X-ray data refinement of perovskite-like compounds by FullPROF

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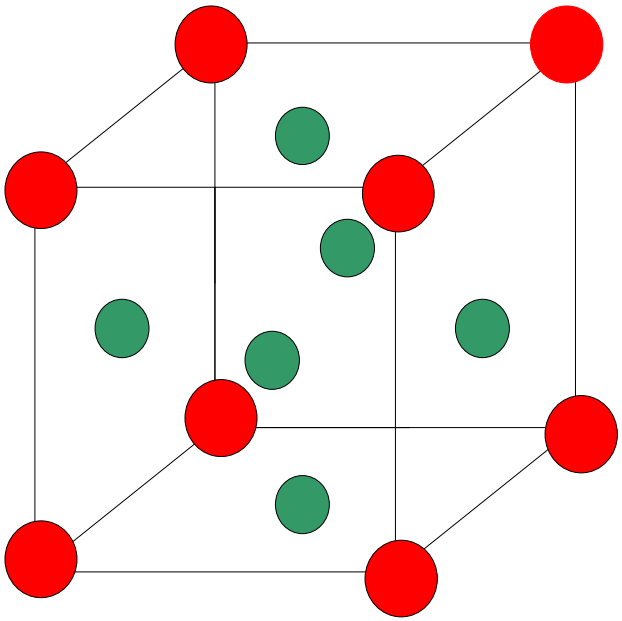
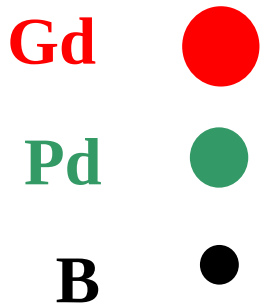
Introduction

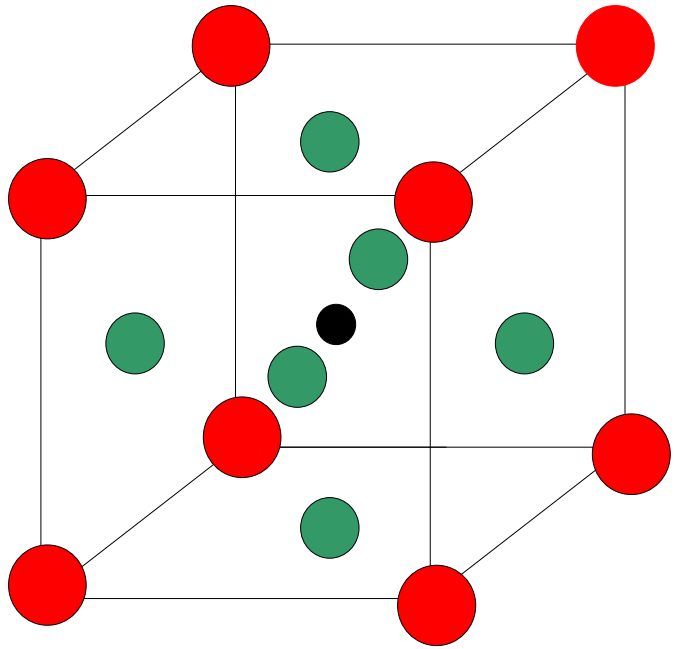
- FullPROF can be used to refine neutron scattering/ X-RAY diffraction data

- We present here powder X-Ray (Cu-K_α) diffraction data refinement using FullPROF for perovskite-like compounds, (RE)$TM_3B_xC_{1-x}$

Crystal Structure





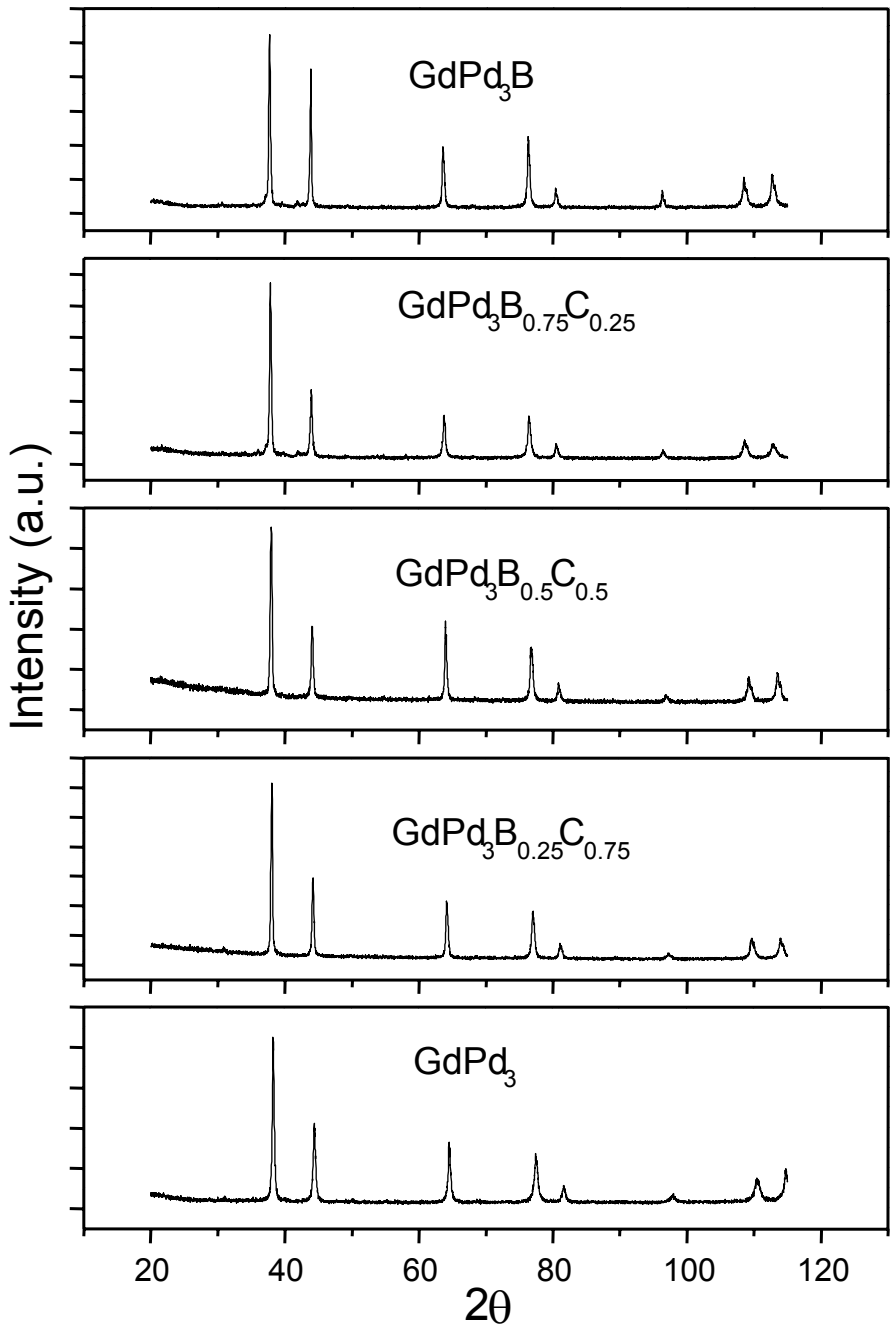


$GdPd_3$
a = 4.09 Å

Space group: *Pm-3m*

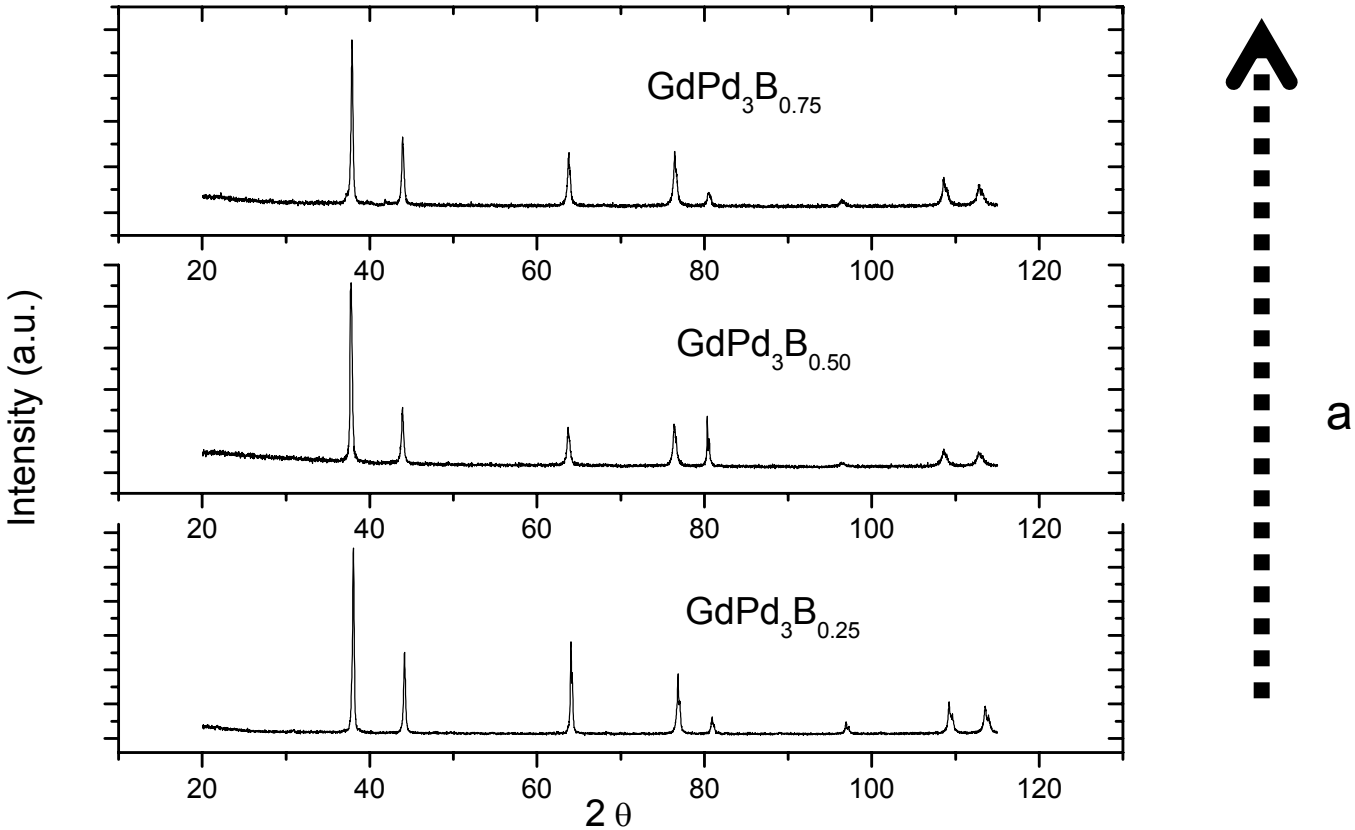
$GdPd_3B$
a = 4.14 Å

X Ray Diffraction Measurements

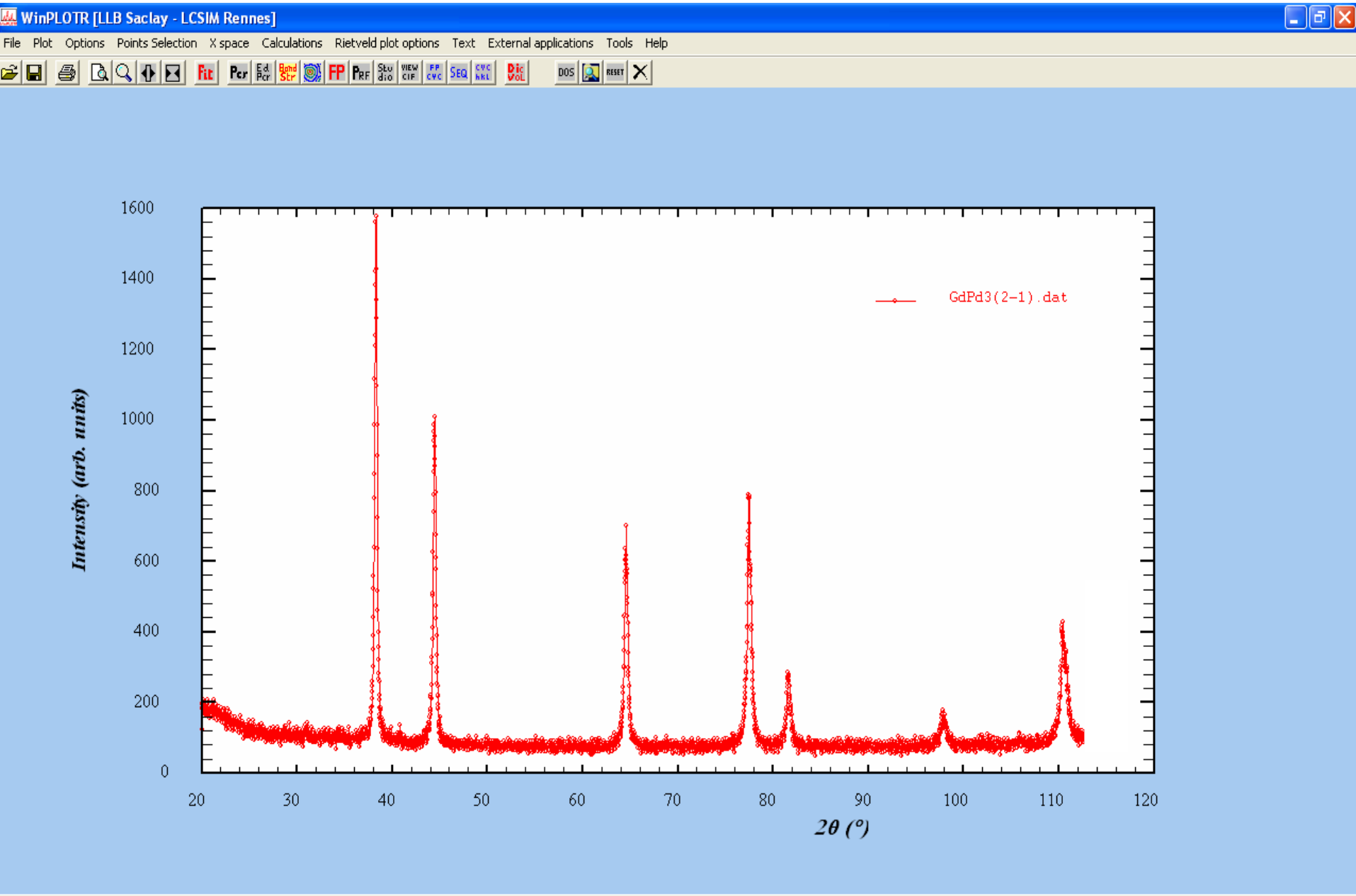


a

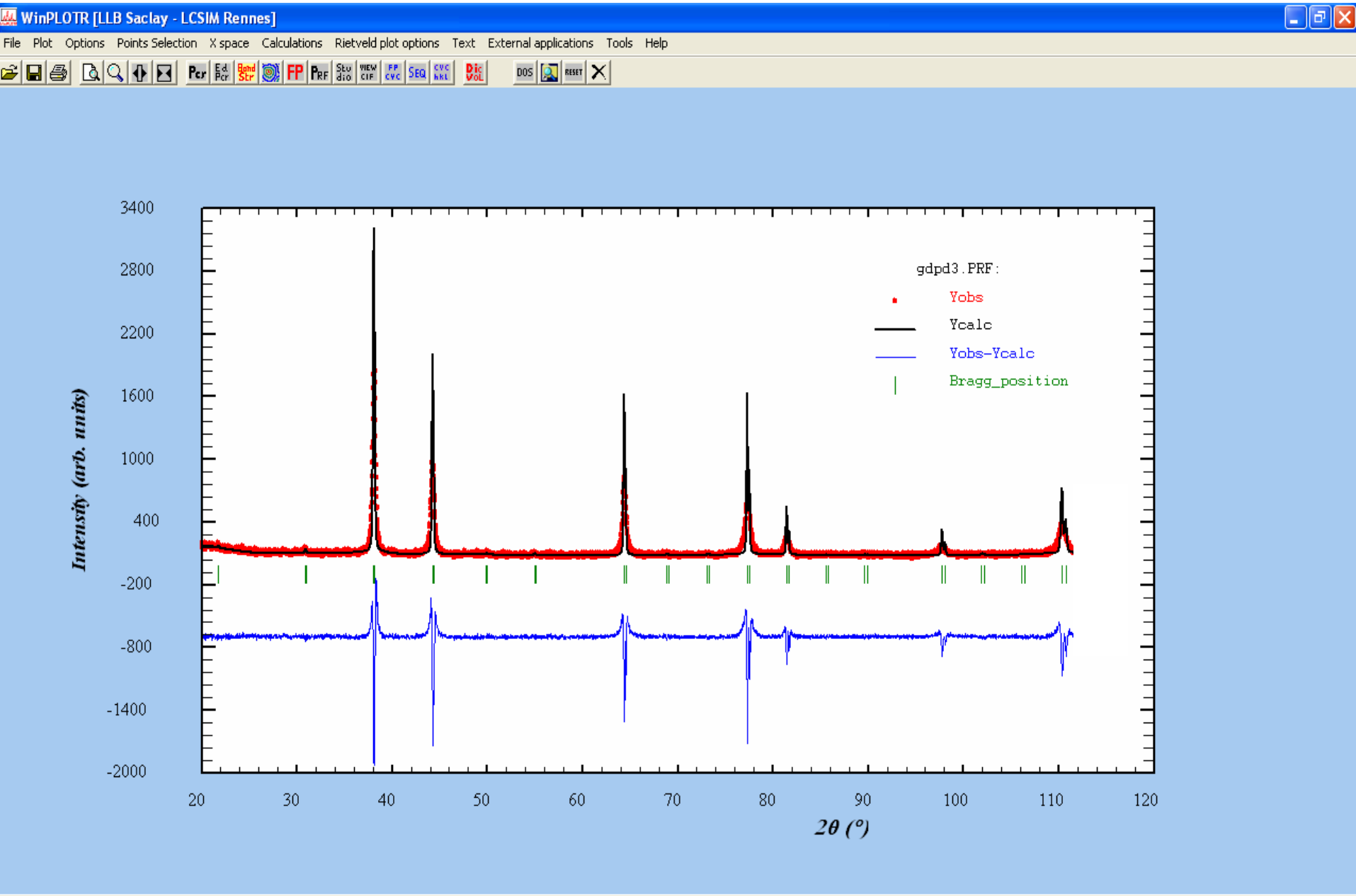
X Ray Diffraction Measurements



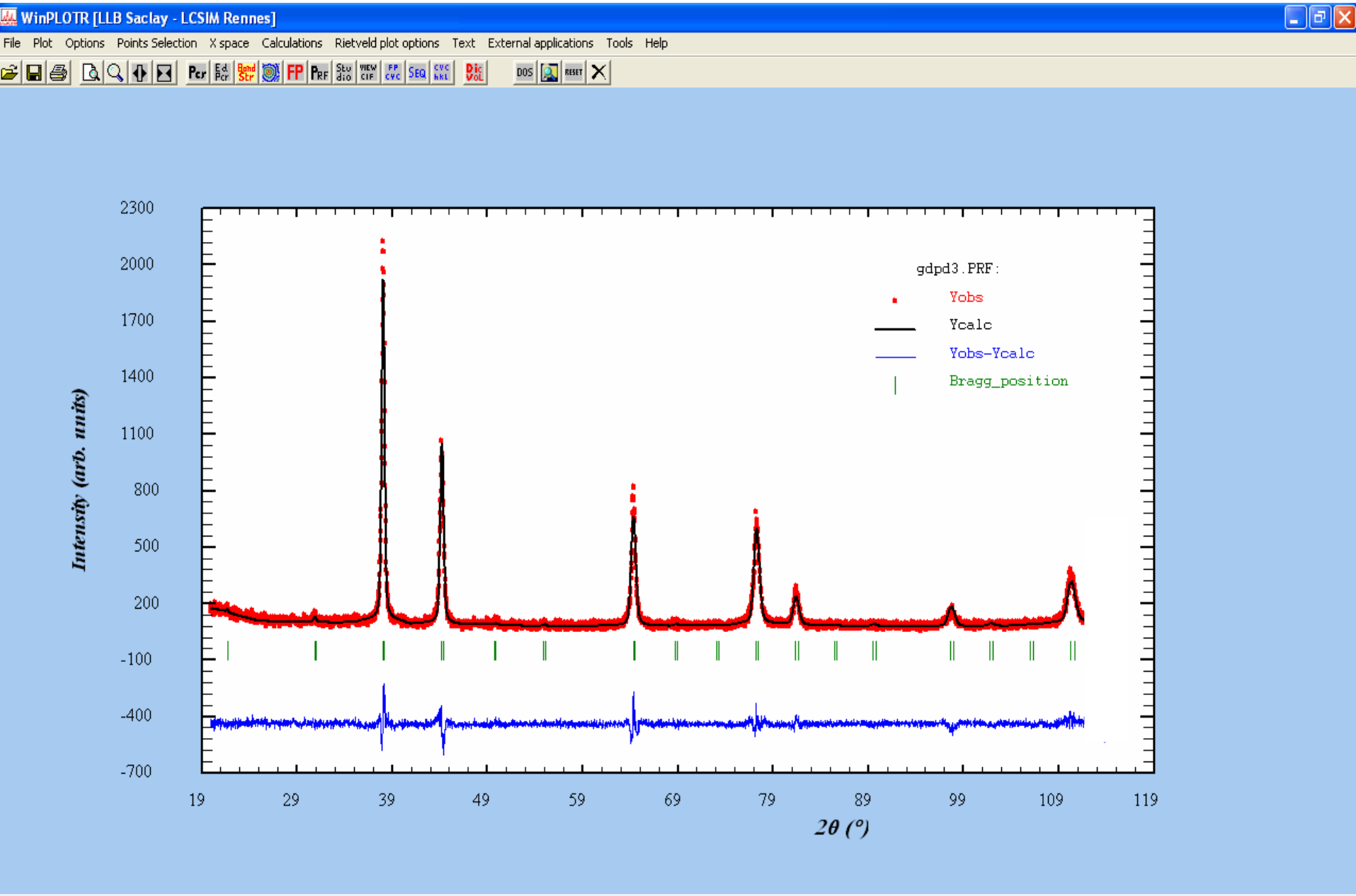
Raw X- ray diffraction data-$GdPd_3$



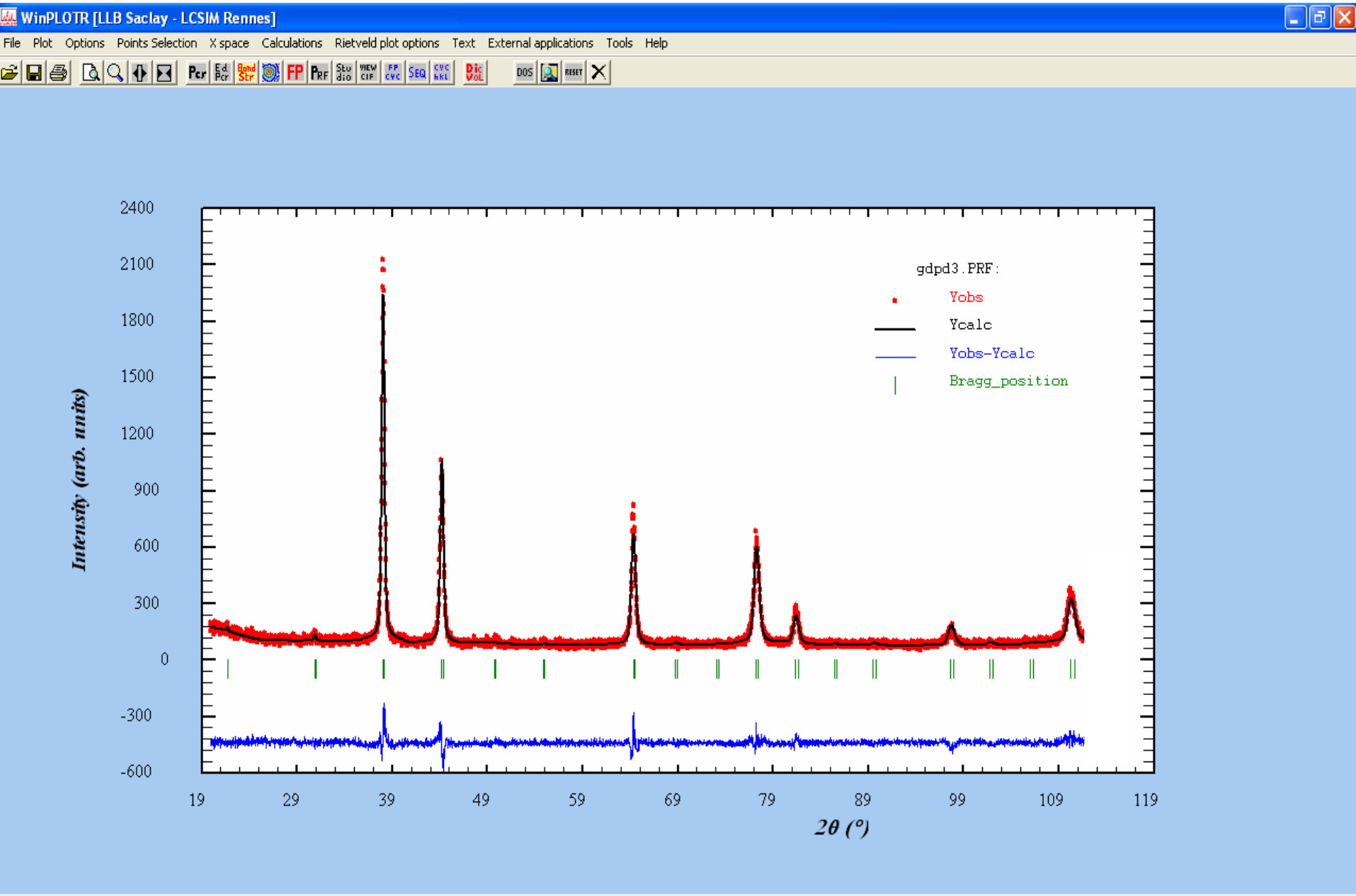
Fitting by using space group symmetry



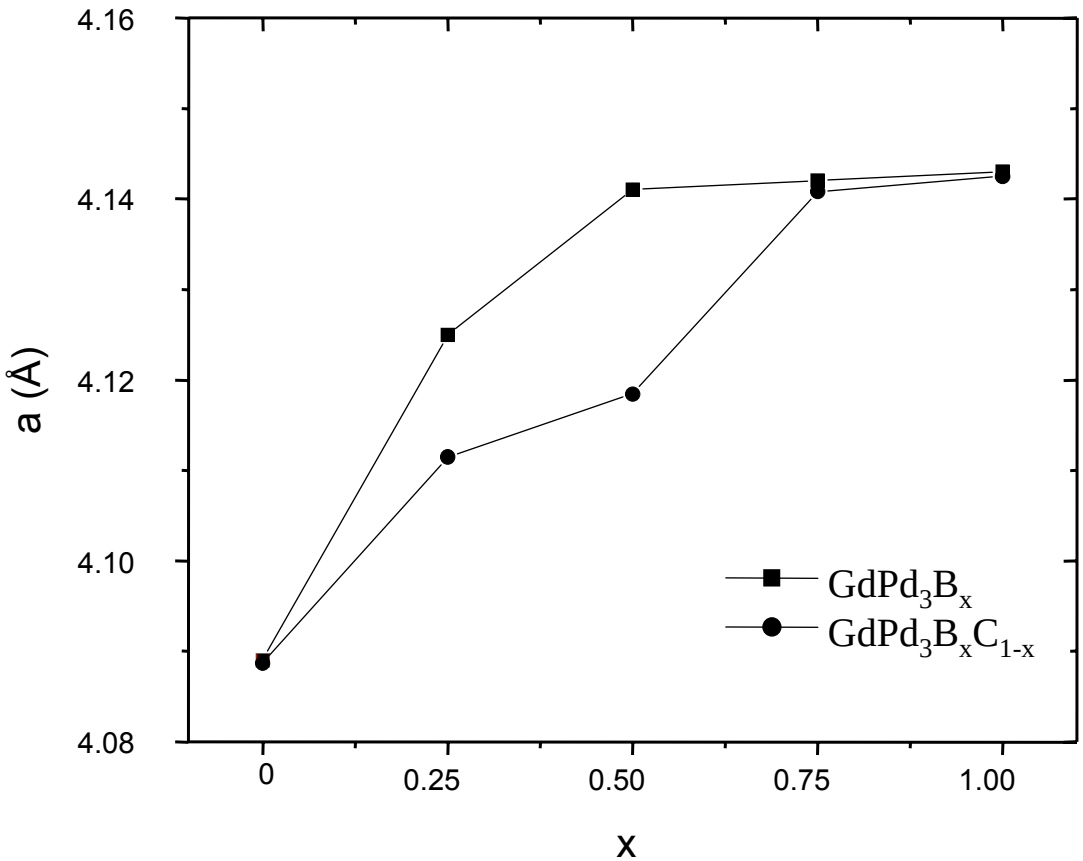
Refined parameter: lattice constant (a)



Refined parameter: instrumental parameters (u, v, w) and shape



Variation of lattice parameter with boron concentration



Thank You