

1.0 MANUAL FOR THE PARENT AUSTENITE RECONSTRUCTION GRAPHICAL USER INTERFACE FOR MTEX

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1.1 Introduction

This is the manual for using the graphical user interface intended for parent austenite reconstruction via iterative OR determination and MCL. The purpose of this manual is to walk you through the reconstruction of the demo file with MTEX and explain the functionality of the buttons. **With this in mind, only a cursory explanation of the methods and algorithms is provided.** If you are interested in the theory behind the iterative OR determination, MCL clustering algorithm or the combined methodology, you can check these resources:

OR determination and reconstruction:

T. Nyysönen, M. Isakov, P. Peura, and V.-T. Kuokkala, Metall. Mater. Trans. A, 2016, vol. 47 (6), pp. 2587–2590.

Nyysönen, T., Peura, P. & Kuokkala, VT. Metall and Mat Trans A (2018) 49: 6426.

<https://doi.org/10.1007/s11661-018-4904-9>

Markov clustering:

S. van Dongen, Graph Clustering by Flow Simulation, Ph.D. thesis, University of Utrecht, 2000.

<https://micans.org/mcl/index.html>

Demonstrations of MCL on parent austenite reconstruction:

E. Gomes and L. A. I. Kestens, IOP Conference Series: Materials Science and Engineering, 2015, vol. 82 (1), p. 012059.

T. Nyysönen, Quenching and Partitioning of High-Aluminum Steels, Ph.D. thesis, Tampere University of Technology, 2017.

In this text, martensite grains are in some cases mentioned. This term refers to the orientation clusters determined using the grain reconstruction feature of MTEX.

Before you proceed to the next page, read the “README.MD” and the “LICENCE.TXT” files.

1.2 Software requirements

The GUI has been created and tested with the App Designer feature of Matlab R2017b running MTEX 5.1.1.

1.3 Importing the EBSD data

Before you can begin, you need to load ebsd data into the workspace and then introduce it to the GUI. Follow these instructions to load the included demo file:

1. Navigate to the folder containing the PAG_GUI.mlapp, the demo file and the associated scripts.
2. Run the script pag1_import_data.m.
3. Run PAG_GUI.mlapp. The window shown in Figure 1.1. will open.
4. The text entry field already contains the default name “ebsd”. Click the button “Get Phase List”.
5. There should now be two identical list of phases in the list boxes. The last phase is selected for both martensite and austenite. You need to change the selections by clicking on the correct option. Click “Iron bcc (old)” in the left list box.
 - a. If you have your own data, it is possible that you do not have any austenite in your phase list. If that is the case, check the box “Select to add austenite to phase list”. Otherwise leave it alone.
6. Check the text entry “Currently selected phases”. It should show the selections “Martensite: Iron bcc (old)” and Austenite: Iron fcc.
7. Proceed to the window “PAGs via MCL”.

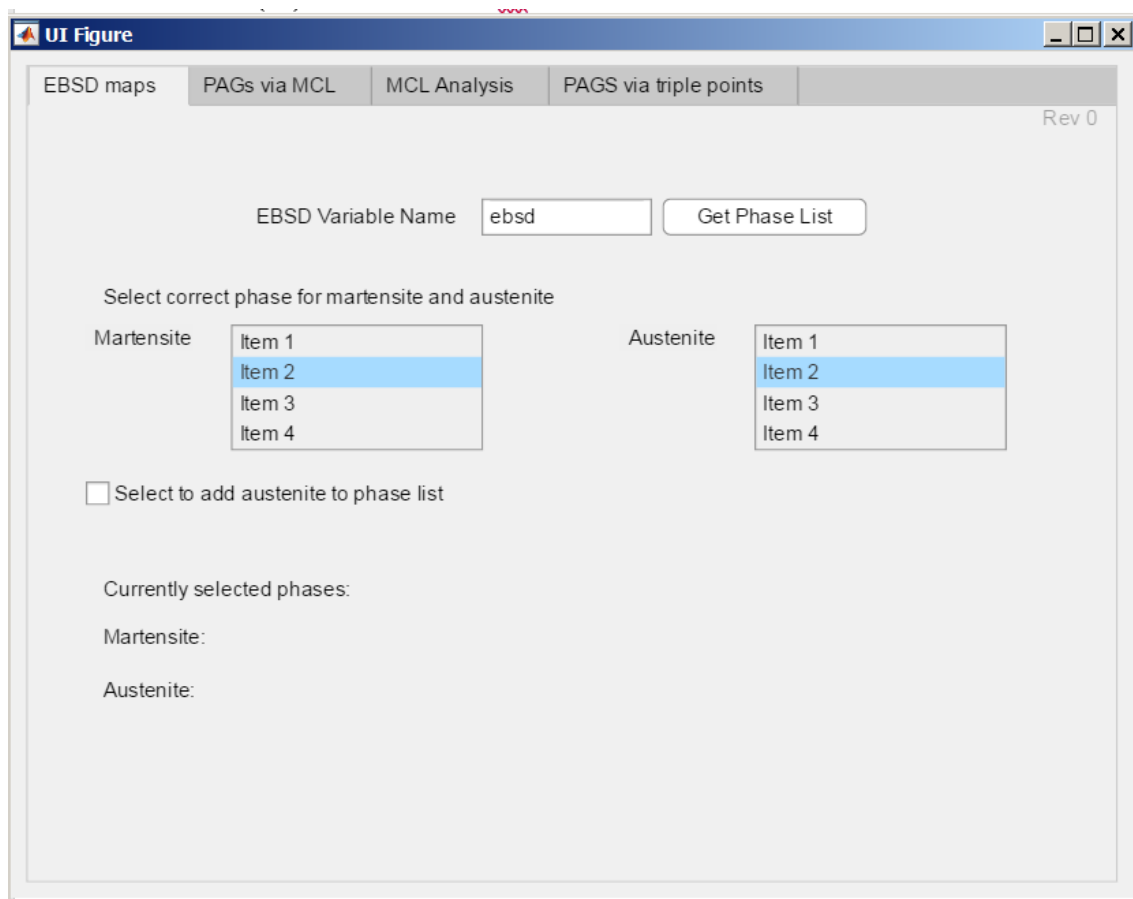


Figure 1.1 The initial window for loading EBSD data.

1.4 Determining the orientation relationship between martensite and austenite

To improve the quality of the reconstruction, it is necessary to determine the orientation relationship (hereafter OR) between austenite and martensite as accurately as possible. This is accomplished by determining the correct symmetry operators of each intergranular misorientations necessary to obtain that misorientation from a predetermined OR (here, the Kurdjumov-Sachs orientation relationship is used). This will allow the determination of a new OR that will be a better match for the experimentally observed misorientations. After an iterative process, an accurate orientation relationship is obtained corresponding to the experimental data.

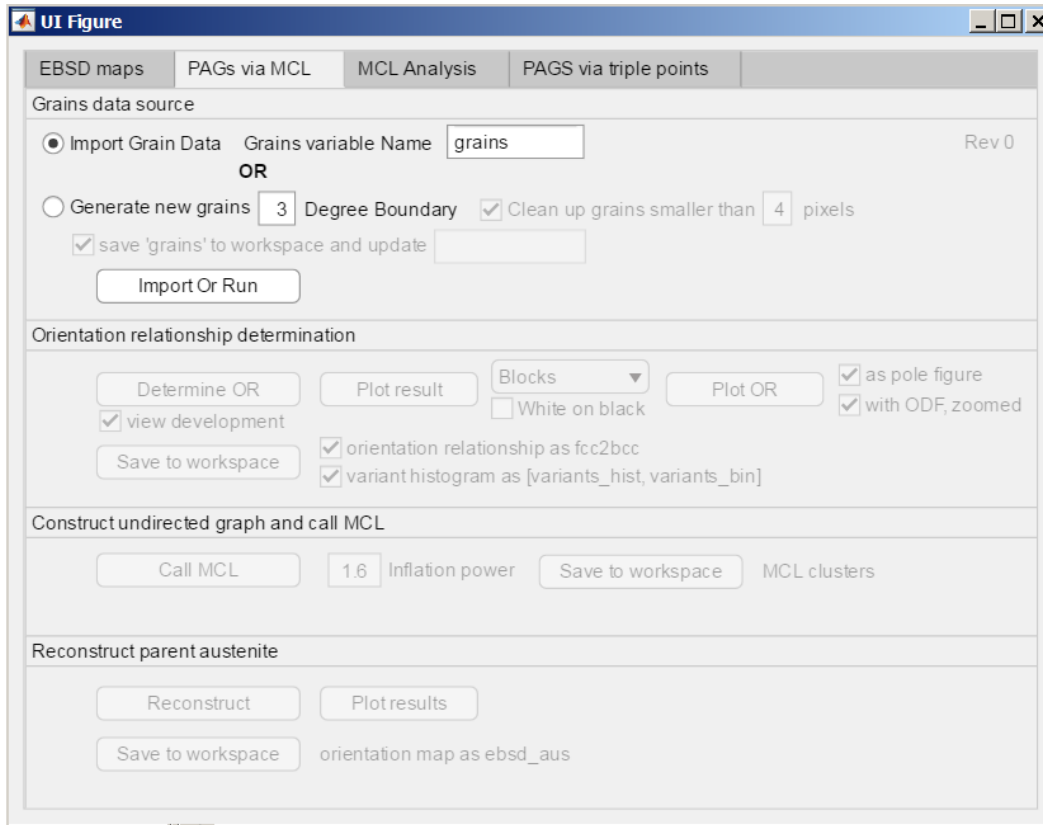


Figure 1.2 The initial window for loading EBSD data.

You will see the window shown in Figure 1.2. Follow the itemized steps to proceed:

1. Generate a grain map for the algorithm. Select the radio button “Generate new grains”. You can perform a cleanup that will remove small grains and save the grains to workspace. Both checkboxes are selected as default. Leave them as is for the demo file.
 - a. You can import a grains object you have preprocessed yourself. In that case, select the radio button “Import Grain Data”.
2. Press the button “Import Or Run”. The button will turn green to indicate completion.
3. The button “Determine OR” will be enabled. Run the iterative OR determination algorithm by pressing it. Leave the checkbox “view development” selected.
 - a. Figure 1.3. shows the development of the iterative algorithm. The upper window will show the developing angular deviation between the near-parallel close-packed planes and directions between the austenite and martensite phases predicted by the iterative OR. The

lower window will show a histogram describing the indexation of each boundary misorientation as one of the V1-V24 type misorientations described by Morito et al. [1].

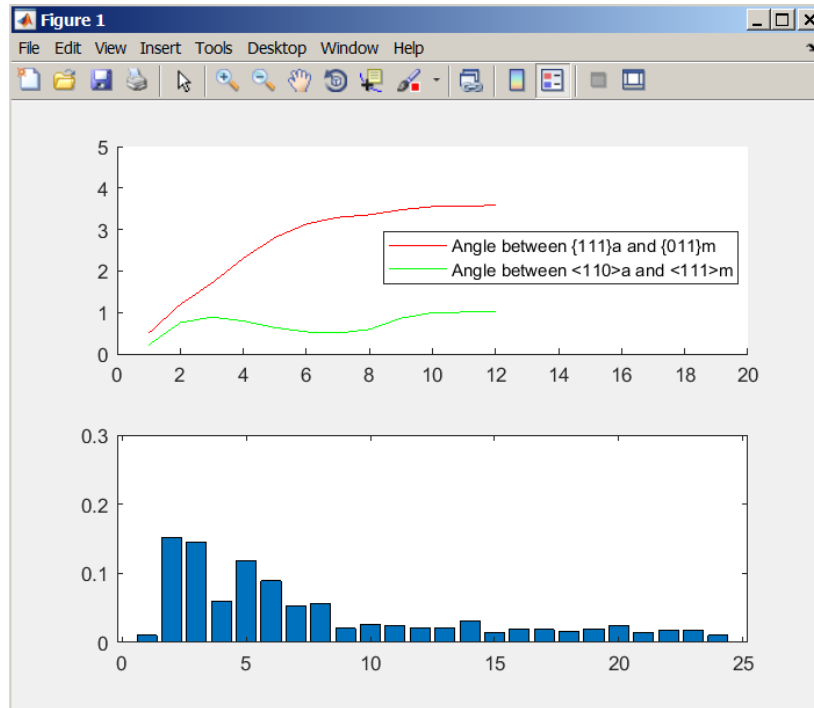


Figure 1.3 The window showing the progress of the reconstruction.

The button “Determine OR” will turn green to indicate completion. New buttons are enabled for analyzing and verifying the result. One way to do so is to use the OR to index all boundary misorientations as PAG boundaries, block boundaries or packet boundaries. You can press the “Plot result” button to view a band contrast image (NOTE: this will require data generated with Oxford Instruments systems) overlaid with indexed grain boundaries. Dark boundaries indicate PAG boundaries, red boundaries packet boundaries and green boundaries block boundaries. The resulting image should present a credible representation of the structure, indicating a successful OR determination. An example generated from the demo file is shown in Figure 1.5. You can try different representations by manipulating the drop down menu and the checkbox.

Another way to visualize the OR is to view the deviation between near-parallel planes and directions of the austenite and martensite phases on a pole figure. You can do this by selecting “Plot OR”: The last figure will show all 24 variant martensite orientations that can be generated from an austenite orientation on three pole figures. The first two figures will show the zoomed-in austenite (111) and [-101] on an austenite stereographic projection, along with corresponding martensite (011) and [-1-11].

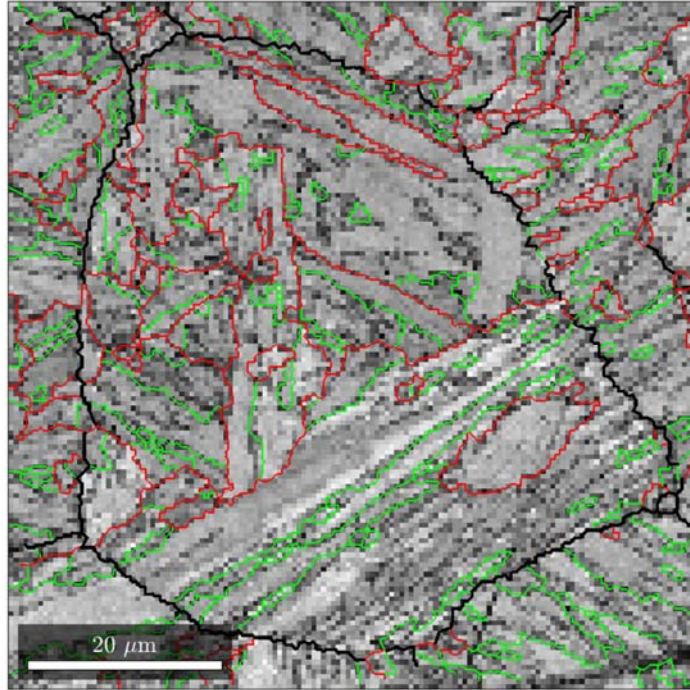


Figure 1.4 A band contrast image overlaid with grain boundaries indexed as block (green), packet (red) and PAG (black).

1.5 MCL algorithm and parent austenite reconstruction

The black grain boundaries in Figure 1.4 present a partially completed parent austenite grain map. However, some boundaries that (based on visual observation) are likely to be parent austenite grain boundaries are mistakenly indexed as block or packet boundaries. These connections need to be severed in some manner before the calculation of prior austenite orientations can take place. Here, the MCL algorithm is used for that purpose.

You can save the orientation relationship and the variant histogram shown in the development window to workspace by pressing the “Save to workspace” button. Proceed by following the itemized list:

1. The button “Call MCL” should now be enabled. Press the button to run the script “mcl_func.m” which contains the algorithm. The button will turn green to indicate completion.
 - a. You can change the inflation power to a desired value. A higher power will produce finer clusters but also increases the time needed for reconstruction and may result in misindexed austenite values in some cases. A lower power will result in larger clusters and will speed up reconstruction time. You will need to experiment to find the right value. 1.6 is usually a good place to start.
2. The prior austenite orientations can now be calculated separately for each set of discrete clusters. Press the button “Reconstruct” to run the script “recaus.m” that will reconstruct the austenite orientation map. A progress bar will pop up. The button will eventually turn green to indicate completion.
3. View the resulting prior austenite grains overlaid with the PAG boundaries from the iterative determination procedure by pressing “Plot results”. There should be good correlation between the iteratively determined PAG boundaries and the reconstructed austenite grain map.
4. Save the reconstructed austenite orientation map to workspace by pressing “Save to workspace”.

1.6 Analysis

Navigate to the “Analysis” tab. In the “Reconstruction quality” field, you will find text describing the average angular deviation from the experimentally observed OR. This value is the mean of the misorientation angles between the austenite orientations calculated for each martensite grain and the austenite orientations calculated for the entire corresponding clusters.

You can use this grain-specific value to color the grain map by pressing the “Plot grain by grain” button. Figure 1.5 shows the result. Most of the grains are a dark blue color, indicating good fit with the austenite orientation calculated for the whole cluster. Some grains, however, are a green or a yellow shade, indicating a poor fit. These grains should possibly be excluded in subsequent analysis of the results. For this purpose, the fit values for each grain can be exported to the workspace with the “Save to workspace” button.

In the last field, the variant numbering can be determined for each martensitic orientation pixel. This value corresponds to the variant notation defined by Morito et al. [1] and used by Miyamoto et al. [2], [3] in variant analysis of martensite nucleated in deformed and nondeformed austenite. Press the “Calculate” button to perform variant indexation. The button will turn green to indicate completion. You can view the variant selection by pressing the “Plot variants” button. There should be good correspondence between the block and packet boundaries determined with the iterative algorithm.

The “Calculate” button also redetermines the orientation relationship between austenite and martensite, based on the direct comparison of each austenite/martensite orientation pixel. This orientation relationship can be viewed by pressing the “Plot OR” button. The default selection will produce similar plots as in the iterative OR determination field in the previous tab. The first selection produces the 001, 110 and 111 pole figures describing each possible distinct martensitic orientation that can be produced from a single austenitic orientation.

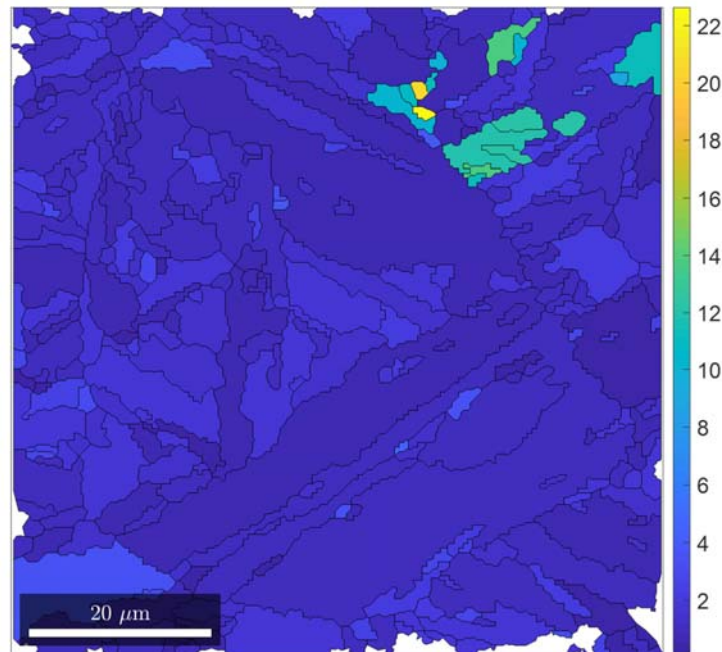


Figure 1.5 The fit values for each grain used to color the grain map.

The second checkbox selection produces zoomed-in pole figures showing martensite (011) planes and [-1-11] directions on a stereographic projection of austenite. An example of this plot is shown in Figure 1.6. In the Figure, the (011) plane can be observed to be nearly but not quite parallel to austenite (111) plane and the martensite [-1-11] direction nearly parallel to austenite [-101] direction. An ODF is included, which has been calculated from all of the austenite/martensite misorientations. The ODF clearly shows the spread in the orientation relationships. It may be helpful to ensure that the ORs determined with the iterative method and after reconstruction are similar.

Finally, the variant indexes and the newly determined orientation relationship can be saved to workspace with the “Save to workspace” button.

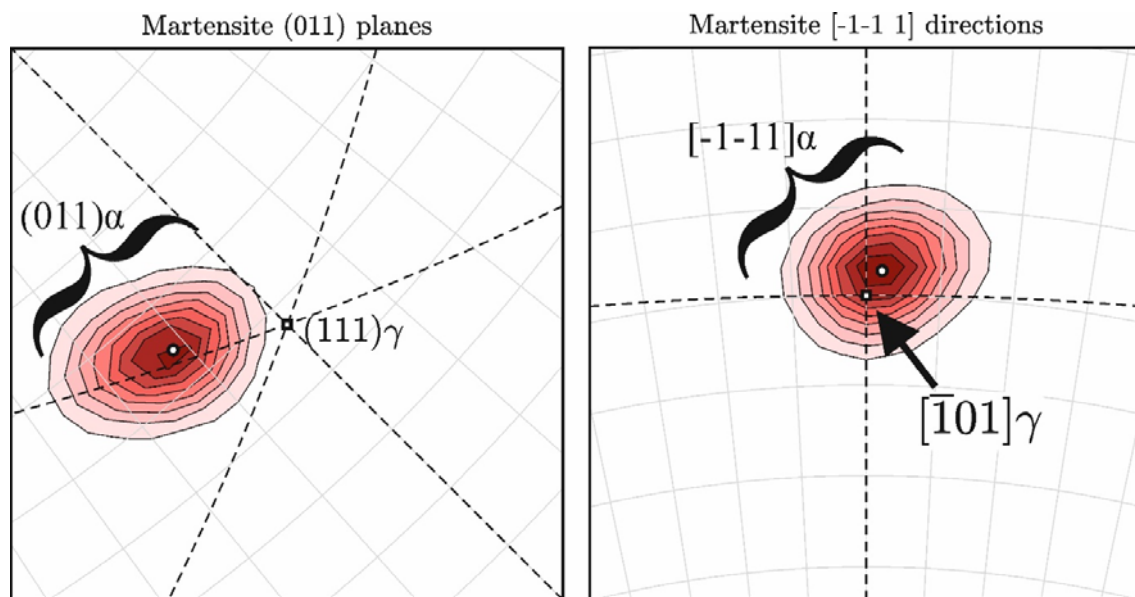


Figure 1.6 Martensite planes and directions plotted on a stereographic projection of austenite.

1.7 PAGs via triple points

The new feature in the GUI calculates the prior austenite orientation for each misorientation individually. It is accessed by opening the final tab “PAGS via triple points”.

1. Press “Determine OR”. You will see a similar development window to the grain-based OR determination algorithm. The difference is twofold:
 - a. all of the necessary symmetry operators for calculating the prior orientations are determined during the OR determination
 - b. Every misorientation between all orientation pixels is examined in the OR analysis.
2. Press “Reconstruct”. The GUI calculates the prior austenite orientations, using the symmetry operators obtained in the previous step.
3. Try out the plotting options to see the differences between various reconstruction methods. You might notice that austenite thermal twins are more readily determined from triple points and individual misorientations. More explanations can be found in the article “Crystallography, morphology, and martensite transformation of prior austenite in intercritically annealed high-aluminum steel” in *Metall and Mat Trans A* (2018) 49: 6426.

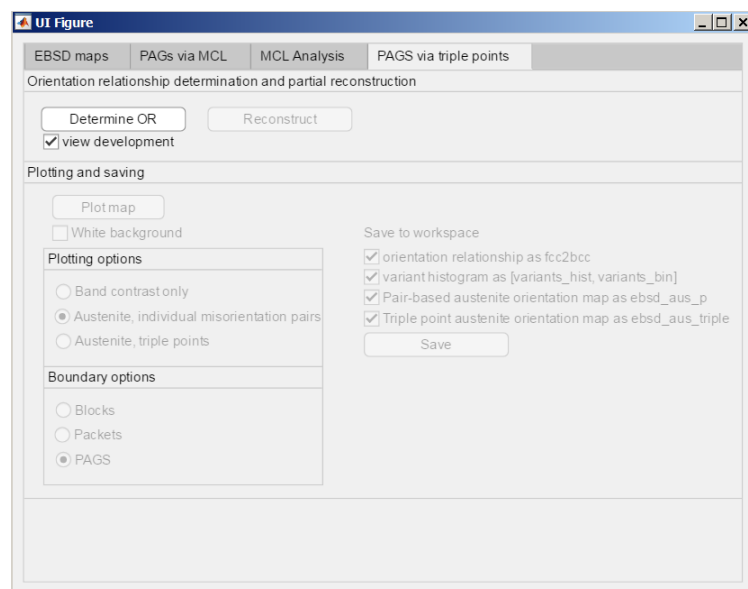


Figure 1.7. The final tab.

1.8 Bibliography

- [1] S. Morito, H. Tanaka, R. Konishi, T. Furuhashi, and T. Maki, “The morphology and crystallography of lath martensite in Fe-C alloys,” *Acta Mater.*, vol. 51, no. 6, pp. 1789–1799, Apr. 2003.
- [2] G. Miyamoto, N. Iwata, N. Takayama, and T. Furuhashi, “Mapping the parent austenite orientation reconstructed from the orientation of martensite by EBSD and its application to ausformed martensite,” *Acta Mater.*, vol. 58, no. 19, pp. 6393–6403, Nov. 2010.
- [3] G. Miyamoto, N. Iwata, N. Takayama, and T. Furuhashi, “Quantitative analysis of variant selection in ausformed lath martensite,” *Acta Mater.*, vol. 60, no. 3, pp. 1139–1148, Feb. 2012.