Precision investigation of modern crystalline material Niobium Carbide by diffraction methods

FRANK LABORATORY OF NEUTRON PHYSICS

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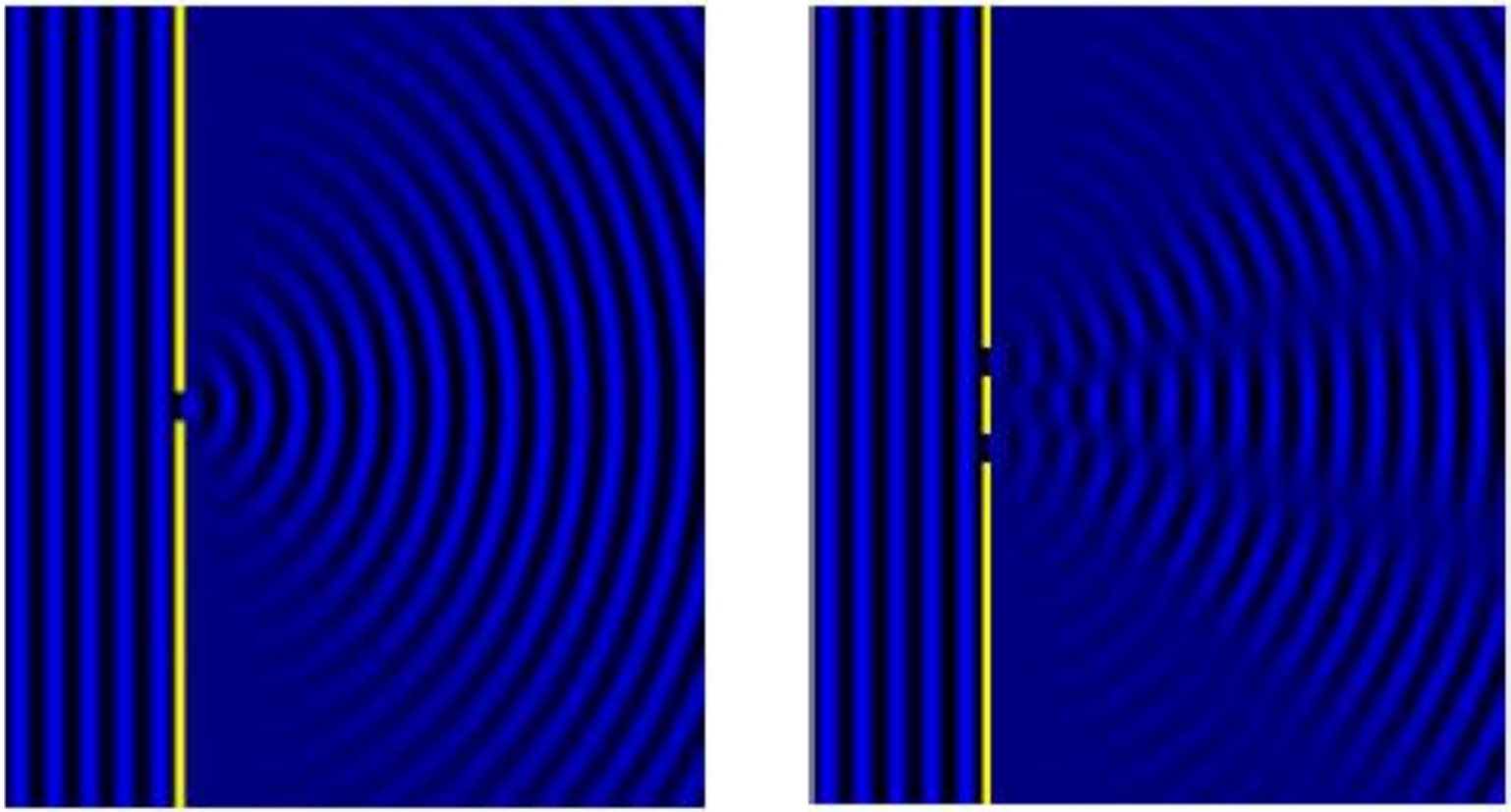
PART I
BASICS OF DIFFRACTION

SPOTOSE LIBO

Diffraction

The bending of waves after passing around small apertures/slits is called the *diffraction*.



Huygens principle

Huygens's principle is a geometric construction for using knowledge of an earlier wave front to determine the position of a new wave front at some instant.

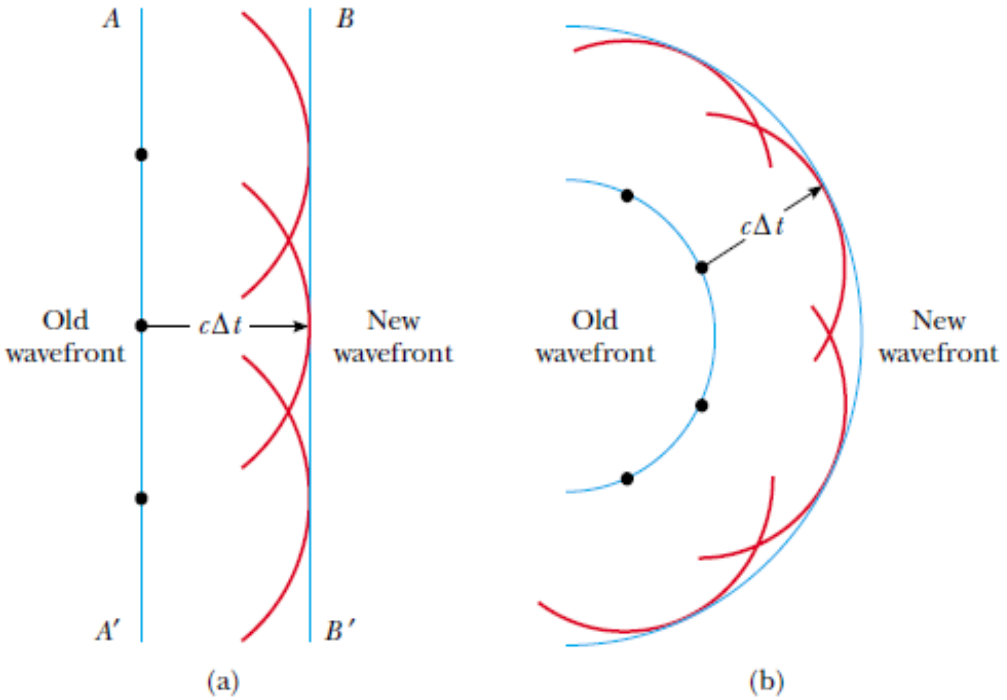
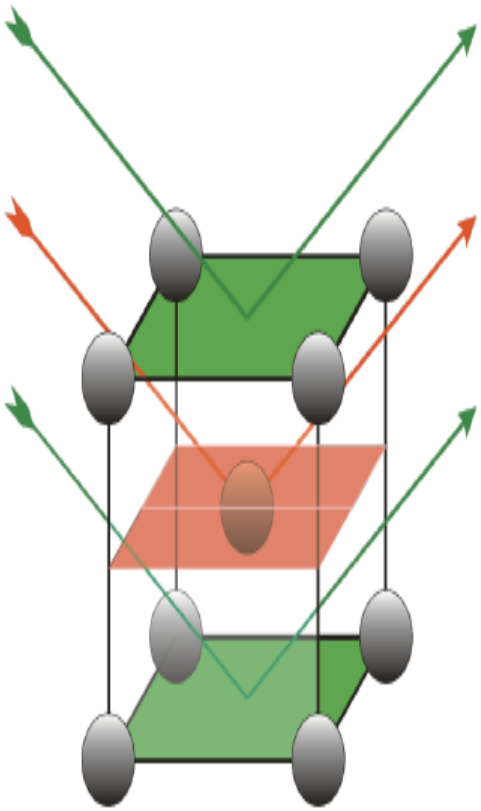


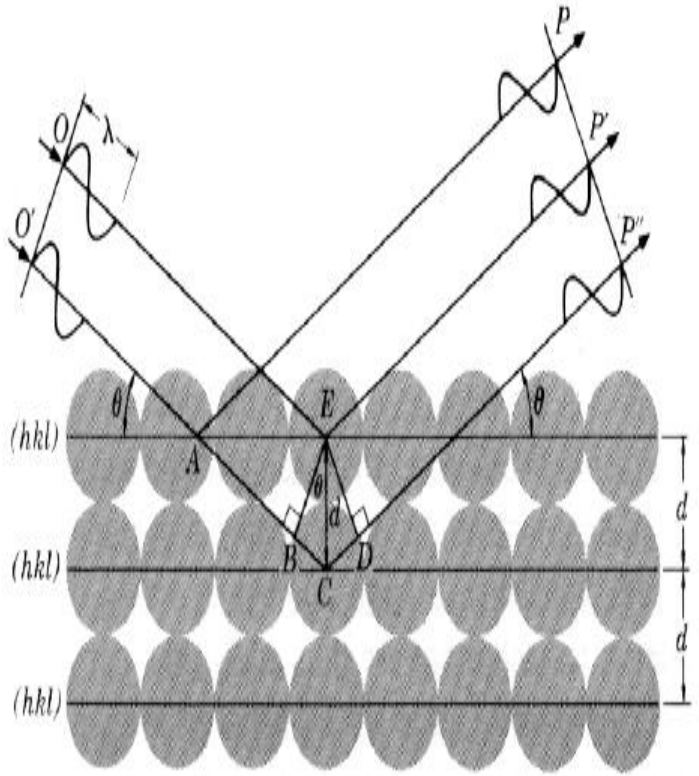
Figure 35.17 Huygens's construction for (a) a plane wave propagating to the right and (b) a spherical wave propagating to the right.

Bragg's Law

Incident beams are reflected in phase if the path difference between them equals an integer multiple of the wavelength

$$2dsin\theta = n\lambda$$





Structure factor

$\varphi = 2\pi(hx' + ky' + lz')$ the *Phase difference* between rays scattered from origin and rays scattered from the atom.

$$F = \frac{amplotude\ of\ waves\ the\ scattered\ atom\ in\ UC}{amplitude\ of\ waves\ scattered\ by\ free\ electrons}$$

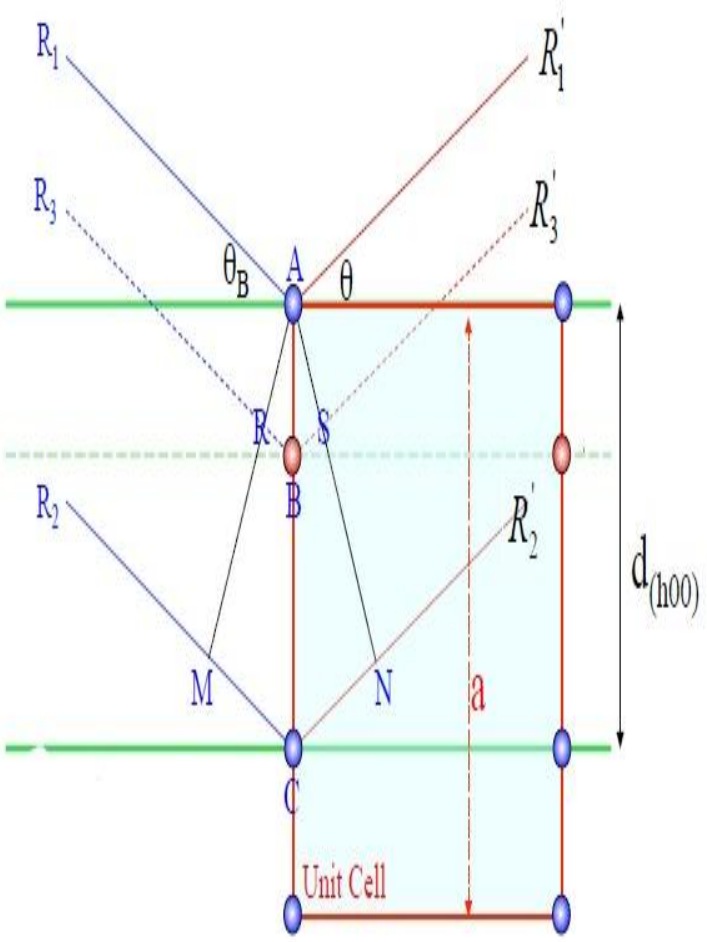
$F = \sum_{j=1}^{n} f_j e^{i\varphi_j}$ for j=1,...,n atoms in the unit cell

For x-rays f_j is an atomic form factor, f_j = f(A).

For neutrons f_j is a scattering length, $f_j \neq$ f(A).

The unit cell scattering factor is called the structure factor.

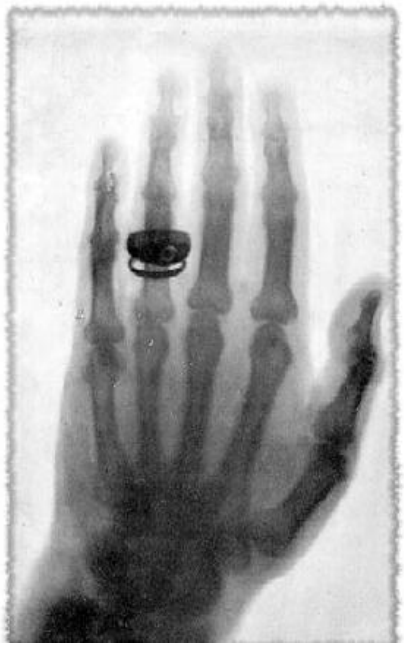
$$I = |F|^2 \delta(\vec{H}_{hkl} - (\vec{k}_i - \vec{k}_f))$$



Diffraction of x-rays

X-ray diffraction is an analytical method used to analyse the material properties like phase composition, structure, texture and many more of powder samples, solid samples and even liquid samples.

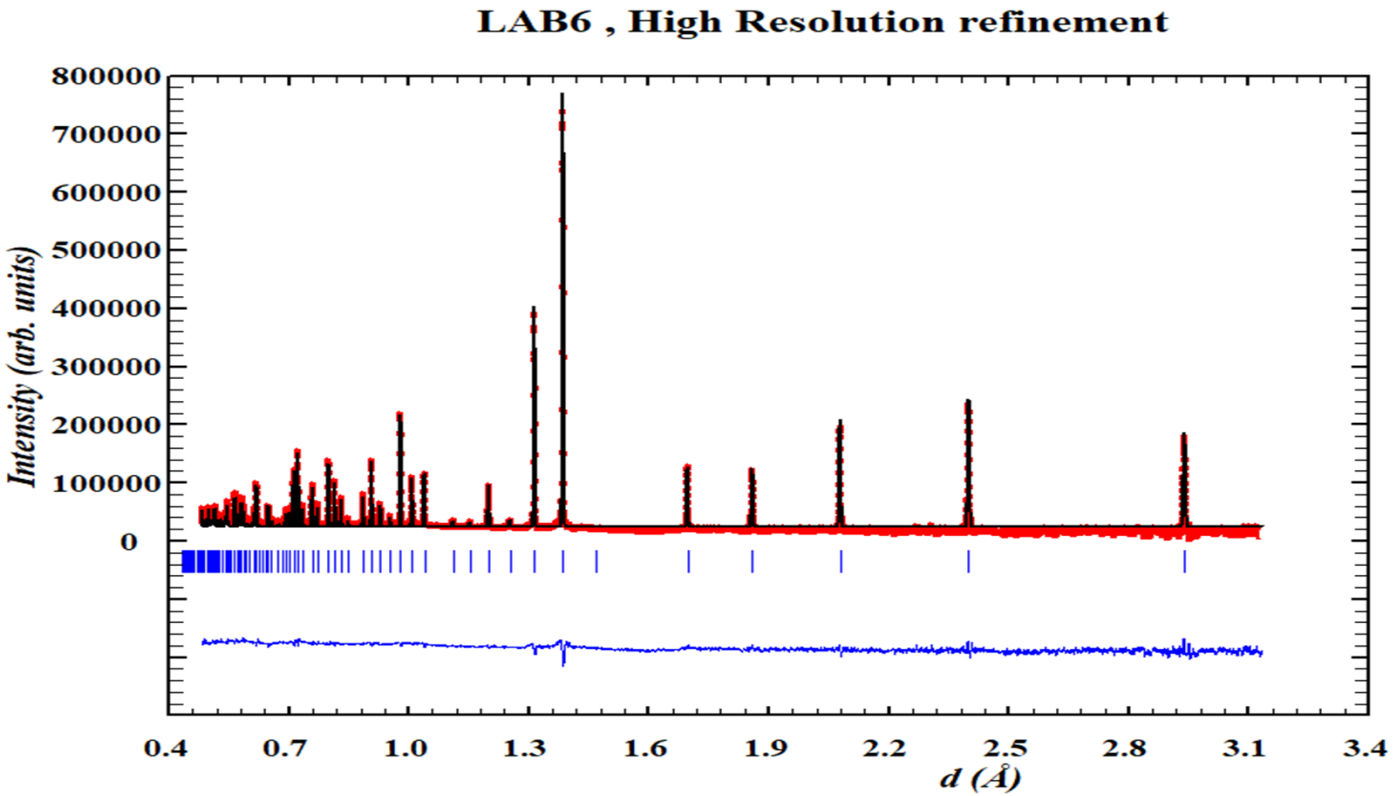
Wilhelm Conrad Roentgen, his wife's hand.



Powder diffraction

In x-ray powder diffraction the sample consists of an infinitely large number of small crystallites, ideally randomly oriented with respect to each other.

Powder diffractogram is obtained by counting the detected intensities as a function of the angle between the incident and the diffracted beam.



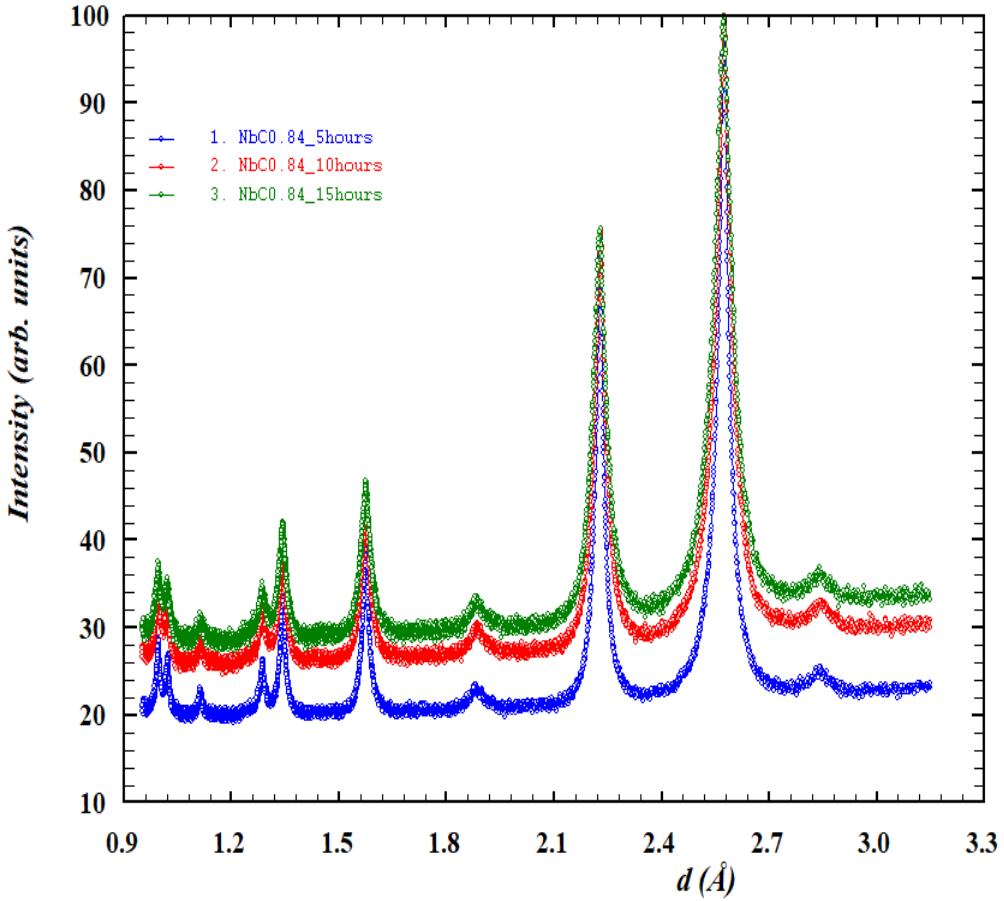
PART II CHARACTERISATION OF NIOBIUM CARBIDE BY X-RAY DIFFRACTION

Kudzai Emmanuel Sithole

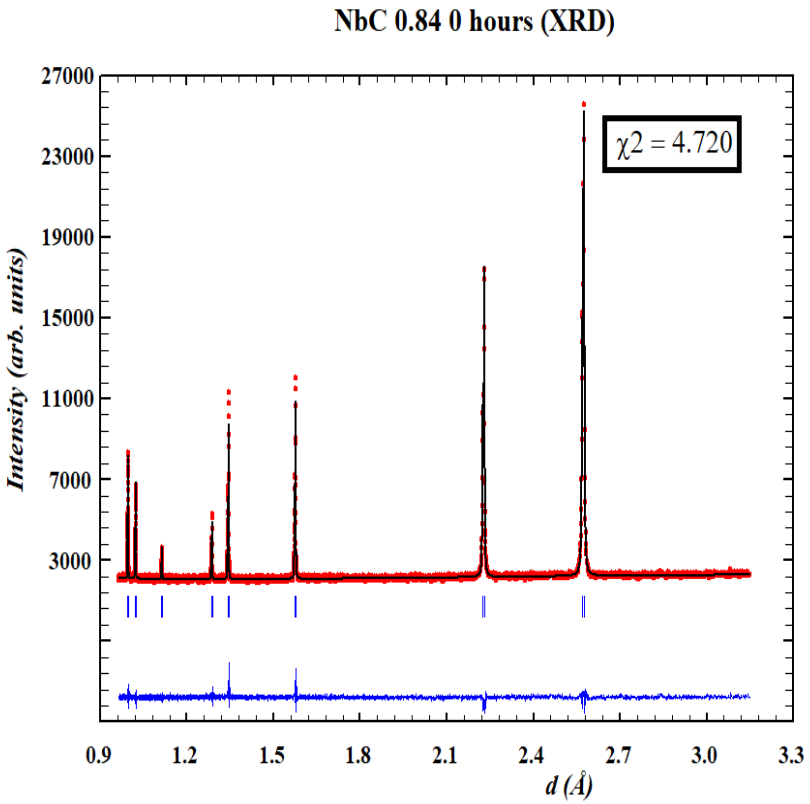
Sample and instruments

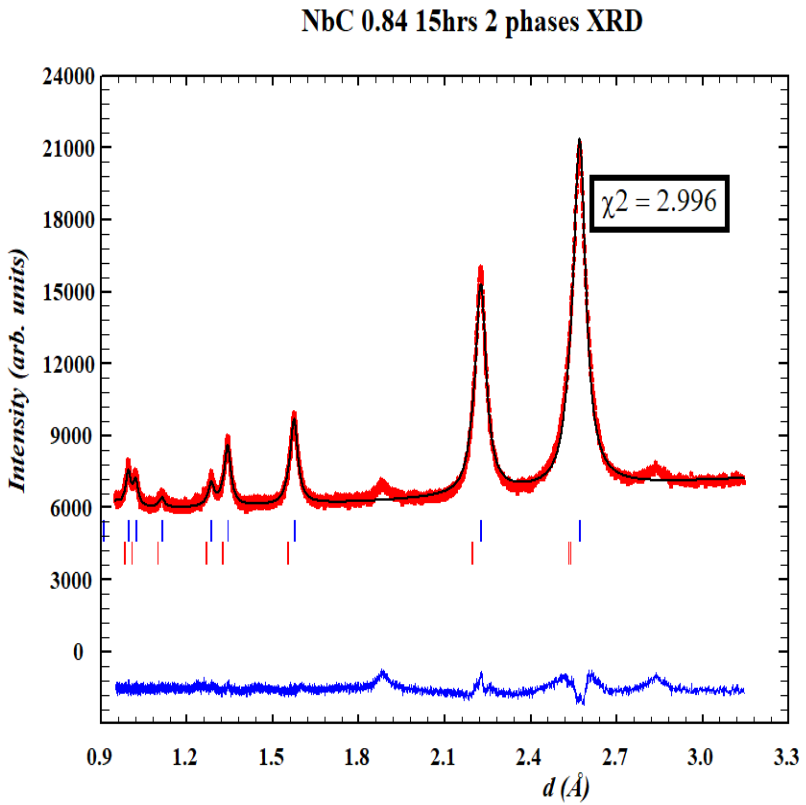
- The non-stoichiometric powder $NbC_{0.84}$ was used
- The powder was milled in a planetary ball mill for 5, 10 and 15 hours
- Panalytical X-ray diffractometer was used to obtain X-ray diffraction spectra

Comparison of the X-ray diffraction spectra

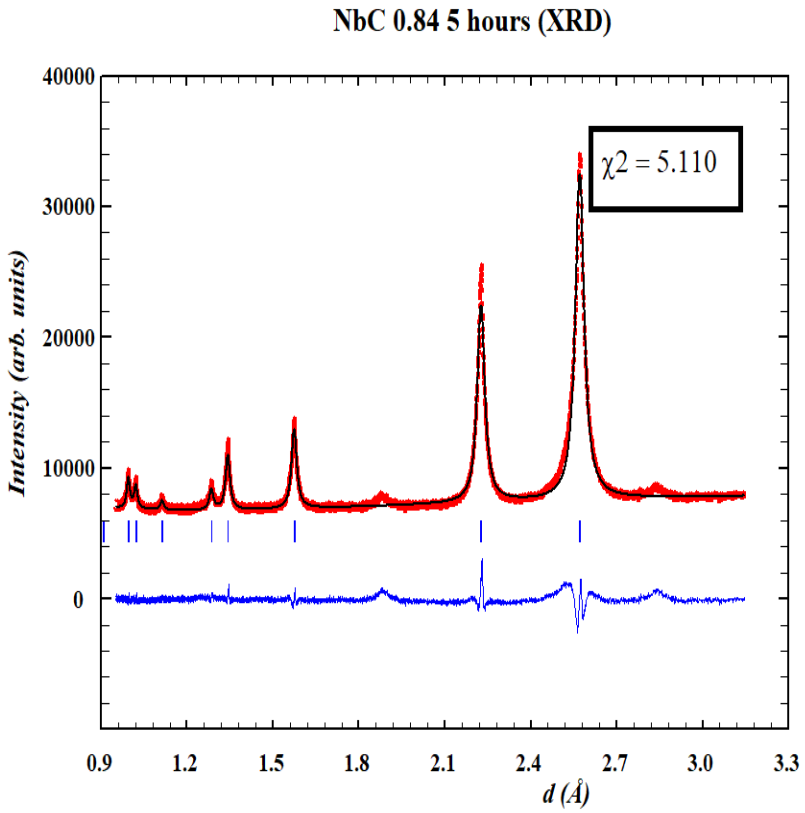


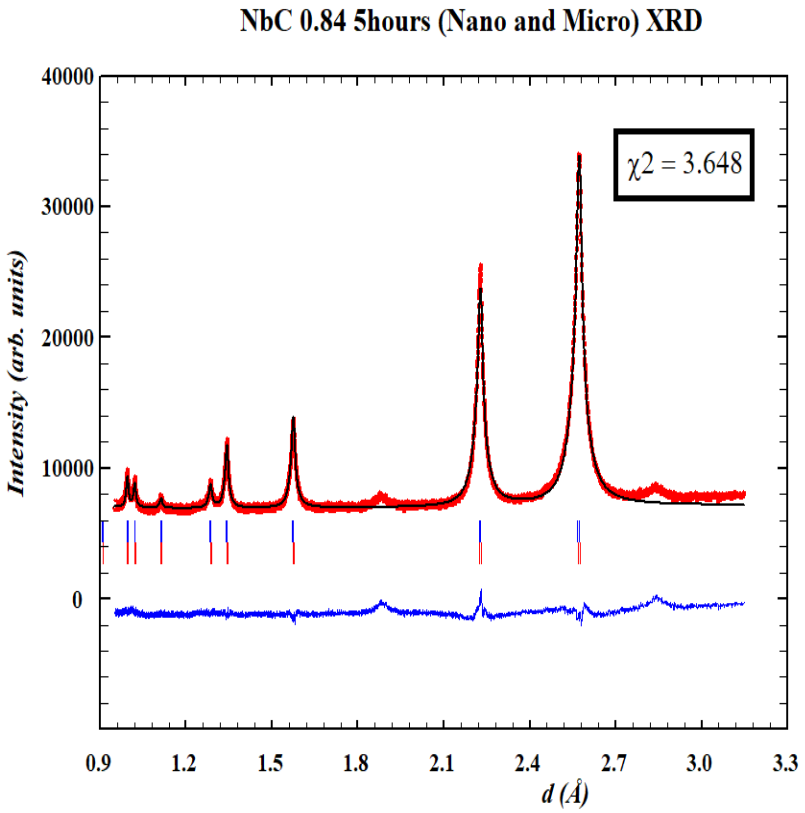
Refinement of NbC milled for 0 hours and for 15 hours with two phases



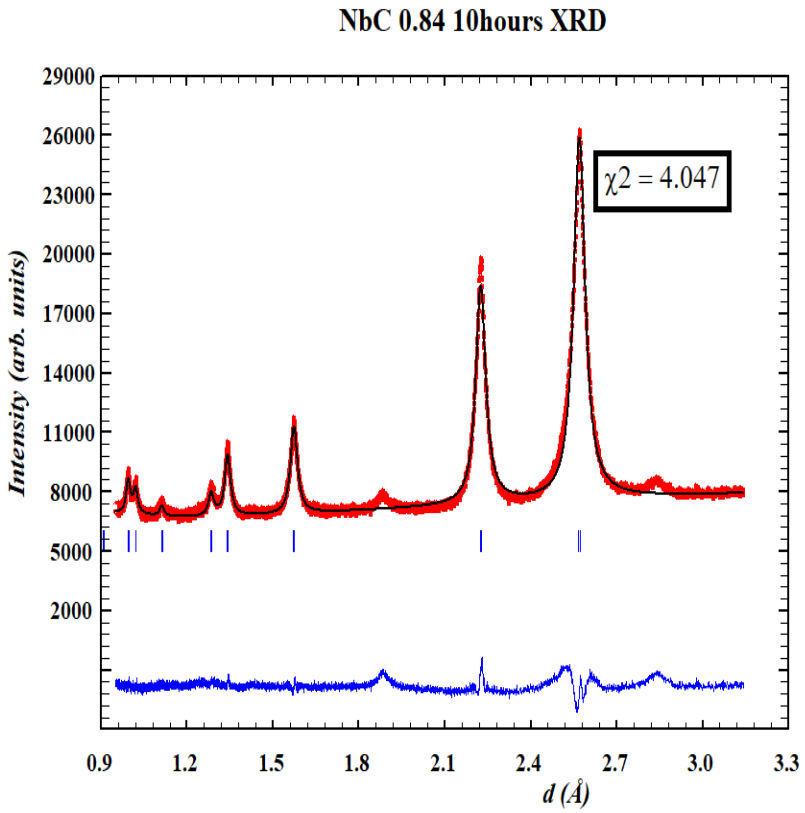


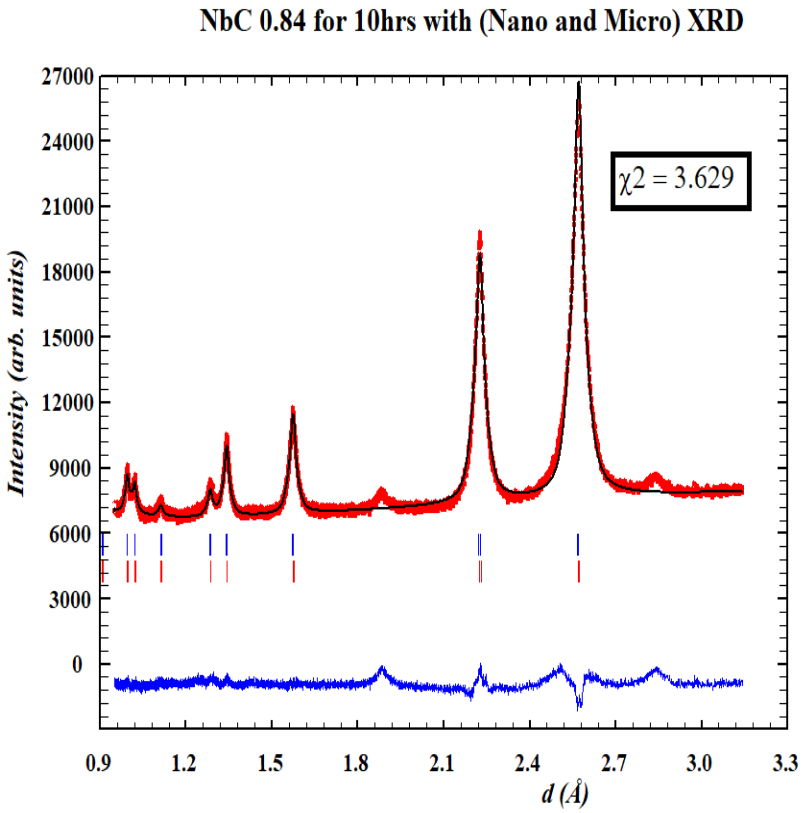
Refinement of NbC milled for 5 hours considering 1 phase and 2 phases



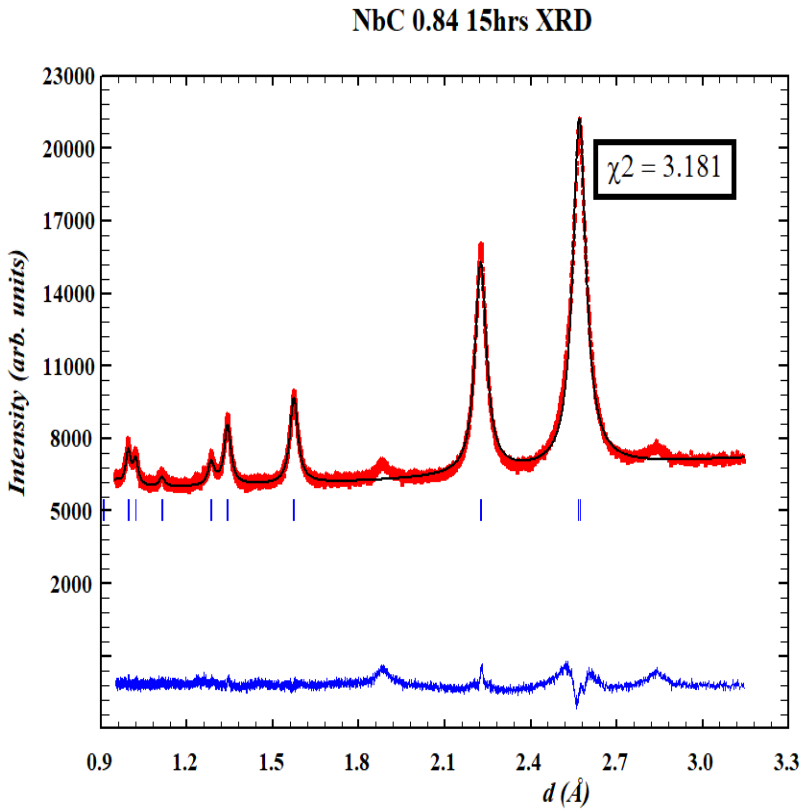


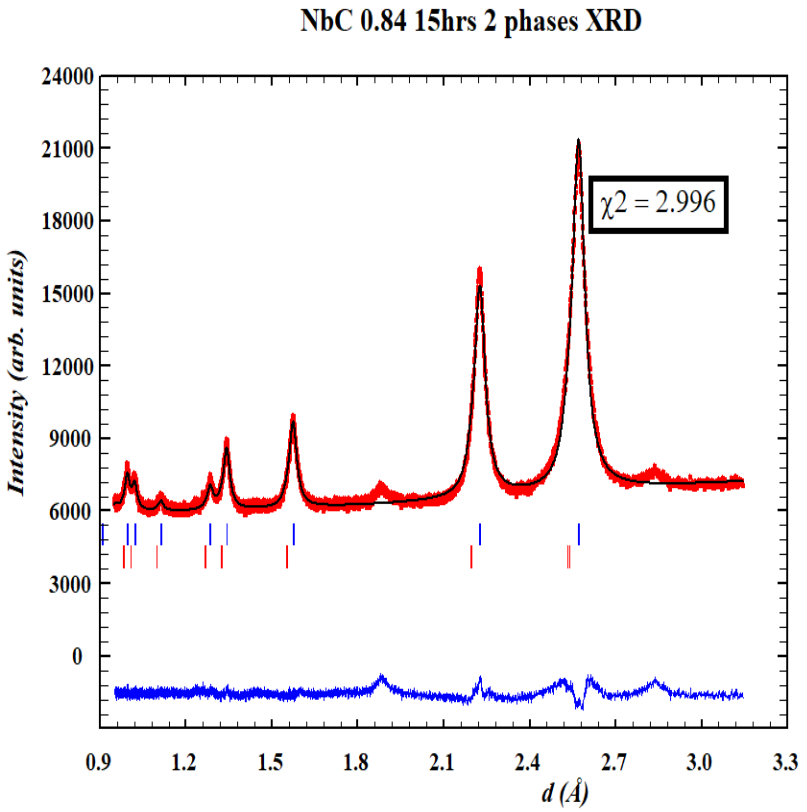
Refinement of NbC milled for 10 hours considering 1 phase and 2 phases



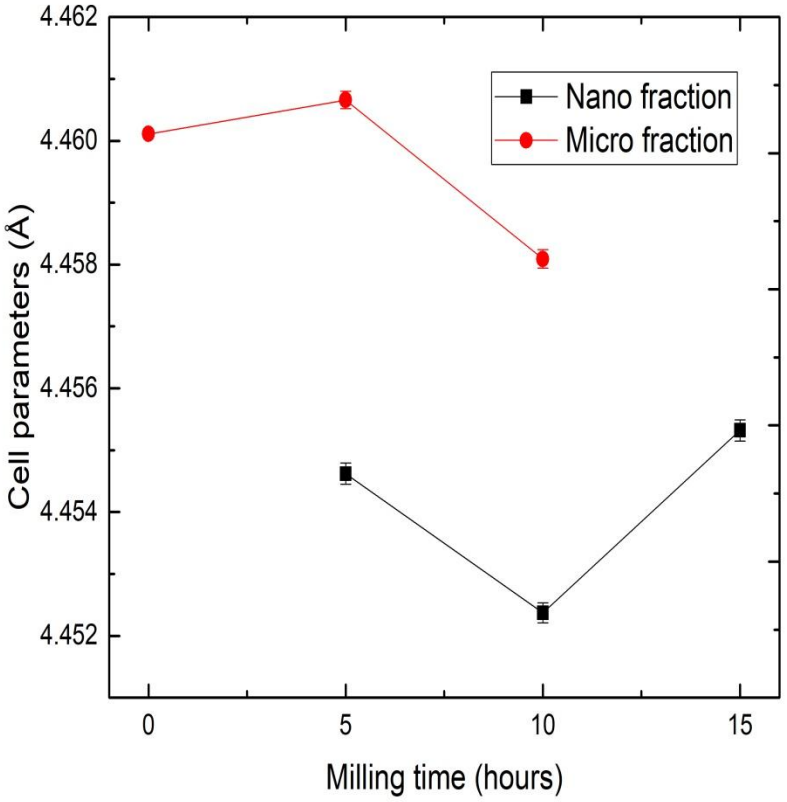


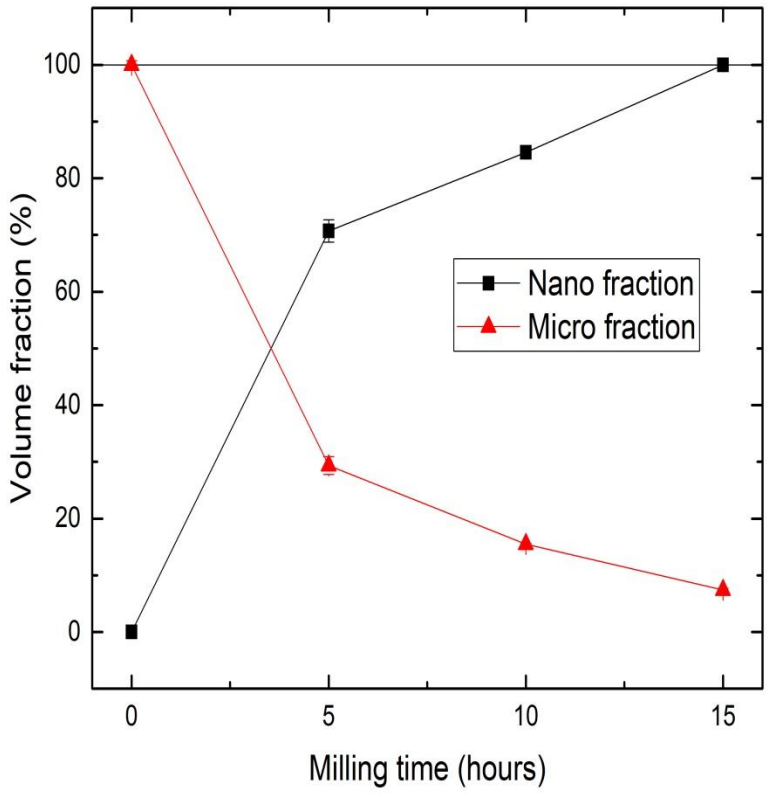
Refinements of NbC milled for 15 hours considering the 1 and 2 phases respectively





Structure parameters obtained from Rietveld refinements

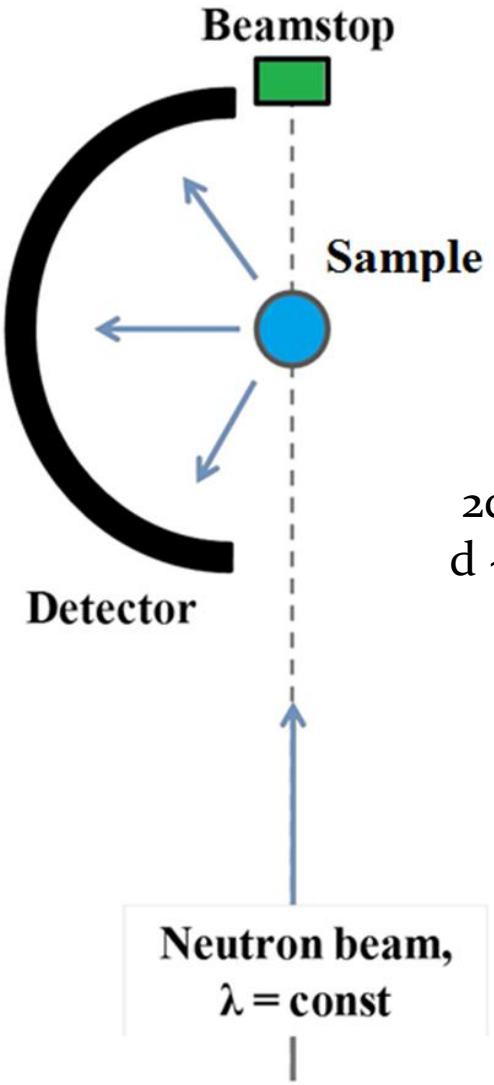




PART III
NEUTRON SCATTERING FOR NIOBIUM CARBIDE

MASHAKA MOLEPO

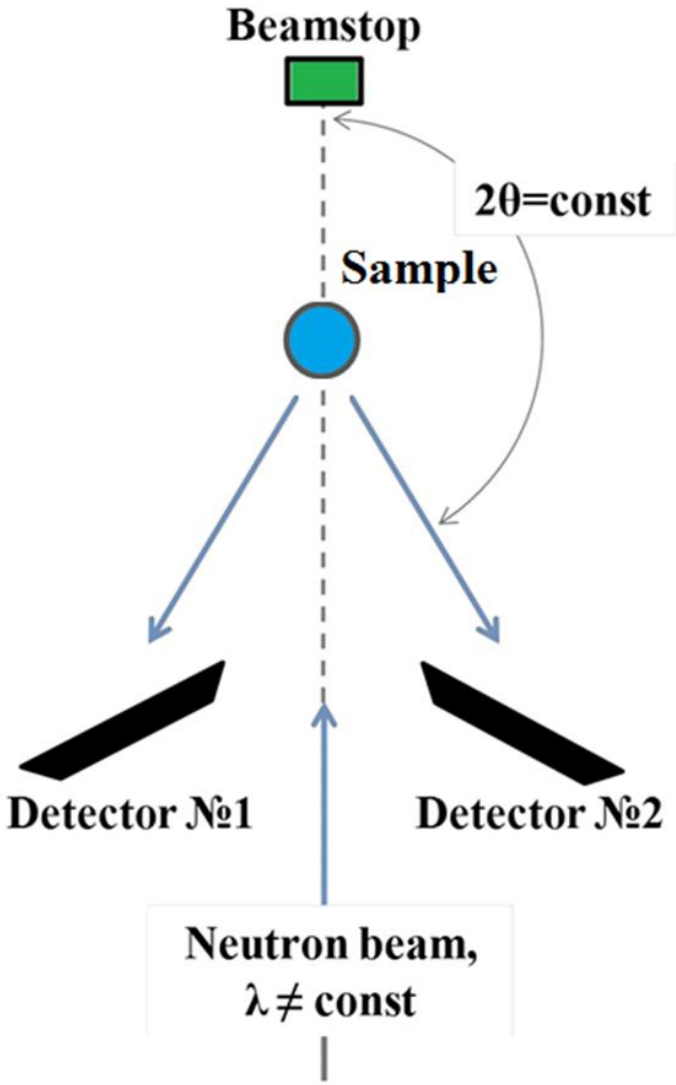
Conventional geometry



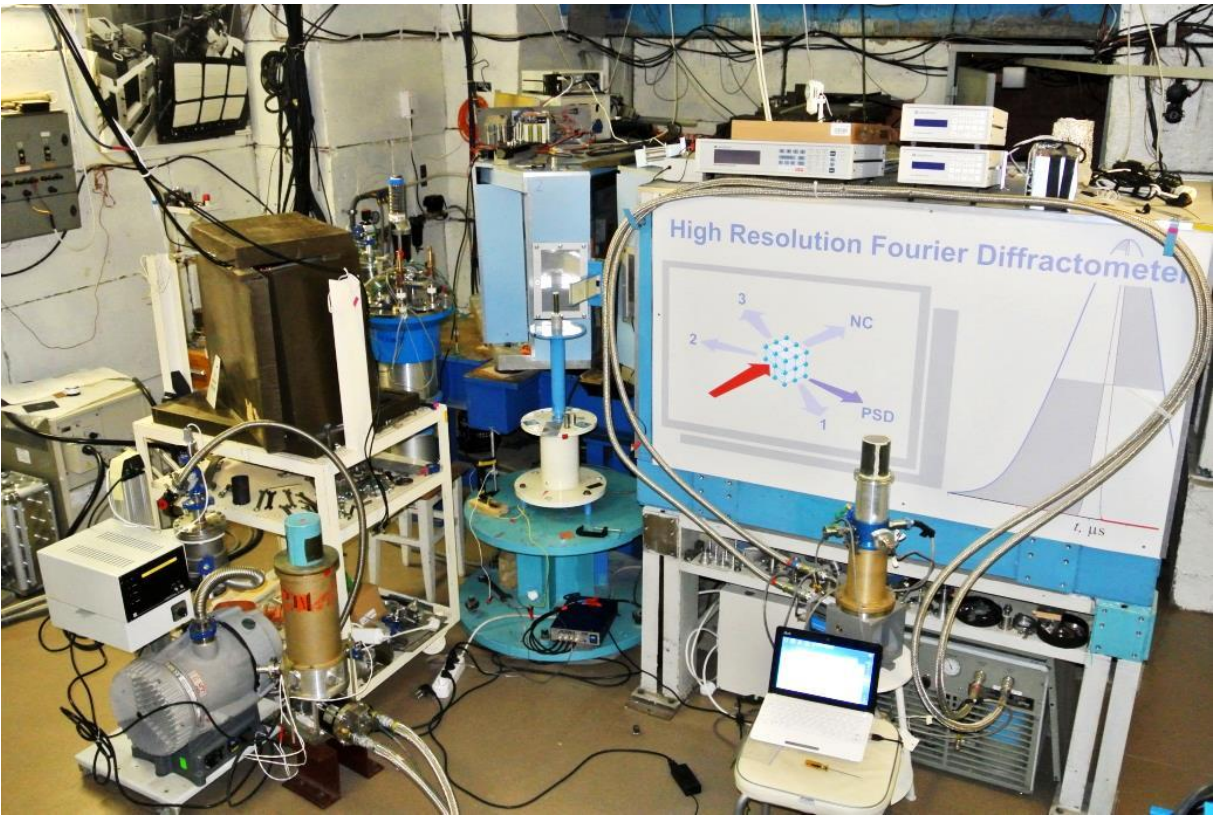
$2d\sin\theta = \lambda,$

$d \sim \lambda\,(E) \sim v = L/t$

Time-of-flight geometry

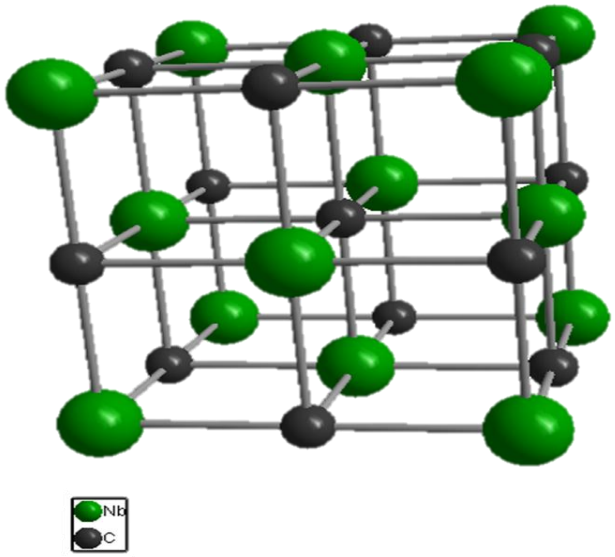


Experimental Setup and Sample

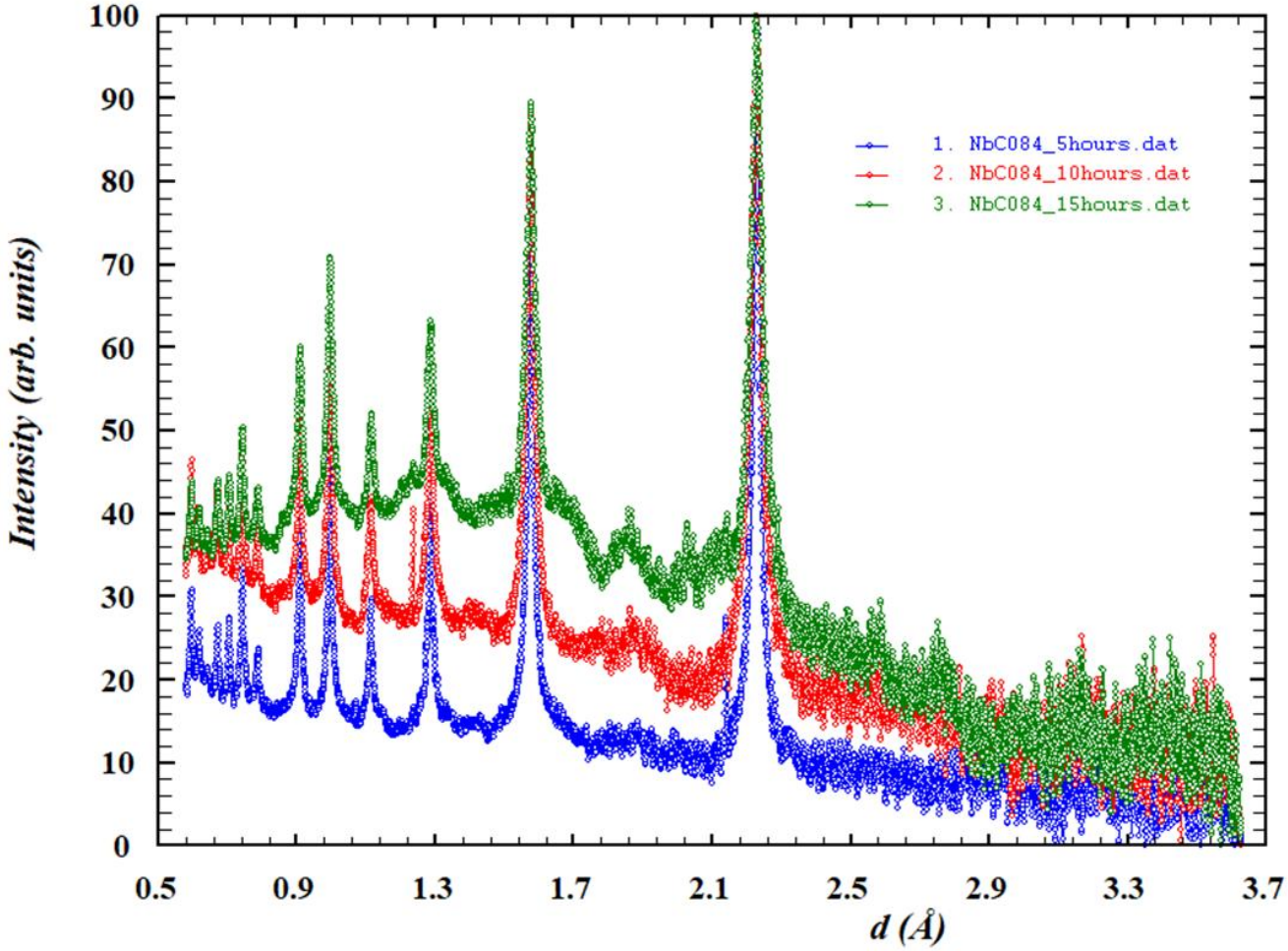


Time-of-flight high resolution fourier diffractometer installed at IBR-2 reactor. Resolution ~ 0.001, almost independent of d spacing.

Niobium Carbide $NbC_{0.84}$

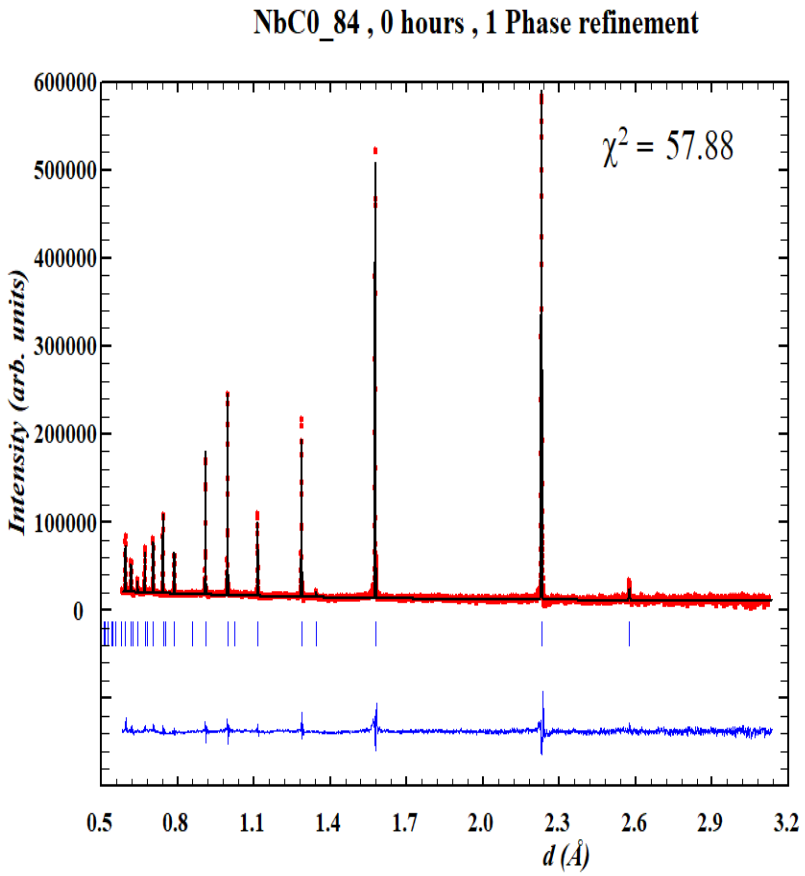


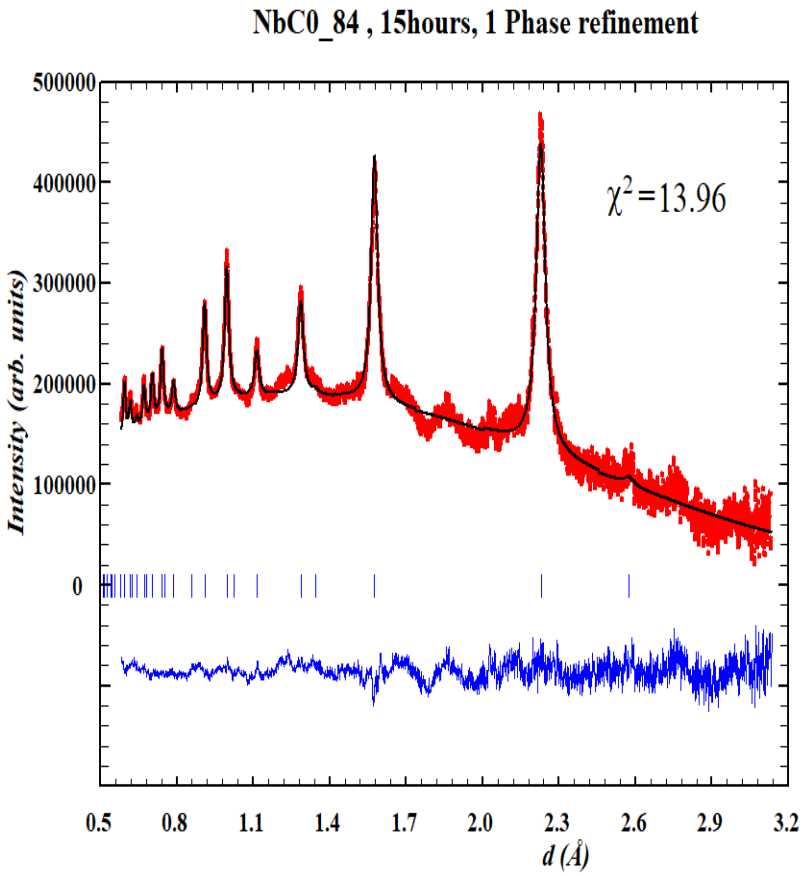
Comparison of diffraction spectra



- In $NbC_{0.84}$, defects only occur in C substructure.
- Neutrons scatter the same on Nb and C atoms while X-rays scatter mostly on Nb.
- BAD : its hard to do refinement compared to X-ray.
- GOOD : It gives more information about the sample.

Refinement of NbC milled for 5 hours in 1 phase and 2 phases





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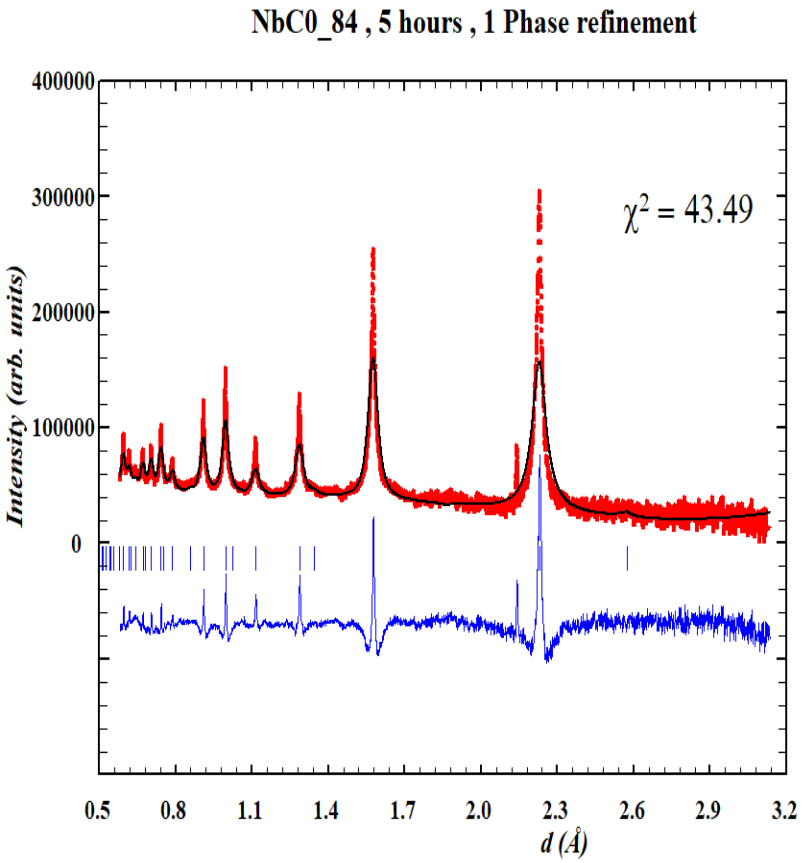
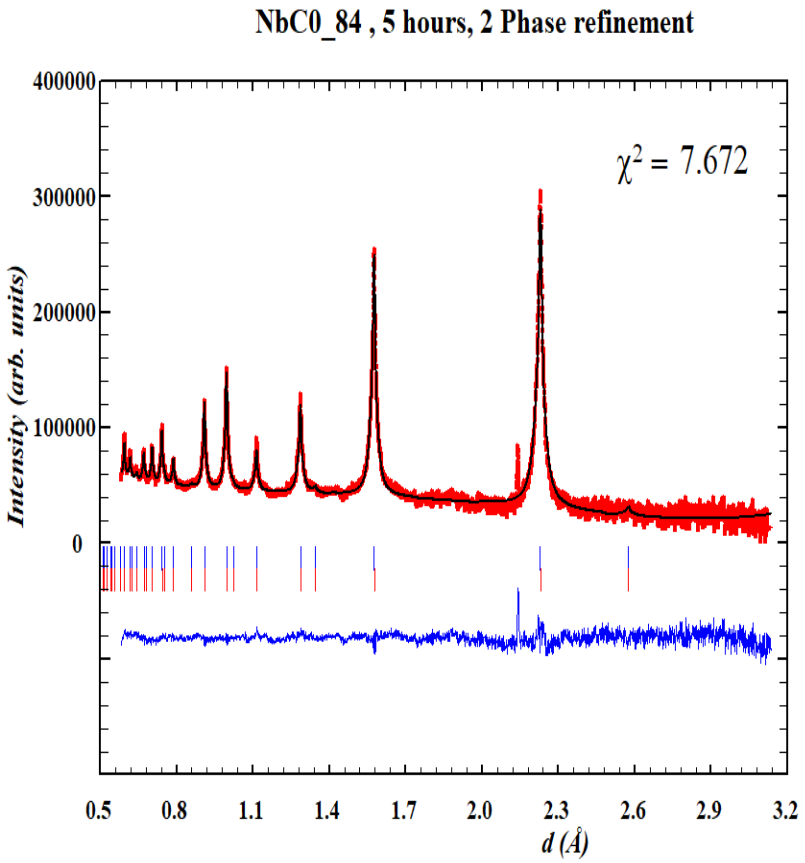
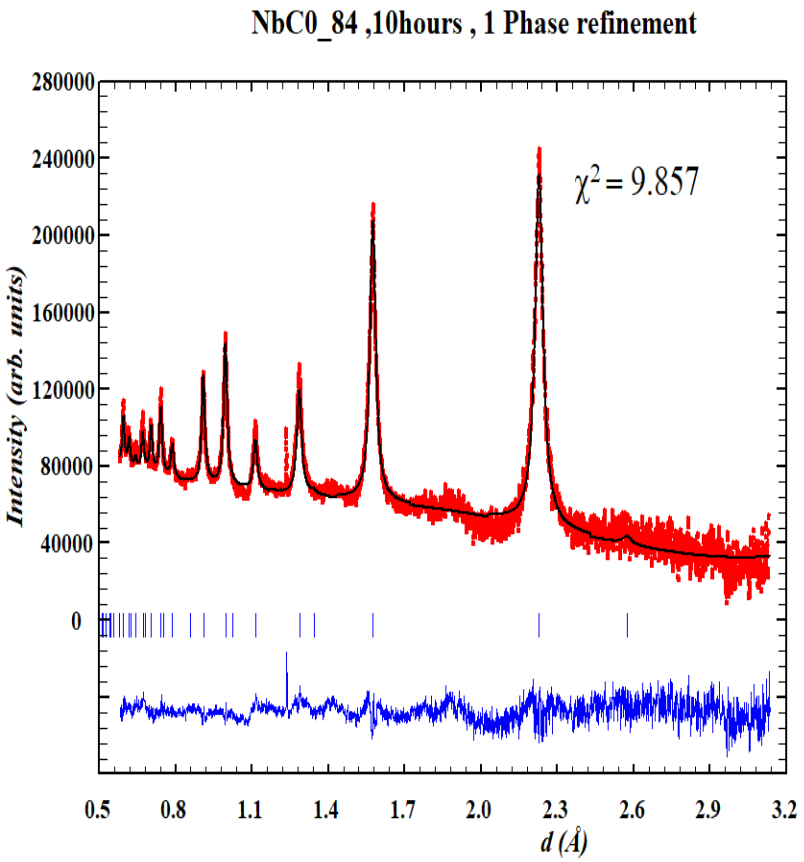
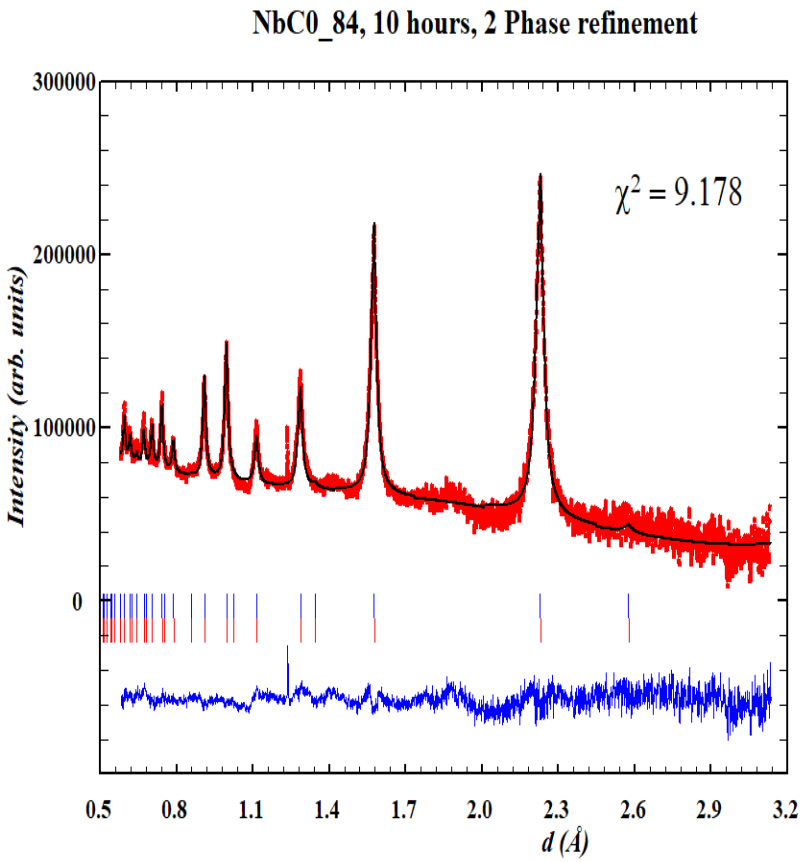


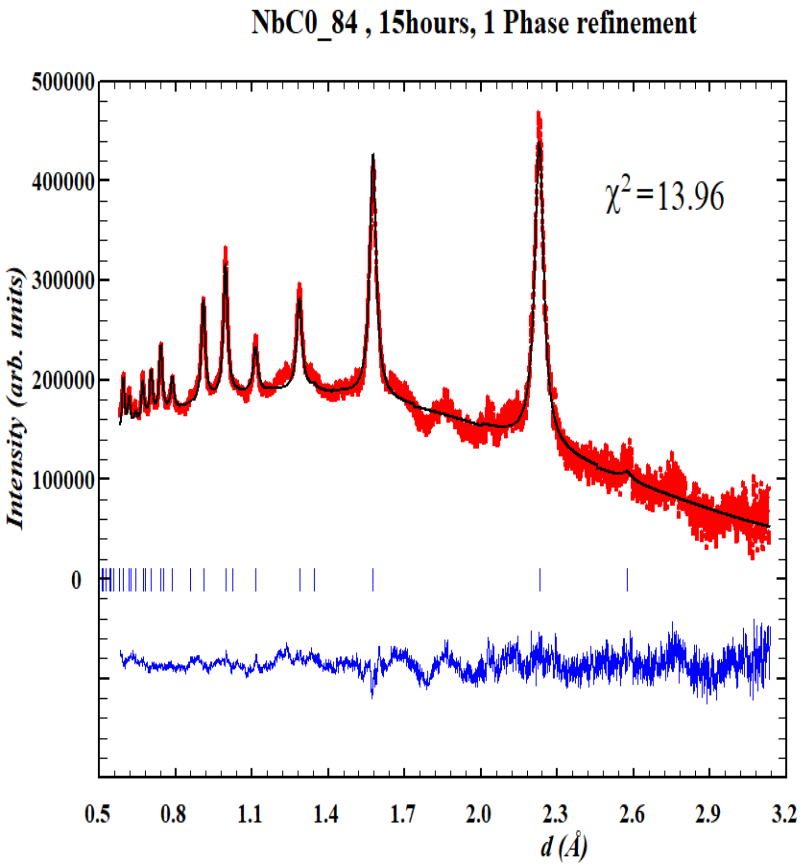


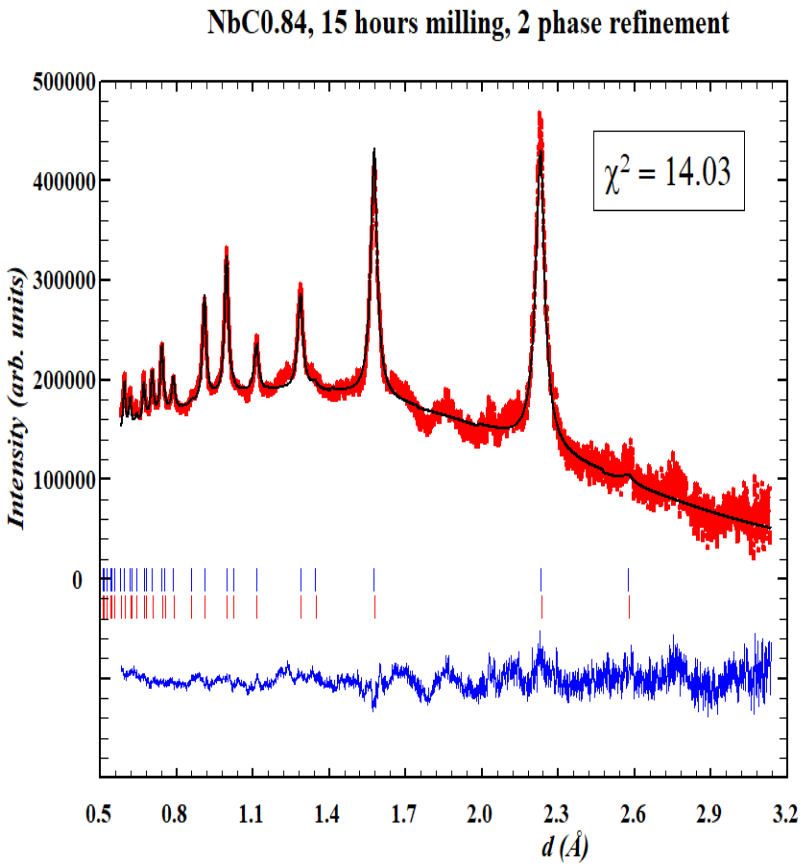
Refinement of NbC milled for 10 hours in 1 phase and 2 phases





Refinements NbC milled for 15 hours for 1 and 2 phases





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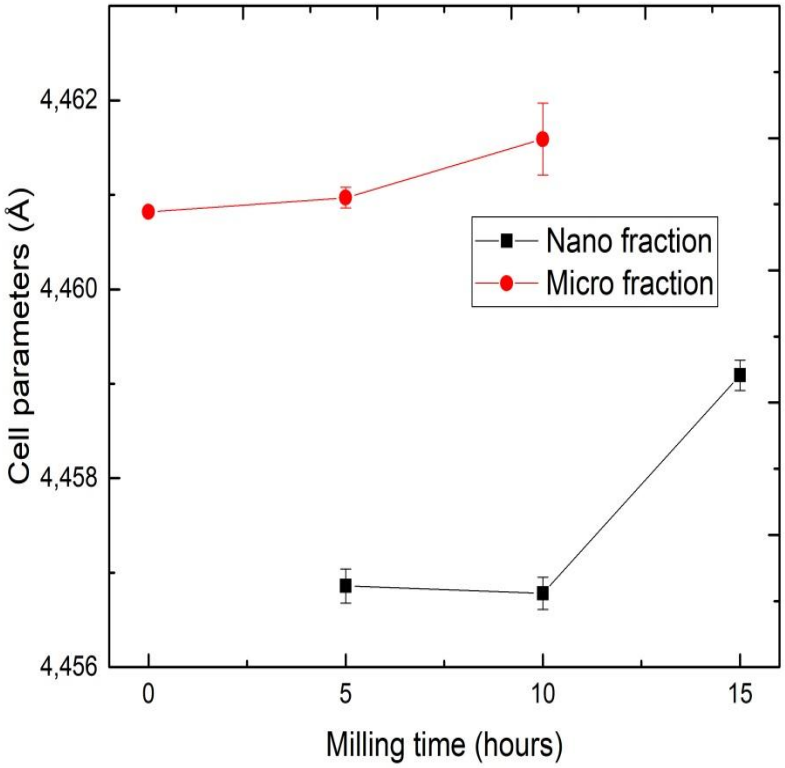

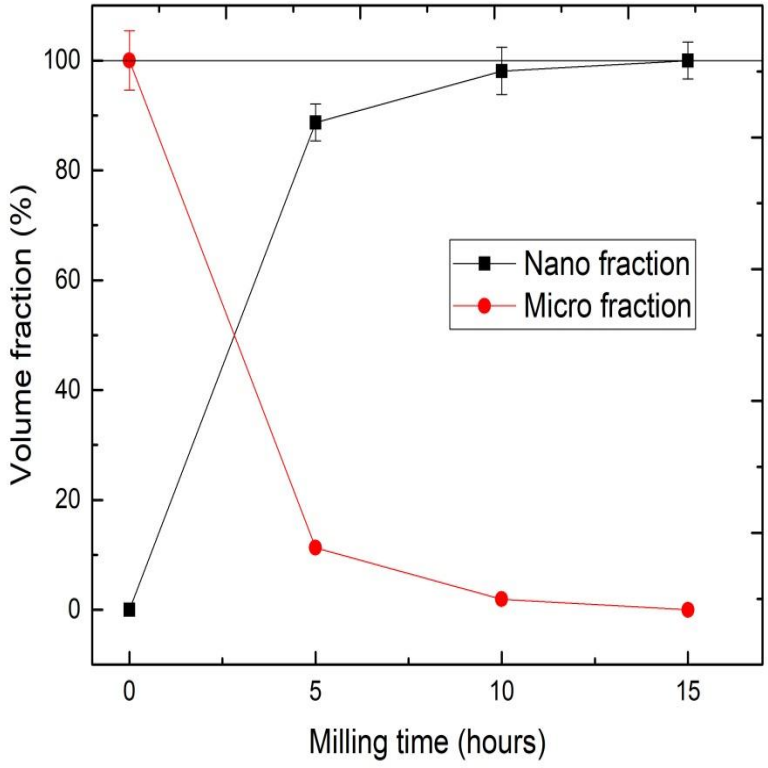

Thank you for attention!

Spasibo za vnimanie!

Ndo livhuwa chifhinga chavho!