweden
Email: stefan.karlsson@ri.se

B. Co-investigator Contact Information

Name: Felix Bengtsson
Institution: Department of Materials Science and Engineering, Solid State Physics, Ångström Laboratory, Uppsala University
Address: Lägerhyddsvägen 1, SE-752 37 Uppsala, Sweden
Email: felix.bengtsson8@gmail.com

C. Co-investigator Contact Information

Name: Ilknur Bayrak Pehlivan
Institution: Department of Materials Science and Engineering, Solid State Physics, Ångström Laboratory, Uppsala University
Address: Lägerhyddsvägen 1, SE-752 37 Uppsala, Sweden
Email: ilknur.bayrak_pehlivan@angstrom.uu.se

D. Co-investigator Contact Information

Name: Lars Österlund
Institution: Department of Materials Science and Engineering, Solid State Physics, Ångström Laboratory, Uppsala University
Address: Lägerhyddsvägen 1, SE-752 37 Uppsala, Sweden
Email: lars.osterlund@angstrom.uu.se

3. Date of data collection: 2020-01-01 to 2021-08-31. The glasses though belonged to a previous study and were melted 2014-2015.

4. Geographic location of data collection: Växjö, Uppsala.

5. Information about funding sources that supported the collection of the data: FORMAS, the Swedish Research Council for Sustainable Development, Grant No. 2018-00707.

SHARING/ACCESS INFORMATION

1. Licenses/restrictions placed on the data: Creative Commons Attribution License (CC BY)

2. Links to publications that cite or use the data:

Bengtsson, F., I.B. Pehlivan, L. Österlund, and S. Karlsson, *Alkali ion diffusion and structure of chemically strengthened TiO₂ doped soda-lime silicate glass*. *Journal of Non-Crystalline Solids*, 2022. **586**: p. 121564. DOI: <https://doi.org/10.1016/j.jnoncrysol.2022.121564>.

3. Links to other publicly accessible locations of the data: N/A

4. Links/relationships to ancillary data sets: N/A

5. Was data derived from another source? No

6. Recommended citation for this dataset:

Bengtsson, F., I. Bayrak Pehlivan, L. Österlund, and S. Karlsson, Dataset: Alkali Ion diffusion and Structure of Chemically Strengthened TiO₂ Doped Soda-Lime Silicate Glass. DOI: <https://doi.org/10.5878/m3y0-kv73>

DATA & FILE OVERVIEW

1. File List:

XPS:

XPS_4.7%TiO2_350degrees_acq1.txt
XPS_4.7%TiO2_350degrees_acq2.txt
XPS_4.7%TiO2_400degrees_acq1.txt
XPS_4.7%TiO2_400degrees_acq2.txt
XPS_4.7%TiO2_450degrees_acq1.txt
XPS_4.7%TiO2_450degrees_acq2.txt
XPS_4.7%TiO2_500degrees_acq1.txt
XPS_4.7%TiO2_500degrees_acq2.txt
XPS_4.7%TiO2_500degrees_acq3.txt
XPS_4.7%TiO2_500degrees_acq4.txt
XPS_9.9%TiO2_350degrees_acq1.txt
XPS_9.9%TiO2_350degrees_acq2.txt
XPS_9.9%TiO2_400degrees_acq1.txt
XPS_9.9%TiO2_450degrees_acq1.txt
XPS_9.9%TiO2_450degrees_acq2.txt
XPS_9.9%TiO2_450degrees_acq3.txt
XPS_9.9%TiO2_500degrees_acq1.txt
XPS_9.9%TiO2_500degrees_acq2.txt
XPS_9.9%TiO2_500degrees_acq3.txt

Raman spectroscopy:

Raman_SLS_500deg_depth6.txt
Raman_SLS_500deg_depth5.txt
Raman_SLS_500deg_depth4.txt
Raman_SLS_500deg_depth3.txt
Raman_SLS_500deg_depth2.txt
Raman_SLS_500deg_depth1.txt
Raman_SLS_450deg_depth1.txt
Raman_SLS_400deg_depth1.txt
Raman_SLS_350deg_depth1.txt
Raman_4.7%TiO2_untreated_depth1.txt
Raman_4.7%TiO2_500deg_depth6.txt
Raman_4.7%TiO2_500deg_depth5.txt
Raman_4.7%TiO2_500deg_depth4.txt
Raman_4.7%TiO2_500deg_depth3.txt
Raman_4.7%TiO2_500deg_depth2.txt
Raman_4.7%TiO2_500deg_depth1.txt
Raman_4.7%TiO2_450deg_depth1.txt
Raman_4.7%TiO2_400deg_depth1.txt
Raman_4.7%TiO2_350deg_depth1.txt
Raman_9.9%TiO2_untreated_depth1.txt
Raman_9.9%TiO2_500deg_depth6.txt
Raman_9.9%TiO2_500deg_depth5.txt
Raman_9.9%TiO2_500deg_depth4.txt
Raman_9.9%TiO2_500deg_depth3.txt
Raman_9.9%TiO2_500deg_depth2.txt
Raman_9.9%TiO2_500deg_depth1.txt
Raman_9.9%TiO2_450deg_depth1.txt
Raman_9.9%TiO2_400deg_depth1.txt
Raman_9.9%TiO2_350deg_depth1.txt

Spectrophotometry:

SLS_AbsorptionCoefficient_untreated.txt
SLS_AbsorptionCoefficient_treated.txt
4.7%TiO2_AbsorptionCoefficient_untreated.txt
4.7%TiO2_AAbsorptionCoefficient_treated.txt
9.9%TiO2_AbsorptionCoefficient_untreated.txt
9.9%TiO2_AbsorptionCoefficient_treated.txt

2. Relationship between files, if important:

Those starting with SLS corresponds to the samples denoted Soda-lime glass or SLS, and those starting with 4.7%TiO2 and 9.9%TiO2 corresponds to the samples denoted the same in the paper:

Bengtsson, F., I.B. Pehlivan, L. Österlund, and S. Karlsson, *Alkali ion diffusion and structure of chemically strengthened TiO2 doped soda-lime silicate glass*. Journal of Non-Crystalline Solids, 2022. **586**: p. 121564. DOI: <https://doi.org/10.1016/j.jnoncrysol.2022.121564>.

3. Additional related data collected that was not included in the current data package: N/A

4. Are there multiple versions of the dataset? No.

METHODOLOGICAL INFORMATION

1. Description of methods used for collection/generation of data:

Please find all relevant information in the following scientific paper:

Bengtsson, F., I.B. Pehlivan, L. Österlund, and S. Karlsson, *Alkali ion diffusion and structure of chemically strengthened TiO2 doped soda-lime silicate glass*. Journal of Non-Crystalline Solids, 2022. **586**: p. 121564. DOI: <https://doi.org/10.1016/j.jnoncrysol.2022.121564>.

2. Methods for processing the data:

Please find all relevant information in the following scientific paper:

Bengtsson, F., I.B. Pehlivan, L. Österlund, and S. Karlsson, *Alkali ion diffusion and structure of chemically strengthened TiO2 doped soda-lime silicate glass*. Journal of Non-Crystalline Solids, 2022. **586**: p. 121564. DOI: <https://doi.org/10.1016/j.jnoncrysol.2022.121564>.

3. Instrument- or software-specific information needed to interpret the data: N/A

4. Standards and calibration information, if appropriate: N/A

5. Environmental/experimental conditions:

Please find all relevant information in the following scientific paper:

Bengtsson, F., I.B. Pehlivan, L. Österlund, and S. Karlsson, *Alkali ion diffusion and structure of chemically strengthened TiO2 doped soda-lime silicate glass*. Journal of Non-Crystalline Solids, 2022. **586**: p. 121564. DOI: <https://doi.org/10.1016/j.jnoncrysol.2022.121564>.

6. Describe any quality-assurance procedures performed on the data:

Please find all relevant information in the following scientific paper:

Bengtsson, F., I.B. Pehlivan, L. Österlund, and S. Karlsson, *Alkali ion diffusion and structure of chemically strengthened TiO2 doped soda-lime silicate glass*. Journal of Non-Crystalline Solids, 2022. **586**: p. 121564. DOI: <https://doi.org/10.1016/j.jnoncrysol.2022.121564>.

7. People involved with sample collection, processing, analysis and/or submission:

- A. Stefan Karlsson
- B. Felix Bengtsson
- C. Ilknur Bayrak Pehlivan
- D. Lars Österlund

DATA-SPECIFIC INFORMATION FOR: XPS

Filenames:

XPS_4.7%TiO2_350degrees_acq1.txt

XPS_4.7%TiO2_350degrees_acq2.txt
XPS_4.7%TiO2_400degrees_acq1.txt
XPS_4.7%TiO2_400degrees_acq2.txt
XPS_4.7%TiO2_450degrees_acq1.txt
XPS_4.7%TiO2_450degrees_acq2.txt
XPS_4.7%TiO2_500degrees_acq1.txt
XPS_4.7%TiO2_500degrees_acq2.txt
XPS_4.7%TiO2_500degrees_acq3.txt
XPS_4.7%TiO2_500degrees_acq4.txt
XPS_9.9%TiO2_350degrees_acq1.txt
XPS_9.9%TiO2_350degrees_acq2.txt
XPS_9.9%TiO2_400degrees_acq1.txt
XPS_9.9%TiO2_450degrees_acq1.txt
XPS_9.9%TiO2_450degrees_acq2.txt
XPS_9.9%TiO2_450degrees_acq3.txt
XPS_9.9%TiO2_500degrees_acq1.txt
XPS_9.9%TiO2_500degrees_acq2.txt
XPS_9.9%TiO2_500degrees_acq3.txt

Filename coding: XPS_XX%TiO2_YYYdegrees_acqZ.txt

XX= TiO2 content in mol%

YYY: temperature of the ion exchange treatment.

Z: wet etch depth starting with 0 μm and then following Table 2 in Bengtsson, F., I.B. Pehlivan, L. Österlund, and S. Karlsson, *Alkali ion diffusion and structure of chemically strengthened TiO2 doped soda-lime silicate glass*. Journal of Non-Crystalline Solids, 2022. **586**: p. 121564. DOI: <https://doi.org/10.1016/j.jnoncrysol.2022.121564>.

1. Number of variables:

11

2. Number of cases/rows:

Data: 201, Total: 205

3. Variable List:

Variable 1: KE_Ti 2p 8, Description: Kinetic Energy, Unit: eV

Variable 2: BE_Ti 2p 8, Description: Binding Energy, Unit: eV

Variable 3: CPS_Ti 2p 8, Description: Ti XPS spectra, Unit: Counts per s

Variable 4: Ti 2p_1_Ti 2p 8, Description: Ti^{4+} $2p_{3/2}$ deconvolution, Unit: Counts per s

Variable 5: Ti 2p_2_Ti 2p 8, Description: Ti^{4+} $2p_{1/2}$ deconvolution, Unit: Counts per s

Variable 6: Ti 2p_3_Ti 2p 8, Description: Ti^{3+} $2p_{1/2}$ deconvolution, Unit: Counts per s

Variable 7: Ti 2p_4_Ti 2p 8, Description: Ti^{3+} $2p_{3/2}$ deconvolution, Unit: Counts per s

Variable 8: Background_Ti 2p 8, Description: Background spectra, Unit: Counts per s

Variable 9: Envelope_Ti 2p 8, Description: Sum of the deconvolutions and background, Unit: Counts per s

Variable 10: Normalised_Residual_Ti 2p 8, Description: Normalised residual spectra, Unit: Counts per s

Variable 11: Residual_Ti 2p 8, Description: Residual spectra, Unit: Counts per s

4. Missing data codes:

N/A

5. Specialized formats or other abbreviations used:

N/A

DATA-SPECIFIC INFORMATION FOR: Raman Spectroscopy

Filenames:

Raman_SLS_untreated_depth1.txt

Raman_SLS_500deg_depth6.txt

Raman_SLS_500deg_depth5.txt
Raman_SLS_500deg_depth4.txt
Raman_SLS_500deg_depth3.txt
Raman_SLS_500deg_depth2.txt
Raman_SLS_500deg_depth1.txt
Raman_SLS_450deg_depth1.txt
Raman_SLS_400deg_depth1.txt
Raman_SLS_350deg_depth1.txt
Raman_4.7%TiO2_untreated_depth1.txt
Raman_4.7%TiO2_500deg_depth6.txt
Raman_4.7%TiO2_500deg_depth5.txt
Raman_4.7%TiO2_500deg_depth4.txt
Raman_4.7%TiO2_500deg_depth3.txt
Raman_4.7%TiO2_500deg_depth2.txt
Raman_4.7%TiO2_500deg_depth1.txt
Raman_4.7%TiO2_450deg_depth1.txt
Raman_4.7%TiO2_400deg_depth1.txt
Raman_4.7%TiO2_350deg_depth1.txt
Raman_9.9%TiO2_untreated_depth1.txt
Raman_9.9%TiO2_500deg_depth6.txt
Raman_9.9%TiO2_500deg_depth5.txt
Raman_9.9%TiO2_500deg_depth4.txt
Raman_9.9%TiO2_500deg_depth3.txt
Raman_9.9%TiO2_500deg_depth2.txt
Raman_9.9%TiO2_500deg_depth1.txt
Raman_9.9%TiO2_450deg_depth1.txt
Raman_9.9%TiO2_400deg_depth1.txt
Raman_9.9%TiO2_350deg_depth1.txt

Filename coding: Raman_XXX_YYYdeg_depthZ.txt

XXX= glass composition with denotation according to Table 1 in Bengtsson, F., I.B. Pehlivan, L. Österlund, and S. Karlsson, *Alkali ion diffusion and structure of chemically strengthened TiO2 doped soda-lime silicate glass*. *Journal of Non-Crystalline Solids*, 2022. **586**: p. 121564. DOI: <https://doi.org/10.1016/j.jnoncrysol.2022.121564>.

YYY: temperature of the ion exchange treatment (and untreated means not ion exchanged).

Z: wet etch depth starting with 0 μm and then following Table 2, see Fig. 7 in Bengtsson, F., I.B. Pehlivan, L. Österlund, and S. Karlsson, *Alkali ion diffusion and structure of chemically strengthened TiO2 doped soda-lime silicate glass*. *Journal of Non-Crystalline Solids*, 2022. **586**: p. 121564. DOI: <https://doi.org/10.1016/j.jnoncrysol.2022.121564>.

1. Number of variables:

2

2. Number of cases/rows:

Data: 890-905, Total: 891-906

3. Variable List:

Variable 1: #Wave, Description: Wavelength, Unit: cm^{-1}

Variable 2: #Intensity, Description: Raman intensity, Unit: Counts per s

4. Missing data codes:

N/A

5. Specialized formats or other abbreviations used:

N/A

DATA-SPECIFIC INFORMATION FOR: Spectrophotometry

Filenames:

SLS_AbsorptionCoefficient_untreated.txt
SLS_AbsorptionCoefficient_treated.txt
4.7%TiO2_AbsorptionCoefficient_untreated.txt
4.7%TiO2_AAbsorptionCoefficient_treated.txt
9.9%TiO2_AbsorptionCoefficient_untreated.txt
9.9%TiO2_AbsorptionCoefficient_treated.txt

Filename coding: XXX_AbsorptionCoefficient_YYY.txt

XXX= glass composition with denotation according to Table 1 in Bengtsson, F., I.B. Pehlivan, L. Österlund, and S. Karlsson, *Alkali ion diffusion and structure of chemically strengthened TiO2 doped soda-lime silicate glass*. Journal of Non-Crystalline Solids, 2022. **586**: p. 121564. DOI: <https://doi.org/10.1016/j.jnoncrysol.2022.121564>.
YYY: untreated means not ion exchanged and treated means ion exchanged at 500 °C.

1. Number of variables:

2

2. Number of cases/rows:

Data: 890-905, Total: 891-906

3. Variable List:

Variable 1: Description: Wavelength, Unit: nm

Variable 2: Description: Absorption coefficient, Unit: cm^{-1}

4. Missing data codes:

N/A

5. Specialized formats or other abbreviations used:

N/A