DISCUS Strained Ellipsoid tutorial

This tutorial is essentially a copy of ELLIPSOID with the additional task:

- apply a strain field throughout the nanoparticle

The main tool for this tutorial is the macro “top.mac” found in the STRAINED_ELLIPSOID folder. This macro again 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/Angstroem2].

Start the discus_suite, navigate to the STRAINED 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 that differ from ELLIPSOID in the following:

In **line 38 to 43** the essential parameters of the strain model are defined. These are two distances and an angle as well as corresponding potential depths for the energy minimization step. The basic idea is to define the regular Gold-Gold distance as half the body diagonal:

P_auau = lat[1]/sqrt(2.0)

The strain is introduced by defining a Gold Sulfur distance (line 39) and a bond angle within Sulfur to the two Gold atoms at the surface (line 40). If the bond angle does not match the lengths in the triangle Au-S-Au, a strain is introduced. In this example, the potential Au-Au is very shallow (line 41) while the Au-S potential is very deep. This will force DISCUS to change the Gold-Gold distance at the surface and as a consequence throughout the entire nanoparticle.

The actual modification of the nanoparticle structure is done in macro “**strain.mac**”.

To speed up the strain relaxation the decoration by the ligand molecule is split into two steps, the decoration with the Sulfur atom macro “decorate_head.mac” (line 56) and the decoration with the remaining Carbon atoms macro “decorate_tail.mac” (line 63).

Finally the macro “**k_compare_pdf**” displays the calculated PDF for the pure ellipsoid and the decorated and strained ellipsoid.

Homework:

- run the macro with different diameters and/or coverage
- modify the distances / potential values (lines 38 to 43). What effect does this have on the
- PDF?