Abstract

The main part of this work concerns so-called orbital mapping. For this imaging method, the transmission electron microscope together with electron energy-loss spectroscopy is employed. By adequately choosing an energy window of the inelastically scattered electrons, the electronic transitions of the sample electrons can be mapped. In many cases, this is equivalent to imaging the spatial distribution of the orbitals which constitute the transitions.
However, even current state-of-the-art electron microscopes are hard pressed to their limits when it comes to orbital mapping. Thus, we have performed extensive simulations in order to optimize the method and make its widespread use better realizable. In order to do so, we have applied several image difference metrics of which the metric based on the "Scale-Invariant Feature Transform" algorithm has yielded the best results. Using this specific metric, three quite different materials were investigated: rutile, graphite and a transition metal oxide heterostructure. The usefulness of parallel, as well as convergent, probe beams were analysed and compared to each other.
The results were used to design and support two experimental applications of orbital mapping. Thus, it proved possible to measure the spatial distribution of π^* and σ^* orbitals in graphene. Further, promising attempts at mapping the, up to now elusive, 2-dimensional electron gas at the interface between anatase and $LaAlO_3$ were made. In the last part of this work, we attempted to improve the simulation process itself by implementing electron-hole interaction into the simulation.