

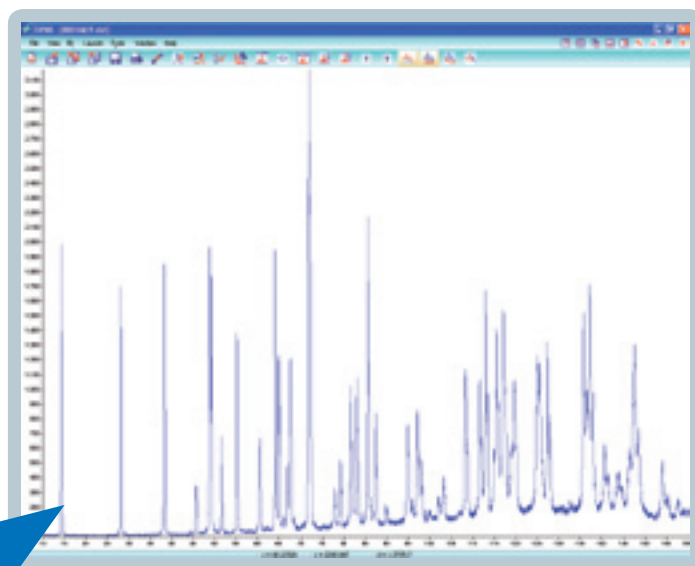
## VARIABLE COUNTING TIME: THE GOLDEN STANDARD FOR X-RAY DATA COLLECTION

Variable Counting Time (VCT) refers to a data collection scheme for X-ray powder diffraction, where the measurement time is systematically increased towards higher angles  $2\theta$ . As a result the natural steep intensity fall towards higher angles  $2\theta$  is compensated, leading to drastically improved data quality for all kinds of profile fitting applications.

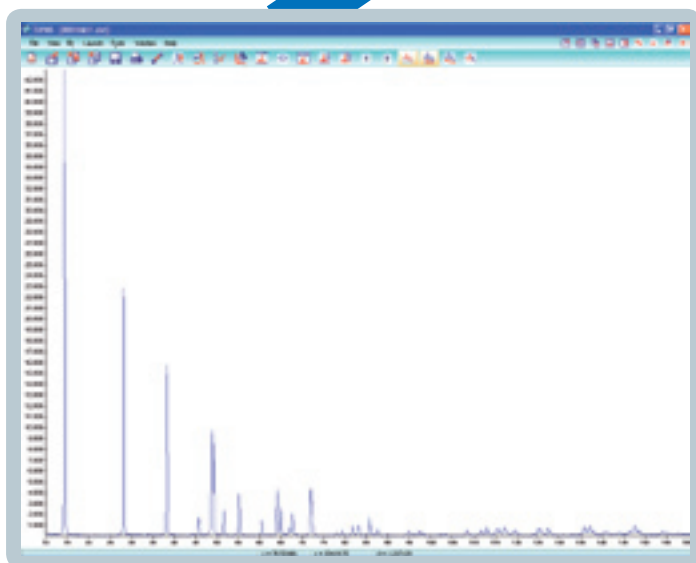
Generally, with VCT full advantage can be taken of the substantial amount of peak information present at higher angles  $2\theta$ , which is otherwise lost in conventional constant counting time measurements.

Now fully supported by the XRDWizard V2.9 and TOPAS V4

VCT Enhance your results



Same sample recorded with variable counting time



Typical diffraction pattern recorded with constant counting time

VCT data typically results in:

- Greatly enhanced chance for success in structure determination. Atomic coordinates, occupancy factors and (anisotropic) thermal parameters are better determined, especially in the case of light atoms.
- More stable refinement of atomic coordinates and thermal parameters of light atoms, including hydrogen.
- Substantially lower  $R_{wp}$  indicating a better overall fit.
- A GOF much closer to unity, indicating a better fit of the structural and profile models to the data and that the weights are properly applied.

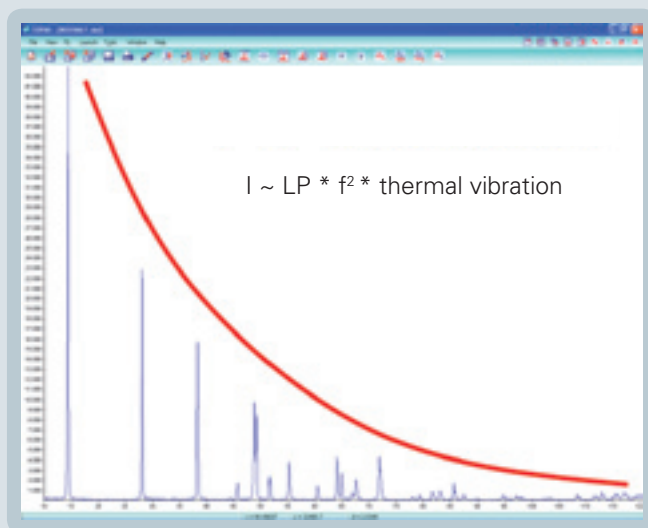
## VCT?

The concept of a Variable Counting Time (VCT) strategy for X-ray powder diffraction data acquisition was introduced by Madsen & Hill (1992, 1994) and David (1992). A VCT strategy is based on a function that increases the counting time used at each step in the scan in a manner that is inversely proportional to the decline in reflection intensity that inevitably results from the combined effects of the Lorentz-Polarisation (LP) factor, scattering factors  $f^2$  (form factor fall-off) and thermal vibration of atoms.

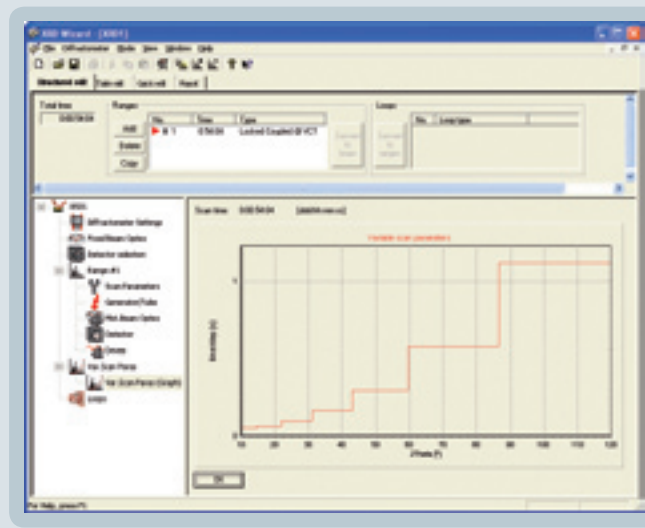
The highly dominating factor of these is the sample / structure independent LP factor, leading to an intensity

decrease by a factor of about 400 (!) as the diffraction angle increases up to about  $100^\circ 2\theta$ ; above this angle, the intensities slowly increase again. The contribution by scattering factors and thermal vibration of atoms is typically an order of magnitude smaller and can therefore be neglected.

In the XRDWizard V2.9 implementation of VCT, the measurement time depends on a function approximately compensating the dominating effect of the LP factor. This allows for a very user-friendly push-button creation of VCT schemes, as no crystal structure information is required.



Intensity loss due to Lorentz-Polarisation, scattering factors and thermal vibration of atoms



Example variable counting time scheme in the XRDWizard V2.9

### References:

Madsen, I.C. & Hill R.J. (1992): „Variable step-counting times for Rietveld analysis or getting the most out of your experiment time.” - Adv. X-ray Anal., 35, 39-47

Madsen, I.C. & Hill R.J. (1994): „Collection and analysis of powder diffraction data with near-constant counting statistics.” J. Appl. Cryst., 27, 385-392

David, W.I.F. (1992): „Accuracy in Powder Diffraction: Optimization of data collection strategies.” - Abstract P2.6, NIST Special Publication No. 846, Page 210

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