DISCUS Ellipsoid tutorial

In this tutorial you will learn to:

- build an ellipsoidally shaped nanoparticle
- decorate its surface with a ligand molecule
- calculate the powder pattern and the powder PDF
- plot the resulting structure with JMOL

The main tool for this tutorial is the macro “top.mac” found in the ELLIPSOID folder. This macro takes 4 parameters and is started as the following example shows:

```
@top.mac   30.00, 30.00, 30.00, 0.01
```

The first three parameters are diameters of the nanoparticle along the axes a, b, c. Values are understood as Angstroem. The fourth parameter is a density of ligands on the nanoparticle surface in units of [Ligands/Angstroem^2].

Start the discus_suite, navigate to the ELLIPSOID folder and try it out.
The macro will be interrupted a few times to give you time to visualize the nanoparticle at intermittent steps in its construction. Try the macro with different parameter values.

Load the file “top.mac” into a suitable text editor on your computer. This file contains all the commands that are passed on to the discus_suite. We will highlight the most important steps in the following:

The first 22 lines all start with “#” and are considered a comment. In this header section a short description and instruction on the use of the macro are provided.

Most of the individual tasks shown in the list at the top of this description are found in further files. DISCUS refers to these files with the command lines that start with the at symbol : “**@**”. This nesting of macros within the top macro serves to break the tasks into smaller portions and to provide a library of macro files that you can modify for your own needs.

In macro “**definitions.mac**” several variables are defined, which are useful throughout the simulation. It is just easier to remember the purpose of a variable with names like “diam_a” than the generic “$1” parameters.

Macro “**prepare_chain.mac**” is used to build a very simple ligand molecule. A task like this does not have to be done each time over, thus you could take this macro on its own and omit it from “top.mac”.

With the command “**discus**” in line 30 we step from the top level discus_suite into the DISCUS section, where we build the particle. In line 53 we step back to the top level again.

DISCUS offers many styles to obtain and read an initial structure, like reading a CIF file, using the DISCUS proprietary format or, as is done in “**prepare_gold.mac**” to build a structure from scratch.

Once the initial gold structure has been defined, actually just the asymmetric unit, **lines 34 to 41** are used to build an initial block of unit cells. By reading a single unit cell we know the lattice parameters and can use this information to calculate the size of the initial block shaped crystal just barely big enough to fit our final nanoparticle inside this block. The line

```
ncell_a = int(max(diam_a,diam_b,diam_c)/lat[1]) + 2
```

calculates the number of unit cells needed along the a-axis. The maximum value of any diameter is divided by the a-lattice parameter, truncated to the next smaller whole number and a safety margin to 2 more unit cells is added. This calculation provides the flexibility to make the initial block big enough as function of the user parameters for the diameters.

Macro "**build_ellipsoid.mac**" performs the task to shape the crystal into the desired ellipsoidal form. Within this macro you will find (optional) steps to display the intermittent crystal structure.

With "**debye.mac**" the powder diffraction pattern is defined and calculated, as well as the powder PDF.

Next, the nanoparticle surface is decorated with the ligand molecules in "**decorate.mac**".

Last, the decorated nanoparticle is displayed ("plot.mac decorated") and the powder pattern/PDF is calculated using "debye.mac" a second time.

Finally the macro "**k_compare_pdf**" displays the calculated PDF for the pure ellipsoid and the decorated ellipsoid.

Homework:

- run the macro with different diameters and/or coverage
- locate the command where the Atomic displacement parameter (ADP) "bvalue" is set and try different values. What effect does this have on the visibility of the Gold-Sulfur peak in the PDF?
- Modify the radiation (neutron, xray, electron). What happens? Why?
- Test the different versions of the "boundary" command.