

DISEMM, a tool for the diffractive investigation of elasto-plastic behavior of polycrystalline alloys

Alexander Heldmann¹, Michael Hofmann¹, Markus Hoelzel¹

¹Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching bei München

DISEMM is a software tool for the investigation of engineering alloys by Neutron or Synchrotron diffraction. The basic concept is to derive the single-crystal elastic constants even in textured multiphase alloys from experimental diffraction data in as few steps as possible. And then use them in elasto-plastic self-consistent modelling and other investigations in a single software package.

The investigation of engineering alloys by diffraction methods has a long history. In particular, well established methods exist to analyze fractions of the constituent phases, textures, residual stresses, microstrains or particle sizes. In the last two decades the investigation of the single-crystal

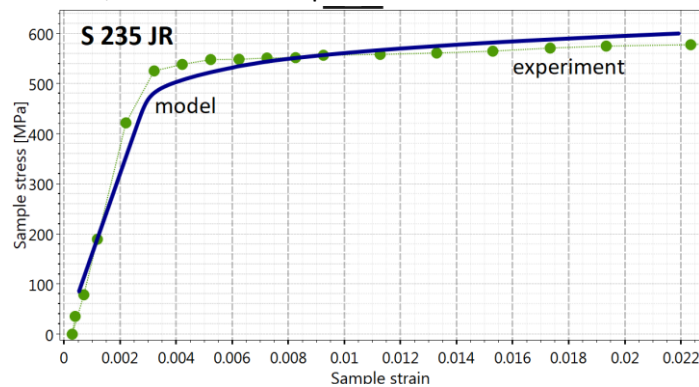


Figure 1 Comparison of the macroscopic stress-strain curve of S 235 JR a ferritic steel to modeled data of DISEMM.

elastic constants by diffraction methods has gained more attention and a method originally proposed by Hauk & Kockelmann has established itself as a reliable method for Neutron or Synchrotron diffraction [1]. The method is in general a reverse of the classical stress analysis and was further developed by Gnäupel-Herold et al. [2]. DISEMM takes the idea further and implements five different grain-to-grain interaction models, namely Reuss, Hill, Kroener, De Wit and Matthies. A novel approach to

include the load-transfer between the present phases and texture are implemented in DISEMM as well. Therefore with DISEMM it is possible to extract single-crystal elastic constants from most of the engineering alloys in-situ not requiring any single crystals as other established methods for example ultra sound techniques [3]. DISEMM can also be used to investigate the plastic deformation behavior with elasto-plastic self-consistent modeling as shown in Figure 1. It is the best possible expansion because it uses the single-crystal elastic constants as input values among different others and the obtained results can be compared to lattice strain measurements in the plastic regime by Neutron or Synchrotron diffraction. These measurements provide information about the stress distribution of investigated materials during plastic deformation. DISEMM uses this information to derive the critical-resolved shear stresses and hardening of the materials. The EPSC model implemented in DISEMM was in detail described by Hutchinson and later extended by various authors. In contrast to finite-element methods the EPSC modelling framework relies on averaging of grain orientations to solve different equations from Eshelby's inclusion model analytically [4].

The software is available for download from <https://github.com/Gipfelgrab/DISEMM>

- [1] Hauk V, Kockelmann H., Ermittlung der Einkristallkoeffizienten aus den mechanischen und röntgenographischen Elastizitätskonstanten des Vielkristalls. Zeitschrift für Metallkunde, 70, 500-502 (1979)
- [2] Gnaeupel-Herold T., Brand P., Prask H., Calculation of Single-Crystal Elastic Constants for Cubic Crystal Symmetry from Powder Diffraction Data. Journal of Applied Crystallography, 31, 929-935 (1998)
- [3] Heldmann A., Hoelzel M., Hofmann M., Weimin G., Schmahl W., Griesshaber E., Hansen T., Schell N., Winfried P., Diffraction-based determination of single-crystal elastic constants of polycrystalline titanium alloys. Journal of Applied Crystallography, 52, 1144-1156 (2019)
- [4] Hutchinson J., Elastic-Plastic Behavior of Polycrystalline Metals and Composites. Proceedings of the Royal Society A, 319, 247-272 (1970)