

2.6. NON-AMBIENT-TEMPERATURE POWDER DIFFRACTION

2.6.8. Temperature accuracy

The accuracy of the temperature measurement of a non-ambient device has to be determined before starting a non-ambient experiment. At present no certified temperature standards for X-ray powder diffraction are available, only commonly used reference materials. A list of these materials can be found at <https://www.xrayforum.co.uk/> and https://bl831.als.lbl.gov/~jamesh/pickup/Snell_SG_change_table.pdf.

A common method for validation of a non-ambient chamber is by determining the thermal expansion coefficient of a reference material as a function of temperature. Another is to determine the transition temperature of well known phase transformations. A third method is the so-called 'differential thermal expansion' method (Drews, 2001). This method utilizes the relative thermal expansion of two diffraction peaks. These peaks can be from the same or different reference material(s) but must be found in a narrow angular range and have different thermal expansion behaviour. Using only the relative separations of the peaks that are closely spaced eliminates the need for full pattern refinement to take into account geometrical aberrations and makes this method fast.

2.6.9. Future

A whole new field of non-ambient experiments has opened up with the study of new applications such as non-ambient PDF (see Section 2.6.7.2) and non-ambient SAXS measurements. And what happens in the nano world when large-scale models no longer hold at ambient and non-ambient temperatures? The future will tell; non-ambient diffraction/scattering experiments are more relevant now than ever before.

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