Segmented ring detector analysis in simulated STEM images investigating medium-range order in amorphous materials

Hilke, S.[1], Kirschbaum, J.[2], Radić, D.[2], Hieronymus-Schmidt, V.[2], Radek, M.[2], Rösner, H.[2], Bracht, H.[2], Wilde, G.[2] and Peterlechner, M.[2]

[1] University of Münster, Institute of Materials Physics, Germany, [2] University of Münster, Institute of Materials Physics, Germany

Properties of amorphous materials such as mechanical behavior or transport are connected to the local structure at the nanoscale, which is typically described in terms of short- and medium-range order (SRO, MRO). Variable resolution fluctuation electron microscopy (VR-FEM) is a sensitive method to characterize the underlying characteristic length scale of MRO of amorphous samples [1,2]. VR-FEM data was acquired using STEM, collecting a large number of nano-beam diffraction patterns (NBDPs) with a various probe sizes. We introduced a method to accelerate the calculation of FEM normalized variance profiles using a newly developed simulation and analysis approach with segmented ring detectors [3] utilizing STEMcl [4]. VR-FEM simulations are based on structures obtained from different relaxation and potential protocols in molecular dynamics (MD) simulations. A comparison between simulated and experimental VR-FEM profiles with respect to peak position, ratio, and shape shows good agreement. Moreover, a crystalline cluster of 1 nm size was embedded into the MD box to test the validity of the paracrystalline approximation suggested by Gibson et al. [2] The corresponding VR-FEM simulation and calculation of MRO yields results very close to the size of the initially embedded crystalline cluster, which supports both the paracrystalline approach by Gibson et al. [2] and the validity of the segmented detector simulation. Moreover, these results indicate the power of the simulation approach and open the possibility to study e.g. small structural heterogeneities by simulations and experiments within reasonable simulation times. Additionally, we are able to conclude that continuous random network (CRN) amorphous silicon models contain more MRO than expected [5].

[1] Daulton, T.; Bondi; K.; Kelton, K.; Ultramicroscopy (2010), 110 (10) 1279 -1289.

[2] Gibson, J.M.; Treacy, M.M.J.; Voyles, P.M.; Ultramicroscopy (2000), 83 169-178.

[3] Hilke, S.; Kirschbaum, J.; Hieronymous-Schmidt, V.; Radek, M.; Rösner, H.; Bracht, H.; Wilde, G.; Peterlechner, M.; to be published.

[4] Radek, M.; Tenberge, J.-G.; Hilke, S.; Wilde, G.; Peterlechner, M.; Ultramicroscopy (2017), submitted.

[5] Rezikyan, A.; Jibben, Z.J.; Rock, B.A.; Zhao, G.; Koeck, F.A.M.; Nemanich, R.F.; Treacy, M.M.J.; Microsc. Microanal. (2015), 21 1455-1474.

Acknowledgement: Financial support by the Deutsche Forschungsgemeinchaft (DFG) under the grant number PE 2290/2-1 is gratefully acknowledged.