What you can, and can't do with *in situ* powder diffraction

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Powder diffraction is particularly powerful for studying samples *in situ* and within a range of sample environments [1]. This has made it an incredibly powerful tool, in particular for studying samples under extreme conditions. But are there any special considerations that you need to make to these data? Generally, yes, and I will describe some of the potential hiccups when approaching data collected *in situ*, and crucially how to describe these to others. A great advantage to powder diffraction data for *in situ* studies, is the ability to visualise data (for instance with thermodiffractorgrams like Figure 1), enabling you to quickly assess the data and its phase transitions. Additionally seeing the fit can be key [2], as relying only on *R*-factors can result in mis-leading results. Increasingly powerful for this is the powder diffraction CIF format (pd\_CIF) [3], which is a useful way to store and deposit your data, and to allow others to easily judge the fit of your data.

![Thermodiffractorgram](image)

**Figure 1.** Example of a thermodiffractorgram, showing variable temperature powder diffraction collected over a large temperature range. This is a particularly useful tool for *in situ* powder diffraction as phase transitions can easily be seen and tracked.


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