**Calculating correlations for atomic displacements**

This routine calculates correlation coefficients $C\left(\vec{n}, R, \vec{n}\_{t},\vec{n}\_{d}\right)$ for atomic displacements as:

$C\left(\vec{n}, R, \vec{n}\_{t},\vec{n}\_{d}\right)=\frac{\left〈\left(δ\vec{r}\_{i}\vec{n}\_{t}\right)\left(δ\vec{r}\_{j(i)}\vec{n}\_{d}\right)\right〉\_{i\in Ω\_{t }}}{\sqrt{\left〈\left(δ\vec{r}\_{i}\vec{n}\_{t}\right)^{2}\right〉\_{i\in Ω\_{t }}\left〈\left(δ\vec{r}\_{j}\vec{n}\_{d}\right)^{2}\right〉\_{j\in Ω\_{d }}}}$ ,

where $δ\vec{r}\_{i}$ is the displacement of the *i*-th atom from its position in the reference configuration.

A reference configuration can be either the initial one or a configuration with the atoms located at the average positions determined for the final refined configuration, which can be obtained using the routine **Thermal\_Ellipsoids**.

The unit vectors $\vec{n}\_{t}$ and $\vec{n}\_{d}$ that describe the directions of the displacement components for which the correlations are sought must be specified in the input file.

A list *Ω*t of atoms to be analyzed (target atoms) can be defined either by specifying the first and the last numbers of these atoms in the configuration file or by providing a list of their numbers in a separate file.

For each atom *i*, the corresponding atom *j*(*i*) is an atom of the user pre-defined type which is displaced relative to the atom *i* by a vector $ R\vec{n}$. ($\vec{n} $ is the unit vector, *R* is the interatomic separation.) The atom *j*(*i*) must simultaneously satisfy the following conditions: (*a*) belong to the set *Ω*d, (*b*) be located within a spherical layer with radii *R*1 and *R*2, which includes atom *i* (*R*1 < *R* < *R*2), and (*c*) be located within a cone directed along $\vec{n}$ and having the angle ϑ.

*Running the program and Input*

To execute the routine Corr\_coeff.exe, the working folder must contain (1) the \*.cor input file, (2) the reference \*.rmc6f file, (3) the \*.rmc6f file that needs to be analyzed and, if relevant, (4) the list of atoms *Ω*t in a separate file.

*Example of the input \*.cor file:*

KNO\_AVERAGE !  *Name of the \*rmc6f file containing the reference configuration*

KNO ! *Name of the \*rmc6f file containing the configuration of interest*

FROM\_START\_FILE ! Legacy keyword, just leave it there

START\_END ! Use this keyword if the list of atoms *i* is defined using the first and last numbers

LIST ! Use this keyword instead of “START\_END” if the list of atoms *i* is defined in a separate file

1 13872 ! First and last numbers of atoms *i* if using the “START\_END” keyword

6 ! number of correlation coefficients to be calculated

 1 13872 ! First and last numbers of atoms j

3.47 4.47 !*R*1 and *R*2 (Angstroms)

1 0 0 $\vec{n}$ (*nx, ny, nz*)

20 ϑ (degrees)

1 0 0 $\vec{n}\_{t}$ (*ntx, nty, ntz*)

1 0 0 $\vec{n}\_{d}$ (*ndx, ndy, ndz*)

The block of keywords marked with the bracket must be repeated for each correlation coefficient.

Two output files **“name”comp.txt, and “name”\_correl.txt** are created, where **“name”** is the name of the configuration .rmc6f file analyzed**.**

The file **“name”comp.txt** contains the atomic displacements (in Angstroms) relative to the corresponding reference positions. The first three columns are the fractional coordinates in the starting configuration, followed by the three columns which contain the corresponding components of atomic displacement.

The file **“name”\_correl.txt** contains the resulting correlation coefficients and input information.