Precision investigation of modern crystalline materials by neutron diffraction method

By : LINDOKUHLE .N.MANANA

Supervisors: Sergey Sumnikov and Ivan Bobrikov

Department of Physics: JINR, Laboratory Physics

2019

Outline

- Objectives of the project
- Introduction
- Equipment
- Results and Analysis
- Conclusion
- References
- Acknowledgements

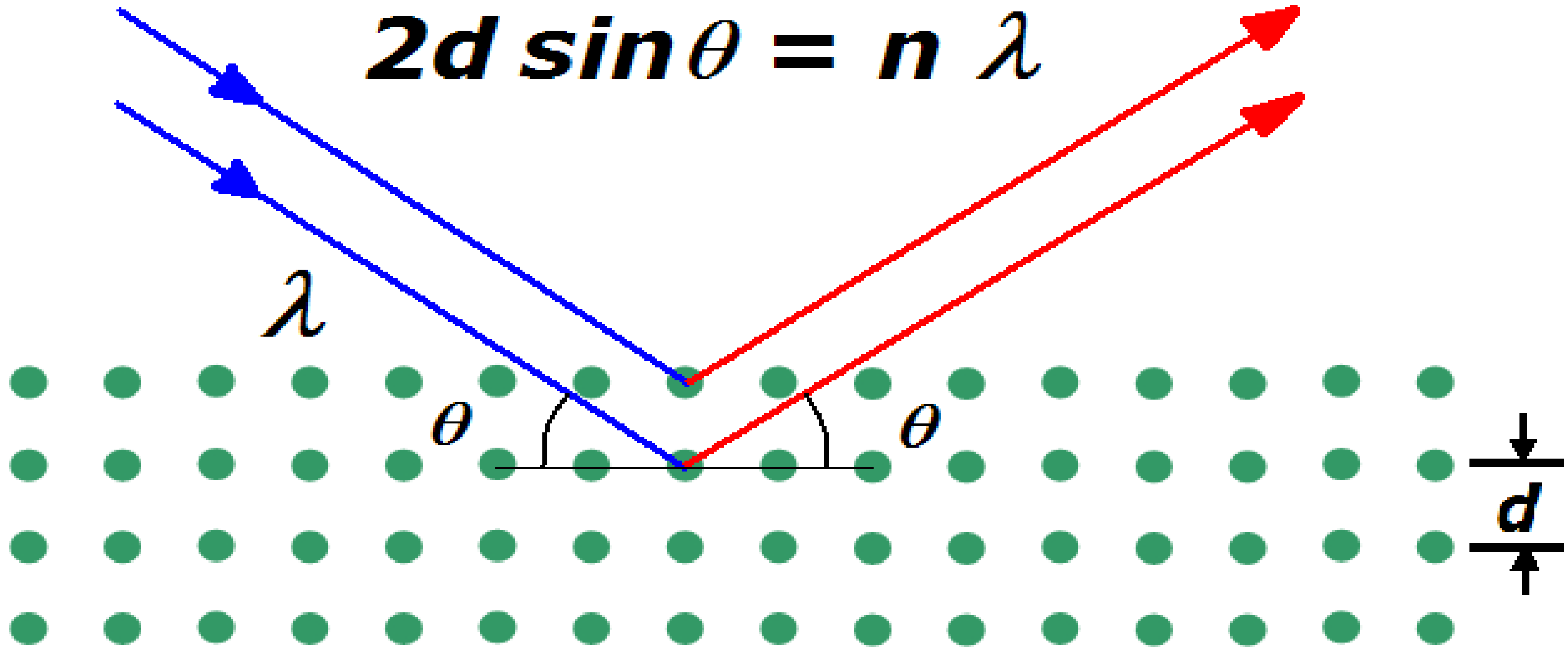
Objectives

- Is to determine the position and motion of an atom in crystal sample structure using neutron diffraction technique.
- To determine the relationship for calculating temperature of sample using diffraction pattern.

Introduction

- Neutrons have high penetration for most elements making neutron scattering a bulk prob.
- High scattering bounce away from nucleus based on brag's law of diffraction.
- Neutron scattering is a technique of choice for studying condense matter
- When the beam of monochromatic is directed to sample it diffract at an angle
- The respond of each grain orientation (hkl) provide distinct peaks
- Neutron have low flux and high cross section area so the information about crystal structure is very specific and useful.

Introduction (cont.)



D= interplaner spacing

n= order of interference

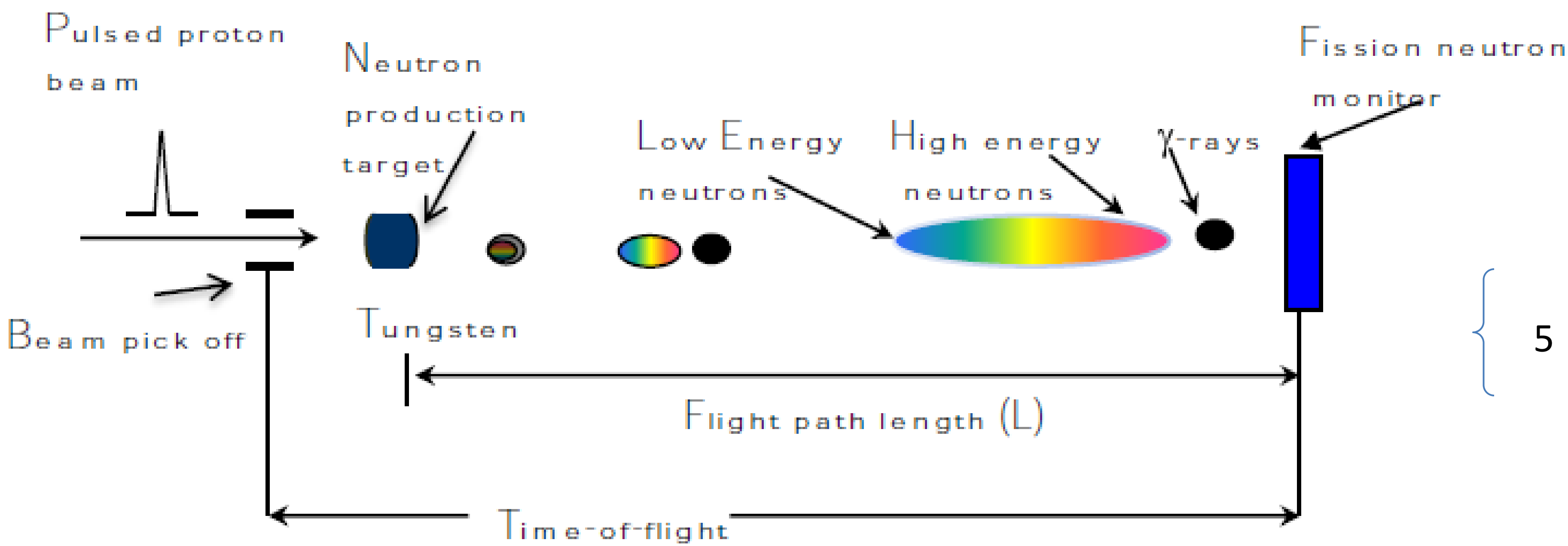
Ө= Bragg angle

λ= wavelength

Neutron diffraction v.s X-ray diffraction

NEUTRON DIFFRACTION	X-RAY DIFRACTION
Neutron particles have magnetic moment, it can be use to study magnetic structure	X-ray does have magnetic moment so you can not use to study magnetic structure
Neutron diffractometer is a complex machine so it more expensive to access it	X-ray have good availability
Neutrons scattered from nuclei and every isotopes have different scattering length, it depends on scattering length.	X- ray scattered from electrons ,so it contains scattering from electron cloud

Time of flight technique



5

Neutron TOF $= \dfrac{72.3\,L}{\sqrt{E_n}}$ (non-relativistic) γ-ray TOF $= \dfrac{L}{c}$ c is velocity of light

Example: $L = 20\,m$ $TOF_\gamma = 67\,ns$ $E_n = 1\,MeV$ $TOF_n = 1.5\,\mu s$

$E_n = 100\,MeV$ $TOF_n = 150\,ns$

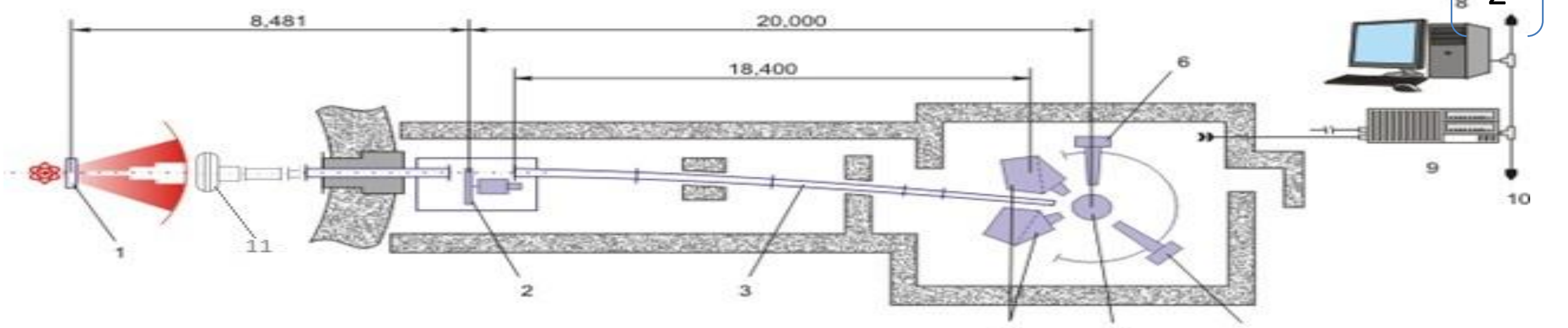
science & technology
Department: Science and Technology REPUBLIC OF SOUTH AFRICA

JOINT INSTITUTE JINR FOR NUCLEAR RESEARCH

NRF National Research Foundation iThemba LABS Laboratory for Accelerator Based Sciences

High Resolution Fourier Deffractometer(HRFD)

2



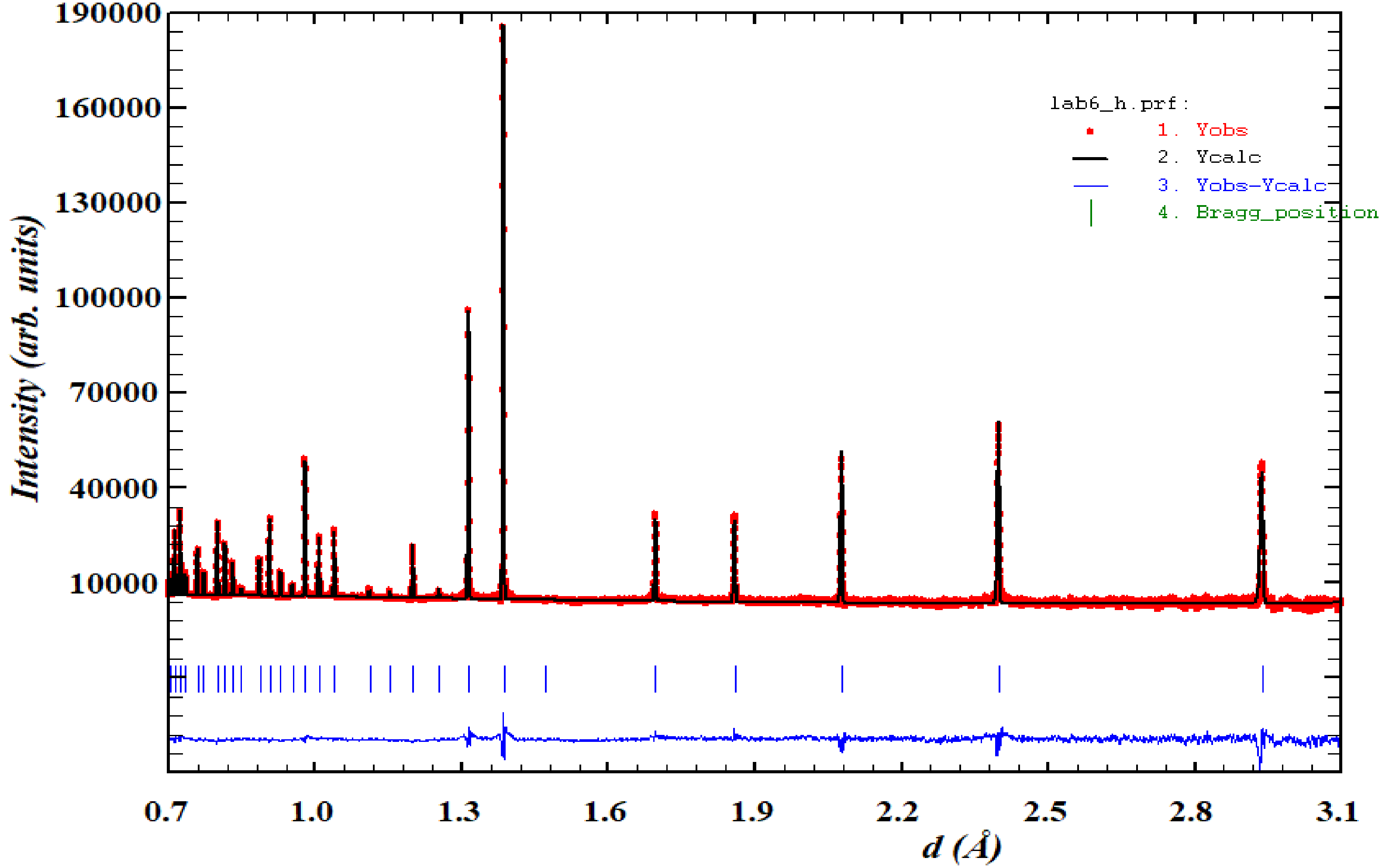
1 – Moderator
2 – Fourier Chopper
3 – Guide Tube
4 – Main Detector
5 – Sample Position
6 – 90°-Detector
7 – PSD Detector
8 – VME Control and Operative Visualization/Analysis
9 – VME Station (OS/9) Data Acquisition
10 – EtherNet Data Transfer
11 - Background chopper

High Resolution Fourier Diffractometer

HRFD

- It was commissioned at the IBR-2 pulse reactor
- It users fast Fourier chopper for modulating primary beam neutron intensity
- It as uses correlation method for data acquisition and has high resolution of about (0.001)
- Flight path between chopper and sample is approximately (20 m).
- The resolution and neutron flux is the most vital parameters in diffractometer experiment.

LaB6 , T=293 K, HRFD-Dubna



science & technology
Department: Science and Technology REPUBLIC OF SOUTH AFRICA

JOINT INSTITUTE FOR NUCLEAR RESEARCH JINR

NRF National Research Foundation

iThemba LABS Laboratory for Accelerator Based Sciences

Furnace

Temperature calibration

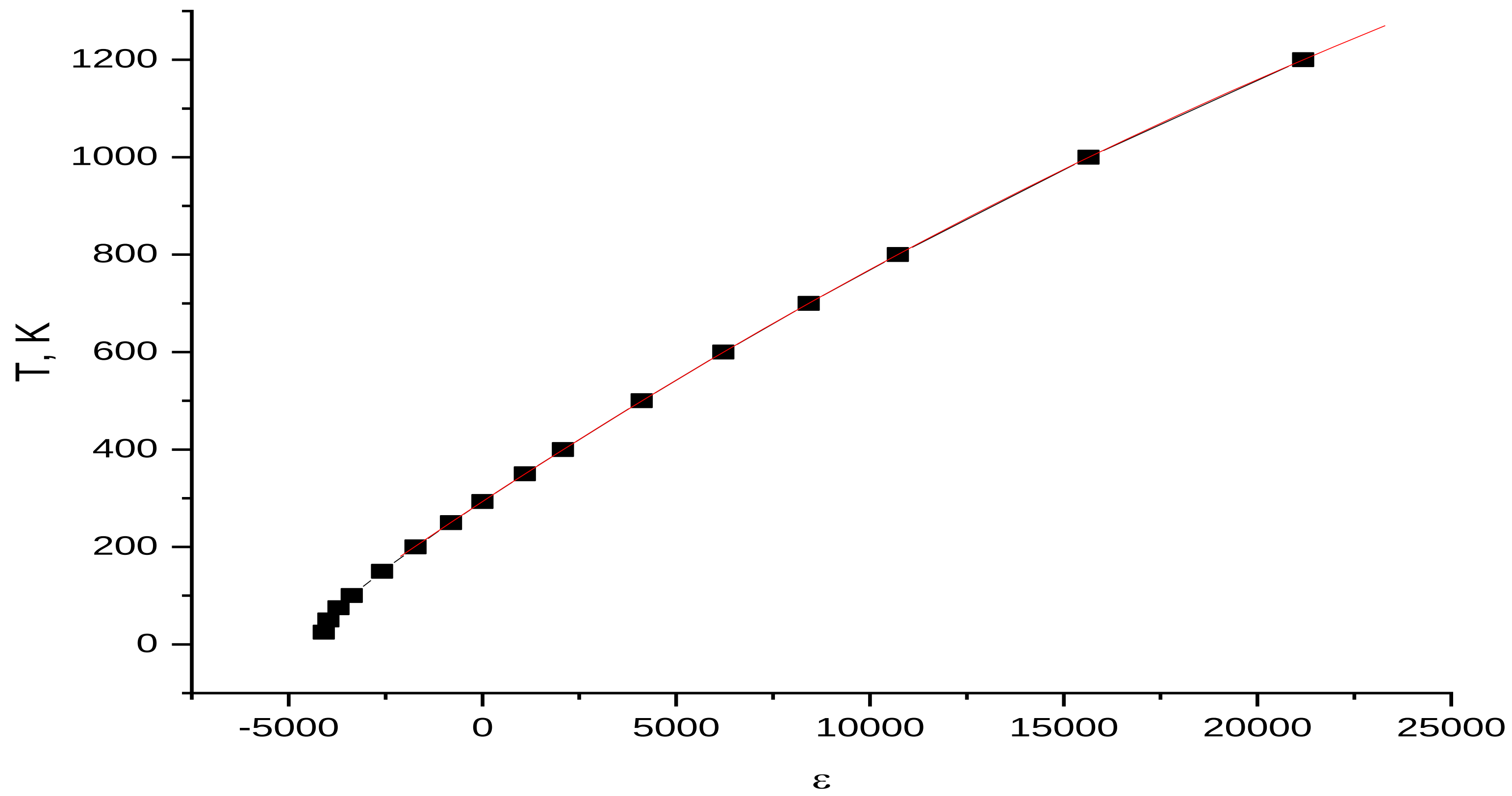
Collect sequence of diffraction patterns for **Silver** .

- Refine unit cell dimensions as a function of temperature
- Calculate ε
- Calculate real T using polynomial coefficients

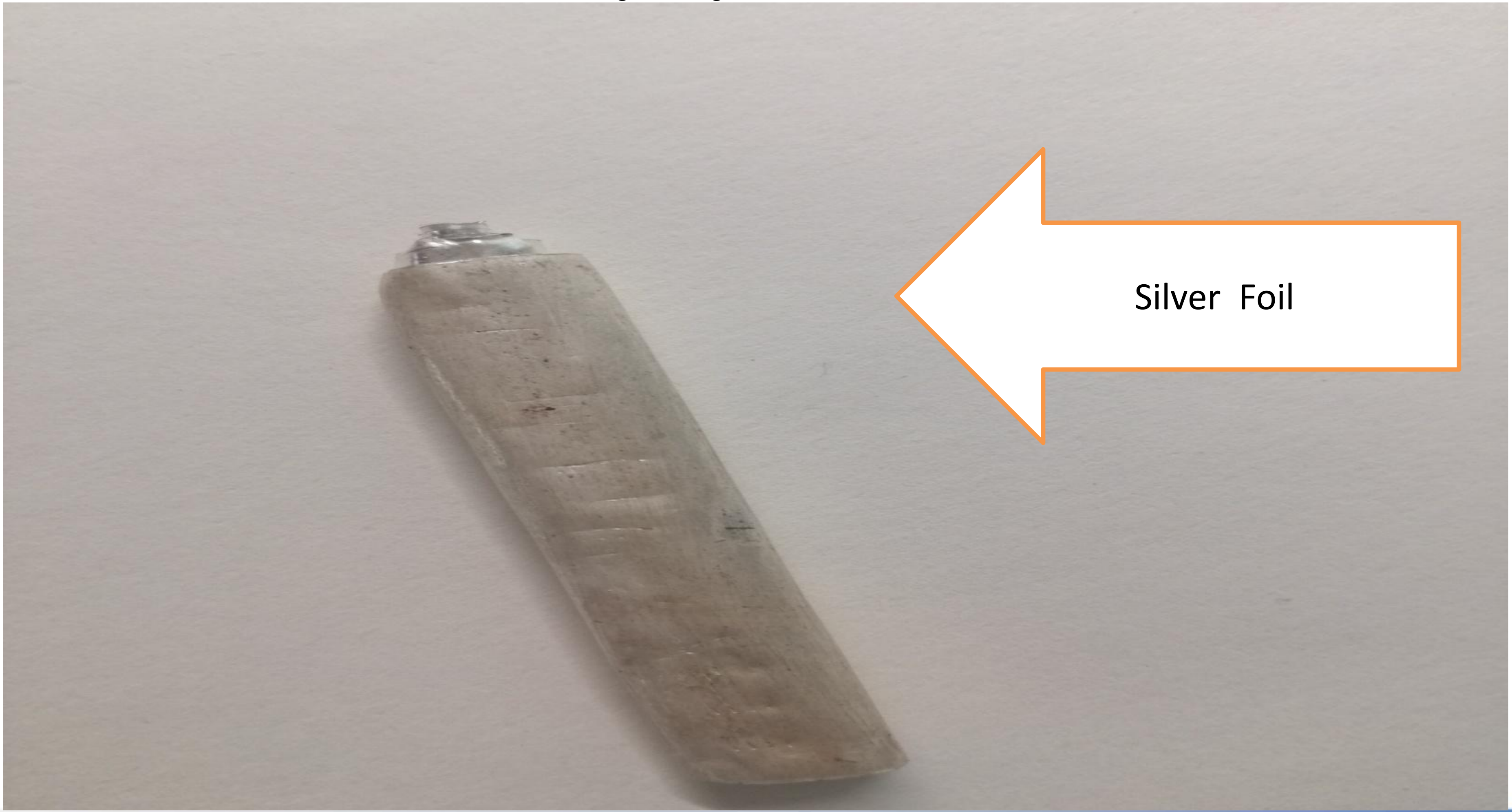
$$\varepsilon = \frac{a - a_{20}}{a_{20}}$$

calibration

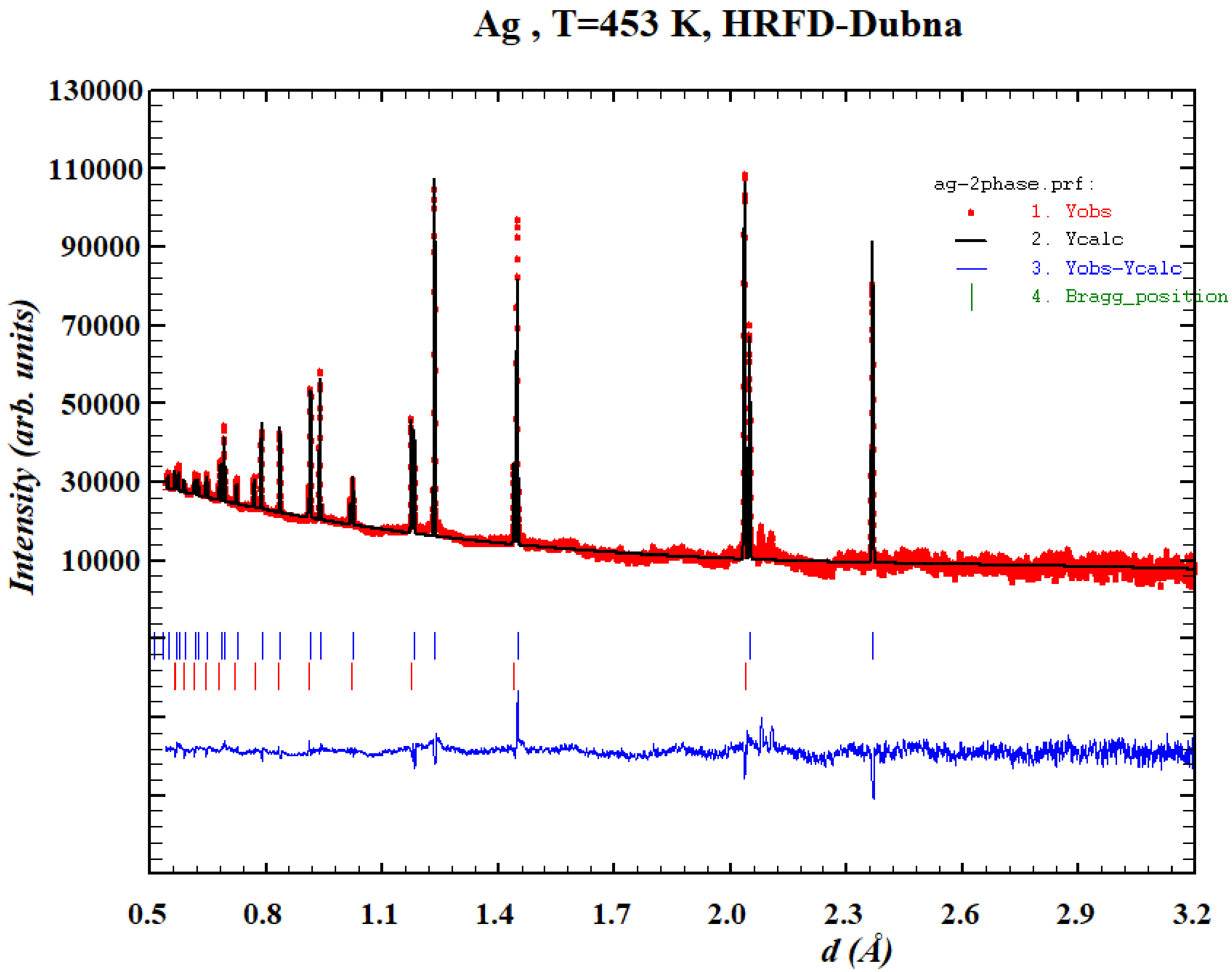
$$T = 293.21939 + 0.05216\varepsilon - 4.63693E\text{-}7\varepsilon^2 + 1.07258E\text{-}12\ \varepsilon^3$$



Equipment



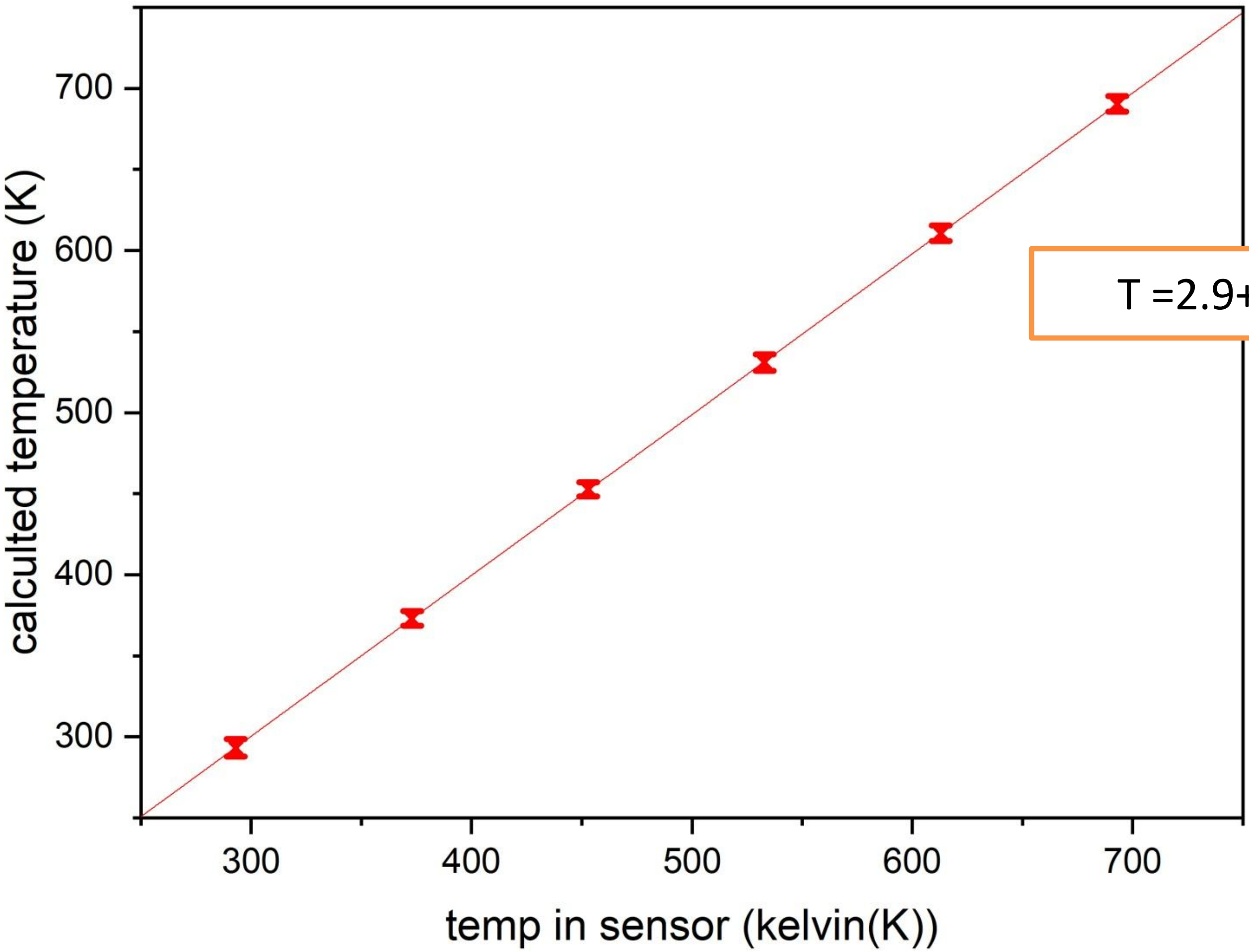
Silver calculated spectrum



Results IN silver sample

TEMPERATURE IN SENSOR(K)	Cell Parameters	Relative elongation unit cell	Calculated temperature(K)
293	4,0871±0.0003	0	293±5
373	4,0934±0.0002	1551,211	373±5
453	4,0999±0.0002	3141,569	452±4
533	4,1065±0.0003	4756,394	530±5
613	4,1134±0.0003	6449,513	610±5
693	4,120±0.0003	8201,354	690±5

Results



$$T = 2.9 + 0.9918t$$

Conclusion

The relation between temperature of sample and a temperature read by a sensor is defined by $T= 2.9 + 0.9918t$ which is leaner relation. In using the neutron diffraction technique the position of an atom was determined and its position changes with temperature .

References

1. https://www.mlzgarching.de/englisch/neutron-research/experimental-methods/inelastic-scattering.html
2. http://flnph.jinr.ru/images/content/ibr2/FDHR.jpg
3. https://upload.wikimedia.org/wikipedia/commons/5/58/Bragg%27s_Law.PNG
4. Texture Investigations by Neutron Time-of-Flight Diffraction by *K.* FELDMANN
5. https://lansce.lanl.gov/facilities/wnr/_assets/images/time_of_flight2.png

Acknowledgements

My Supervisors: Sergey Sumnikov and Ivan Bobrikov

Miss J.Raybeck

Miss Elizabeth

Prof R. Newman

Populace in

JINR institute