During the dissolution at a calcite cleavage face, etch pits open around defects. Atomic steps moving outwards from these pit centres are currently considered the general driving mechanism of this dissolution process that results in heterogeneous material flux from the surface. This means that the defects that generate the etch pits are crucial for the surface evolution. Recent kinetic Monte Carlo (kMC) simulation results indicate that not only the density but also the spatial distribution of defects is critical for the influence on dissolution.

In kMC simulations used for crystal dissolution, defect positions are input and can be defined in various ways, e.g., at pre-defined coordinates or randomly drawn from a distribution. The user is free in defining the defects, although it can generally be considered reasonable to choose defect densities and distributions as close as possible to what is expected to occur in nature and technical systems.

The actual spatial distribution of screw dislocations in calcite and their influence on rate variability are still not entirely known. To make the calcite kMC simulations comparable with experimental results, we experimentally determined the etch pit distributions, analyzed them and subsequently used them as input for further kMC studies.

While the direct measurement of defects in the crystal structure is extremely difficult, the indirect approach of measuring etch pits that have formed around defect outcrops during the beginning of dissolution is more feasible. For this, cleaved calcite single crystals were etched using ultra-pure water for 3 to 4 hours to obtain a significant amount of etch pits on the surface. The topography of the crystal surfaces was analysed using Vertical Scanning Interferometry (VSI). The resulting topography maps were stitched to gain a larger area for better statistics, and the centres of visible etch pits marked. This generates two-dimensional point patterns that describe the actual defect distribution more accurately than purely randomly generated coordinates without further constraints.

Based on data analysis of the experiments, we will show the resulting point distributions and synthetic patterns with similar underlying statistics. Using these as input for modelling, we then
calculate kMC simulations and geometrical models of a system close to the calcite single crystal from our experiment, and compare them also to simulations using different defect positions as input.