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An empirical method to negate Bragg-peak shifts due to partial gauge volume illumination in neutron powder diffraction studies

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Partially filled neutron gauge volumes in neutron powder diffraction experiments lead to anomalous shifts in diffraction peak positions. In stress analyses, these shifts create systematic errors in lattice parameter measurements, potentially leading to incorrect interpretations of strain if left uncorrected. This phenomenon is known as the pseudo-strain effect.

The instrumental gauge volume (IGV) refers to the region which is defined by the intersection of the incident and diffracted neutron beam paths. When this volume is fully embedded in a homogenous sample that does not exhibit large grains or preferred crystallographic orientation, the geometric centre of the IGV closely corresponds to the neutron-weighted centre of gravity (NCOG) of the crystallites being probed. The NCOG represents the effective spatial position within the sample from which the diffracted neutron intensity appears to originate and is influenced by the incident beam intensity distribution, sample geometry, relative sample position / orientation and attenuation cross-sections. In situations where the sample is smaller than the beam, or the beam is not fully embedded in the sample, offsets may exist between the IGV centroid and the NCOG.

To account for the effects of partial illumination, a method was devised to determine the NCOG offsets considering the factors mentioned based on previous investigations \1. In addition, an empirical model, shown in Figure 1, was devised to correct the peak shift due to the combined effect of NCOG offsets and the non-negligible wavelength distribution spread of the incident neutron beam.

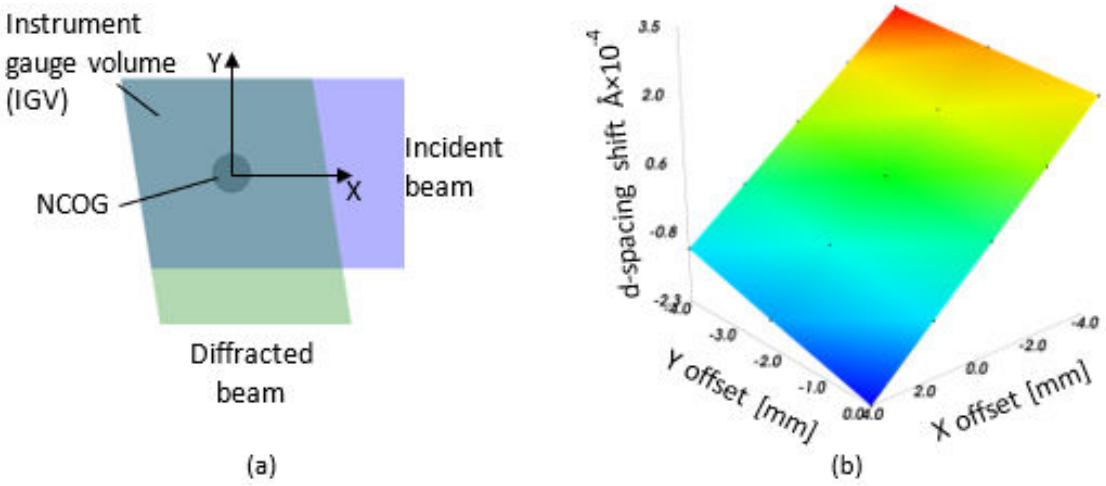

Figure 1: enter image description here

Figure 1. (a) Experimental setup and (b) d-spacing shift due to positional changes of the NCOG within the IGV

\1 D. Marais, Z.N. Sentsho, A.M. Venter. Numerical neutron attenuation correction for partially-illuminated powder samples. Materials Characterization. 153(2019)234-239 (https://doi.org/10.1016/j.matchar.2019.05.011.)

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