Measuring dynamic structural changes of nanoparticles at the atomic scale using scanning transmission electron microscopy

Quantitative analysis of atomic resolution electron microscopy images is commonly used to study the atomic structure of a nanomaterial. When such quantitative analysis is applied to a stationary structure, the insight into the dynamics is lacking. The atomic structure of nanomaterials can change over time via adatom dynamics, surface diffusion, beam effects, or during in situ experiments. Therefore, we propose a quantitative approach specifically designed to analyse the dynamically changing atomic structure using a time series of ADF STEM images [1,2]. The approach is based on the hidden Markov model. We show that the hidden Markov model far exceeds the atom-counting reliability of the existing methods, thanks to the transition probabilities which are used to explicitly model structural changes. In this manner, the hidden Markov model reliably reveals the number of atoms in each atomic column of the nanomaterial in each frame of the time series.

The method can not only be used to obtain reliable counting results, but also allows us to estimate the cross section for dynamical processes such as surface diffusion. This is demonstrated by the application of the novel method to experimental time series of a catalyst Pt nanoparticle on the one hand and of a Pt wedge on the other hand. Dynamic structural changes are determined from the time series analysis using a hidden Markov model, and we can reliably quantify the probability and cross section for surface diffusion. These values are of great importance in order to unravel dominant mechanisms and surfaces in the diffusion process and to gain new insights in surface related phenomena such as catalysis and nanoparticle growth. The hidden Markov model for atom-counting therefore holds promise for a reliable quantification of dynamic structural changes by adatom dynamics, surface diffusion, beam effects, or during in situ experiments. The hidden Markov model was implemented in the freely available StatSTEM software [3].

References

[1] A. De wael et al., Physical Review Letters 124 (2020), p. 106105.

[2] A. De wael et al., Ultramicroscopy (2020), under review with minor revisions.

[3] A. De Backer et al., Ultramicroscopy 171 (2016), p. 104.