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## A Study on Minimizing Measurement Time Based on Active Experimentation for Energydispersive X-Ray Diffraction

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Particularly in laboratory XRD measurements, where the intensities in diffraction experiments tend to be low, an adaption of the exposure time to the investigated microstructure is crucial [1]. An adequately defined counting time is crucial if a high number of measuring points is examined in one measuring cycle. Examples of such cases are texture and residual stress measurements. A counting time that is too short can lead to a poor signal-to-background ratio or too dominant signal noise, which makes the subsequent evaluation more difficult or even impossible. It is then necessary to repeat the measurement with an adjusted, usually significantly longer measurement time [2]. Since the first evaluation steps following the measurement are standardized procedures, they provide an interesting approach for intelligent methods directly embedded in the measurement sequence [3,4]. In the present study, different approaches are investigated that analyze the continuously growing data set during an energy dispersive diffraction measurement on an application like that one shown in [5], and terminate the measurements after a sufficient measurement time is accomplished (this being defined based on data quality). Eventually, different selection strategies are proposed that intelligently choose the next point of investigation utilizing key characteristics of prior acquired data. It is shown that such strategies are able to significantly minimize the required measurement time without losing information and, thus, open up the possibility for active experimental design in the process.

## References

[1] T. Manns, B. Scholtes: Diffraction residual stress analysis in technical components —Status and prospects, Thin Solid Films (2012), doi:10.1016/j.tsf.2012.03.064

[2] B. Breidenstein, S. Heikebrügge, P. Schaumann, C. Dänekas: Influence of the Measurement Parameters on Depth-Resolved Residual Stress Measurements of Deep Rolled Construction Steel using Energy Dispersive X-ray Diffraction, HTM, J. Heat Treatm. Mat., 75 (2020) 6, S. 419-432. DOI: 10.3139/105.110423

[3] K. Dingel, A. Liehr, M. Vogel, S. Degener, D. Meier, T. Niendorf, A. Ehresmann and B. Sick.: AI-Based On The Fly Design of Experiments in Physics and Engineering, IEEE International Conference on Autonomic Computing and Self-Organizing Systems Companion (ACSOS-C) (2021). https://doi.org/10.1109/acsos-c52956.2021.00048

[4] D. Meier, R. Ragunathan, S. Degener, A. Liehr, M. Vollmer, T. Niendorf, B. Sick, Reconstruction of incomplete X-ray diffraction pole figures of oligocrystalline materials using deep learning. In Scientific Reports, 13(1), bl 5410. Springer Nature, 2023, https://www.nature.com/articles/s41598-023-31580-1

[5] A. Liehr, T. Wegener, S. Degener, A. Bolender, N. Möller and T. Niendorf: Experimental Analysis of the Stability of Retained Austenite in a Low-Alloy 42CrSi Steel after Different Quenching and Partitioning Heat Treatments, Adv. Eng. Mater. 2023, DOI: 10.1002/adem.202300380

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