

Description of data for paper titled
**Assessing continuum plasticity postulates with grain-scale stress and strain measurements
in triaxially-compressed sand**

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Data included in this repository included raw and segmented x-ray computed tomography images used in the paper titled “Assessing continuum plasticity postulates with grain-scale stress and strain measurements in triaxially-compressed sand”.

tomo_20mpa.zip, **tomo_30mpa.zip** and **tomo_35mpa.zip** are each .zip files containing raw XRCT images from synchrotron experiments described in the paper. Each raw 16-bit XRCT image is titled **merged2_halfclean_load*.tif** where * represents a load step of the experiment. The load steps are 1, 2, 3, 4, 5, and 6 for 20 MPa, 1, 2, 4, 5, 6, 7, and 8 for 30 MPa, and 1, 2, 3, 4, 5, 6, and 7 for 35 MPa. Step 3 is missing from the 30 MPa dataset because of issues in the reconstruction; no data from this load step were used in analysis presented in the paper. Each XRCT image is actually composed of four independently-reconstructed layers that were stitched together using digital volume correlation (DVC), as described in the *Methods* section of the paper. Each segmented 16-bit XRCT image is titled **segmentednew_clean_load*.tif** where * represents the same load step of the experiment. These images are downsampled from their original size for ease of sharing. The resolution 4.688 microns/pixel.

3dxrd_all.zip contains the raw and processed 3DXRD data used in the analysis in the paper. In each subdirectory labeled **3dxrd_*mpa**, where * represents a stress level, are files labeled **AllGrains.mat** and **tomoToXRD_stress_all.mat**, each of which are MATLAB data files to be opened with the “open(*)” command in MATLAB, where * is the file name. **AllGrains.mat** contains the cell array **allGrainLoad** in which **AllGrainLoad{N}** contains 3DXRD data output from MIDAS for the Nth load step of the corresponding experiment. The lists within **AllGrainLoad{N}** for a given load step N can be accessed via **AllGrainLoad{N}{M}**, where M is the list number. The lists numbered M have the following contents:

- 1: GrainID – arbitrary grain ID assigned by MIDAS.
- 2-10: Components of an orientation matrix, $\mathbf{O}$, providing a transformation from the sample coordinate system to the crystal coordinate system by $\sigma_c = \mathbf{O}^T \sigma_s \mathbf{O}$ and from the crystal to sample coordinate system by $\sigma_s = \mathbf{O}^T \sigma_c \mathbf{O}$. Entries 2-10 are components $O_{11}, O_{12}, O_{13}, O_{21}, O_{22}, O_{23}, O_{31}, O_{32}$, and O_{33} , respectively.
- 11-13: Center of mass positions of the grains in the x, y, and z coordinates.
- 14-19: $a, b, c, \alpha, \beta, \gamma$ lattice parameters inferred from fitting diffraction peaks. Not directly used.
- 20-22: DiffPos, DiffOme, DiffAngle parameters output by MIDAS. Not used.
- 23: Equivalent grain radius inferred from diffraction spot sizes by MIDAS. Not directly used.

- 24: Confidence in grain fitting generated by MIDAS, equivalent to a completeness score.
- 25-33: Strain components $\epsilon_{11}, \epsilon_{12}, \epsilon_{13}, \epsilon_{21}, \epsilon_{22}, \epsilon_{23}, \epsilon_{31}, \epsilon_{32}, \epsilon_{33}$ fit by MIDAS using the inferred lattice parameters. Not used.
- 34-42: Strain components $\epsilon_{11}, \epsilon_{12}, \epsilon_{13}, \epsilon_{21}, \epsilon_{22}, \epsilon_{23}, \epsilon_{31}, \epsilon_{32}, \epsilon_{33}$ fit by MIDAS using equations equivalent to strain gauges along scattering vectors. This strain is used in the calculations in the paper and is preferred by beamline scientists because it provides more stable results.
- 43: RMS strain error calculated by MIDAS.
- 44: Phase number (1 for all grains in this case).
- 45-47: Euler angles about the x, y, and z axes corresponding to the orientation of the grain. Not used.
- 48-56: Stress tensor components $\sigma_{11}, \sigma_{12}, \sigma_{13}, \sigma_{21}, \sigma_{22}, \sigma_{23}, \sigma_{31}, \sigma_{32}, \sigma_{33}$ in the sample coordinate frame obtained by $\sigma = C: \epsilon$ where C is the stiffness tensor for quartz from [1]. Note that the strain tensor components used in this calculation must be transformed to the crystal coordinate frame via $\epsilon_c = O^T \epsilon_s O$ before this calculation and the result must be transformed back to the sample coordinate frame via $\sigma_s = O^T \sigma_c O$ after the calculation.
- 57: ID of paired grain used internally in our calculations to find twinned quartz crystals.
- 58: Flag indicating the presence of a twinned crystal.
- 59: Measure of stress difference between sub-crystals of a twinned crystal. Not used in calculations.

tomoToXRD_stress_all.mat contains the cell structure **tomoToXRD** which contains a list for each load step analyzed in the paper for a given sample. The length of each list is the number of labelled grains in the segmented XRCT image. The entry for a given row of a list is the ID in the 3DXRD data that corresponds to the stress in the corresponding grain in the **allGrainLoad** cell structure. For instance, if **tomoToXRD{1}{50}=100**, this means the grain labelled “50” in the 16-bit image **segmentednew_clean_load01.tif** has a σ_{11} in the sample coordinate system of **allGrainLoad{1}{48}(100)**. **tomoToXRD_stress_all.mat** also contains arrays labeled **strains**, **strSampQ**, **strSampXX**, **strSampXY**, **strSampXZ**, **strSampYY**, **strSampYZ**, and **strSampZZ** which contain, respectively, arrays holding macroscopic sample strain and average deviatoric, xx, xy, xz, yy, yz, and zz stresses as computed by: (1) for sample stress tensor components – taking a simple arithmetic average of the corresponding stress tensor components for all grains found in 3DXRD analysis; (2) for deviatoric stress – using the stress tensor computed by averaging in (1) and computing the deviatoric part of it.

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References

- [1] P. Heyliger, H. Ledbetter, and S. Kim, “Elastic constants of natural quartz,” *J. Acoust. Soc. Am.*, vol. 114, no. 2, pp. 644–650, 2003.