Utility for Calculating Displacement Correlations for RMCProfile Configurations

Routine AtomCorr.exe calculates atomic correlation parameters for the .cfg files used by RMCProfile. These parameters are calculated as

$$C(\mathbf{n}_1, \mathbf{n}_2, \mathbf{R}) = \frac{\langle (\mathbf{u}_i \mathbf{n}_1)(\mathbf{u}_j \mathbf{n}_2) \rangle}{\sqrt{\langle (\mathbf{u}_i \mathbf{n}_1)^2 \rangle \langle (\mathbf{u}_j \mathbf{n}_2)^2 \rangle}}$$

where $\mathbf{u}_i$ is the displacement of the *i*-th atom in the refined configuration relative to the position of this atom in the initial configuration (average crystal lattice), $\mathbf{n}_1$ and $\mathbf{n}_2$ are the unit vectors along the directions of interest, and <> denote the average over configuration.

A set of atoms *i* is selected by specifying a range of their sequential numbers (first and last) in the *.cfg file, whereas a set of atoms *j* is selected by specifying (*1*) a range of their sequential numbers (first and last) in the .cfg file and (*2*) a volume delimited by an intersection of a spherical layer around atoms *i* (radii r_{min} and r_{max}) and a cone (axis **R** and angle θ) having its vertex at atoms *i*.

To use this utility, the *.cfg files containing the starting and the refined configurations must be in the same directory with the **AtomCorr.exe** file. The input for **AtomCorr** can be entered either manually, following the on-screen instructions, or using a text file having an extension "**.cor**". This input file has the following structure:

```
Initial          ! .cfg filename (no extension) for an initial configuration
Final            ! .cfg filename (no extension) for a final configuration
1    4096        ! range of atoms i in the .cfg file
4097  12288      ! range of atoms i in the .cfg file
3.5    4.5       ! rmin and rmax in Å
1 1 2            ! component of vector R in Å
20               ! Angle θ (degrees)
1 0 1            ! components of vector n1
1 0 -1           ! components of vector n2
```

Vectors **R**, $\mathbf{n}_1$, and $\mathbf{n}_2$ are normalized by the program and, therefore, only relative values of their components are important. The program generates two output files: **finalcomp.txt** and **final_correl.txt**.

The **finalcomp.txt** file contains the coordinates of all atoms in the **initial.cfg** file (RMC units) plus three components of the corresponding atomic displacements relative to the initial positions (Å) (the results are arranged in a six-column table). The file final_correl.txt file contains calculated values of the correlation parameters and the *rms* displacements of atoms *i* ($\sqrt{\langle (\mathbf{u}_i \mathbf{n}_1)^2 \rangle}$) and *j* ($\sqrt{\langle (\mathbf{u}_i \mathbf{n}_1)^2 \rangle}$).