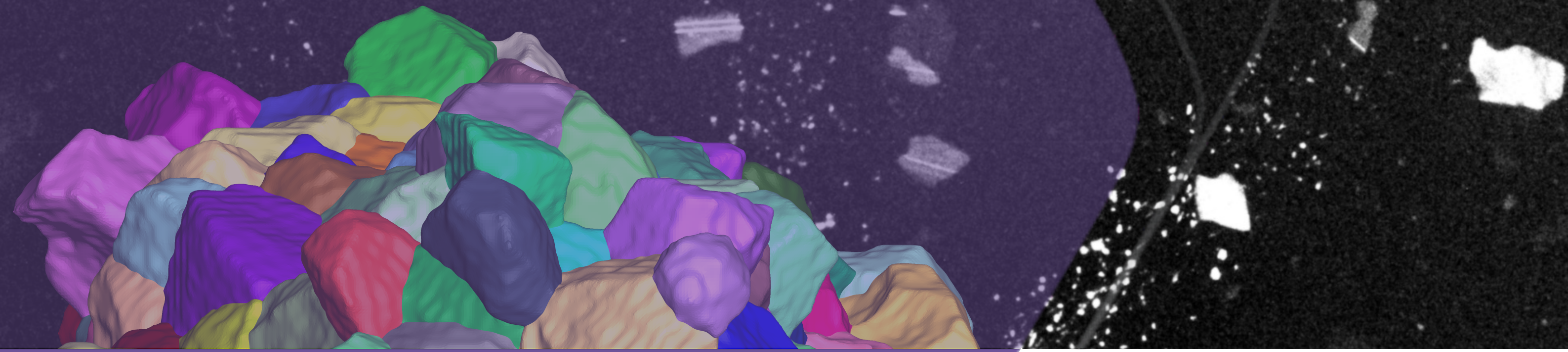

Application Note

Neper pipeline for LabDCT

Coupling grain mapping to modelling

Crystallographic orientations are critical in understanding the physical, chemical, and mechanical properties of materials, as well as in building models to predict how these properties evolve under external stimuli like mechanical deformation or thermal conditions.

Crystal-plasticity finite-element (CP-FE) simulations offer the ability to predict how the grain structure evolves during deformation. CP-FE models can be instantiated from synthetic grain structures, both random and with tailored properties like grain size distributions and textures, as well as from experimentally determined grain structures.

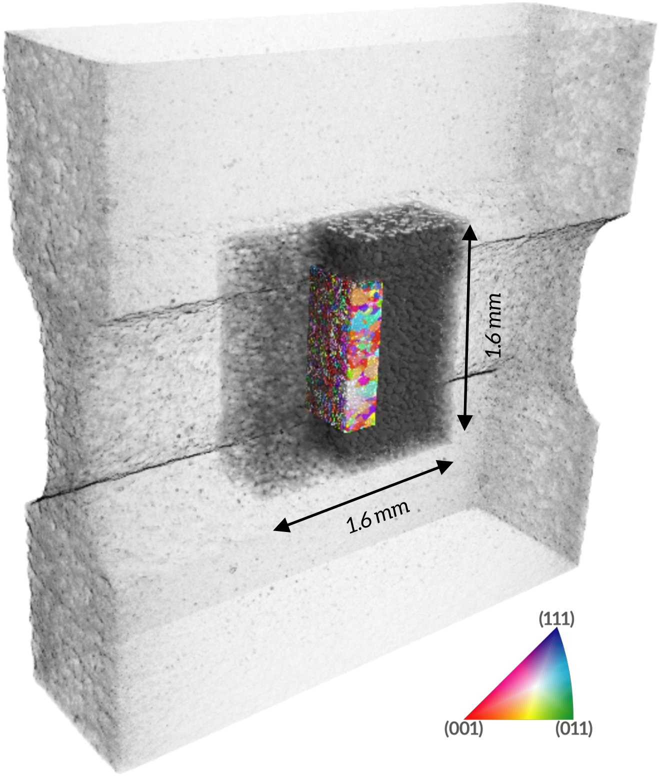

Fig. 1 *6016 T4 Aluminum alloy. Average grain size 40 μm. Wide dogbone shape to fulfil plane strain conditions during tensile deformation [4]. Original LabDCT map dimensions 0.5 × 1.6 × 1.6 mm³ (x,y,z) shown in greyscale representing map completeness. Cropped region of interest (ROI) comprising 1666 grains shown in IPF color along the tensile z-axis, c.f. Fig. 2.*

Neper pipeline for LabDCT

LabDCT provides a unique, non-destructive approach to experimentally determine the crystal orientations of materials experimentally. While the LabDCT output from GrainMapper3D is a voxellated volume, CP-FE models typically require the simulation input to be a mesh.

Here we demonstrate how the open-source software Neper [1], can be used to go from a voxellated LabDCT grain map to a simulation-ready input mesh. The full pipeline instructions are available from github [2], while example data (*c.f.* Fig. 2) can be downloaded from the Materials Data Facility [3].

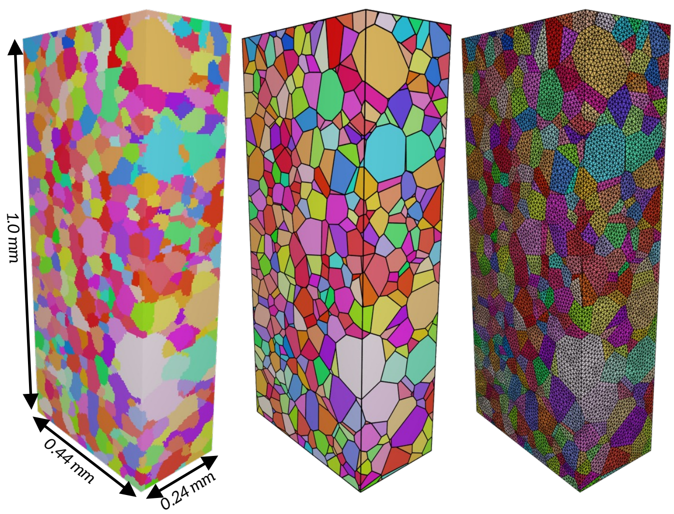

Fig. 2 *Left: Cropped LabDCT ROI for the Neper pipeline of dimensions 0.44 × 0.24 × 1.00 mm³ (x,y,z). This is approx. six grains in thickness along the y-direction of near-zero strain in the plane strain condition (tensile z-axis, c.f. Fig. 1). Center: Neper tessellation of the LabDCT ROI. Right: Neper mesh of the tessellation.*

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Neper pipeline in detail

After converting the LabDCT result file to a Neper input file using the python script provided on github, the Neper pipeline comprises the following steps:

- Cleaning the grain structure,
- Determining the tessellation domain,
- Tessellating the grain structure, and
- Meshing the tessellated grain structure.

In addition, Neper has functionality to visualize the output of each step along the way as shown in Fig. 2 and Fig. 3. All steps, including the visualizations, are detailed in the github instructions [2].

Example data for the Neper pipeline

The example data stems from a larger study of 3D strain heterogeneity and fracture under plane strain condition by M. Gille *et al.* [4], *c.f.* Fig. 1.

There, the microstructure of the undeformed specimen was first obtained using LabDCT. Absorption contrast tomography (ACT) was then used to measure the natural speckle of intermetallic particles in the material bulk during an in-situ tensile test performed for twelve loading increments up to fracture. Taking advantage of the plane strain condition, the evolution of the internal strain field was determined by two-dimensional digital image correlation (DIC) on the ACT measurements. Finally, the LabDCT microstructure was tessellated and meshed using Neper, and crystal CP-FE simulations were performed and compared with the experimental DIC results.

The findings of the study support the hypothesis that crystallographic effects are responsible for early strain heterogeneities, which precede localization and the final failure path.

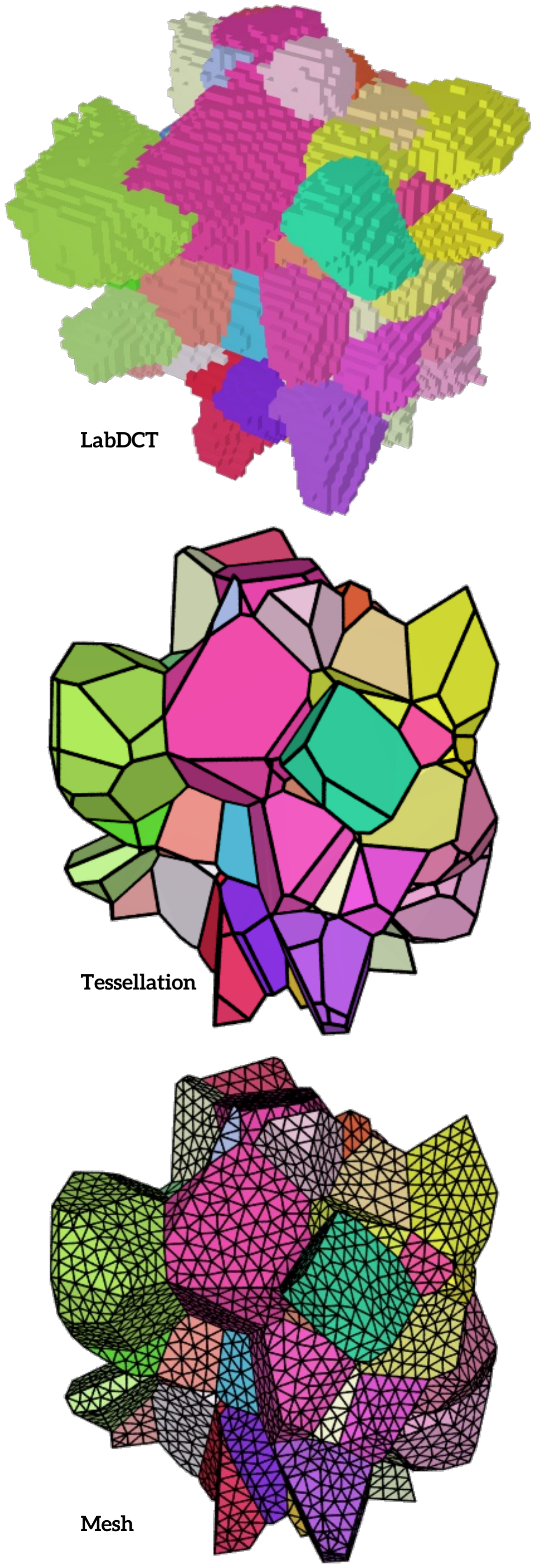

Fig. 3 *Cluster of grains in the center of the example grain map plotted as: voxellated LabDCT reconstruction (Top), tessellation (Center) and mesh (Bottom).*

References:
[1] R. Quey & L. Renversade, Comput. Methods Appl. Mech. Eng. 330, 308 (2017)
[2] https://xnovotech.github.io/gm3dh5/user/neper
[3] https://doi.org/10.18126/yc1m-nk41
[4] M. Gille et al., Int. J. Plasticity, 183, 104146 (2024)

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