DISCUS RefineZnSe tutorial

In this tutorial you will learn to:

- refine parameter values that describe an ellipsoidally shaped nanoparticle with stacking faults and distance dependent peak width to obtain a good fit to an actual experimental PDF

The final result will be a nanoparticle with stacking fault content along the c-axis. To obtain a good fit using the REFINE section, one needs to perform the refinements in steps.

The initial macro "**refine_step_1_sphere.mac**" restricts the model to a perfect, spherically shaped nanoparticle. This initial step allows to get better estimates for the lattice parameters, the Zn-position and a rough particle diameter.

A main shortcoming of this model is the imperfect fit at very low distances and ath higher distances.

To remedy the latter, one can use the result of the first macro "refine_new.res" as a template for the refinement of further parameters. Macro "**refine_step_2_ellips.mac**" essentially is a copy of this first result macro. Compared to the first step, we start at the resulting parameters and refine independent diameters in the a-b-plane and along the c-axis.

The third step "**refine_step_3_cquad.mac**" refines the "corr_quad" parameter. This applies an empirical sharpening to PDF peaks ar short interatomic distances, to mimick acoustic phonon like behavior of first neighbors.

Finally "**refine_step_4_stack.mac**" we refine a stacking fault probability. As an individual nanoparticle with just a few layers (roughly 10 to 15 in our case) is not a good representation of the many different stacking fault conformations DISCUS simulates several individual nanoparticle and averages their respective PDFs. This gives the best fit, of course at the expense of much more computing time.