Exercise: GBCD of Y-doped alumina

The aim of this exercise is to calculate and plot the grain boundary plane distribution (GBPD) and the grain boundary character distribution (GBCD) of Y-doped alumina, using the method and data presented in the paper "*Influence of Y and La Additions on Grain Growth and the Grain-Boundary Character Distribution of Alumina*" [1].

Plot:

- Misorientation distribution
- GBPD independent of misorientation
- GBCD at a 60°/[0001] misorientation
  GBCD at a 144.2°/[1-210] (near Σ11) misorientation
  GBCD at a 38.2/[0001] (Σ7) misorientation

Instructions:

1. **Download segment files:**
   Download the individual segment files (for 1500°C or 1600°C) from:
   http://mimp.materials.cmu.edu/~gr20/Grain_Boundary_Data_Archive/alumina_Y_doped/alumina_Y_doped.html
2. **Process segment files:**
   Copy the downloaded segments into the *2_condition_segments* folder. Edit the input file accordingly, then run *condition_segs.exe*
3. **Calculate distributions:**
   Copy the newly generated file *all_segments.txt* file into *3_calc_discrete_dist* folder: Edit the input file accordingly, then run *calc_discrete_dist.exe*
4. **Plot distribution graphs:**
   Copy the newly generated files *all_segments_gbcd.txt* and *all_segments_gbpd.txt* files into *4_graph_discrete_dist* folder. Edit the input file based on the distribution you want to plot, then run *graph_discrete_dist.exe*.

Conversion of Miller-Bravais indices [hkil] to Cartesian coordinates

$$x = a \times (h - \frac{k}{2} - \frac{i}{2})$$

$$y = \frac{\sqrt{3}}{2} \times a \times (k - i)$$

$$z = l \times c$$

Lattice parameters α-alumina

a = 4.758 Å

c = 12.991 Å

[1] Bojarski SA, Stuer M, Zhao Z, Bowen P, Rohrer GS (2013): Influence of Y and La Additions on Grain Growth and the Grain-Boundary Character Distribution of Alumina. Journal of the American Ceramic Society, Vol 97(2), 622–630. https://doi.org/10.1111/jace.12669.