Investigation of the reactor neutron irradiated Si single crystal by a low energy neutron scattering.

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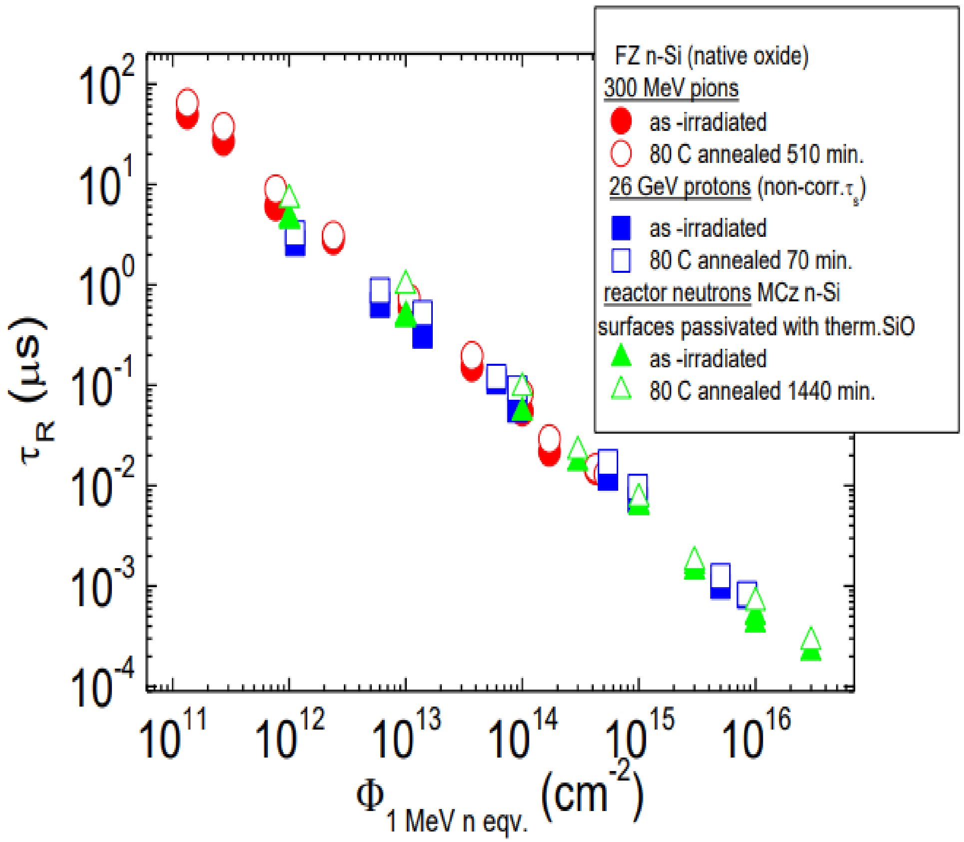
Outline

- Motivation:
  - Why was this research performed?;
  - Why neutrons … ?
- Experiment
- Results and discussion
- Future …
- Acknowledgements

Si irradiated by reactor neutrons



The free carrier lifetime dependence on the hadron fluence. E.Gaubas et al
https://indico.cern.ch/event/456679/contributions/1126323/

1. Many researchers teams have investigated the irradiated Si, and it was not found any local level which concentration linearly depended on hadron fluence.

2. Measurement of parameters of the centers, **as proposed related to the clusters in the irradiated Si,** gave **similar vaues for the capture cross-sections of the electrons and holes**

In the existing recombination center models **the capture cross-sections of the electrons and holes are always very different**, according to their polarity,

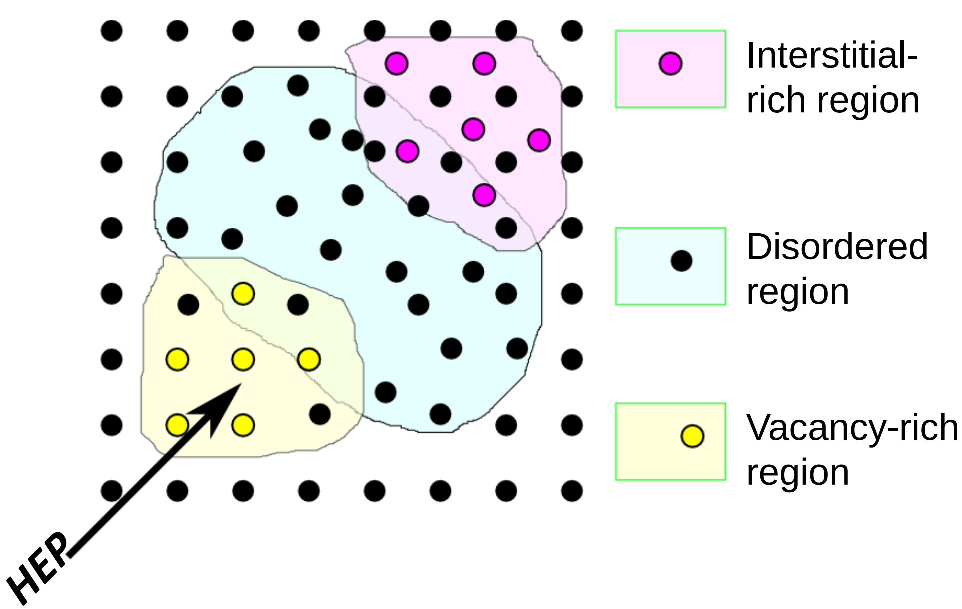
$\sigma_n \ll \sigma_p$ OR $\sigma_n \gg \sigma_p$

(Si vacancy – Si interstitial) Cluster Model

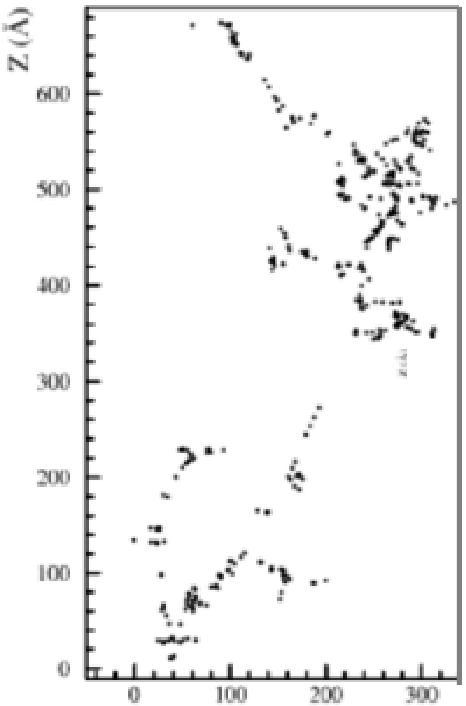
In the paper [1] and presentation [2] we proposed the cluster model that predicts the similar capture cross-sections of the electrons and holes.

This idea was confirmed by simulation using the density functional means. [1] E.Zasinas, J.Vaitkus, Disordered small defect cluster in silicon. Lithuanian J. Physics, 55(4): 330-334 (2015); [2] E.Zasinas, J.Vaitkus. https://rd50.web.cern.ch/rd50/ 26th RD 50 Workshop, Santander, Spain.

High Energy Particle (HEP) destroys the lattice:

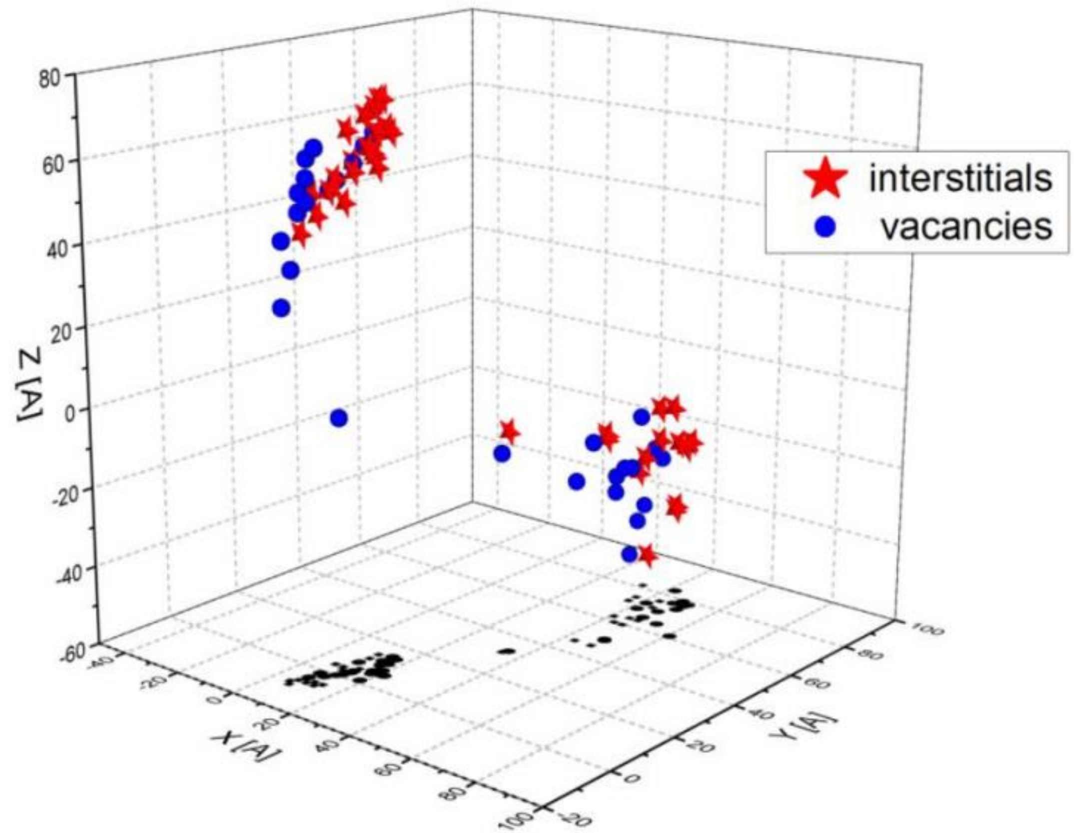


Si irradiated by high energy hadrons *simulation*



M. Huhtinen, NIMA 491, 194–215 (2002).

A projectionn of vacancies distribution in the cluster. *(Z=14, A=28, E=50 keV, 505 vacancies.*



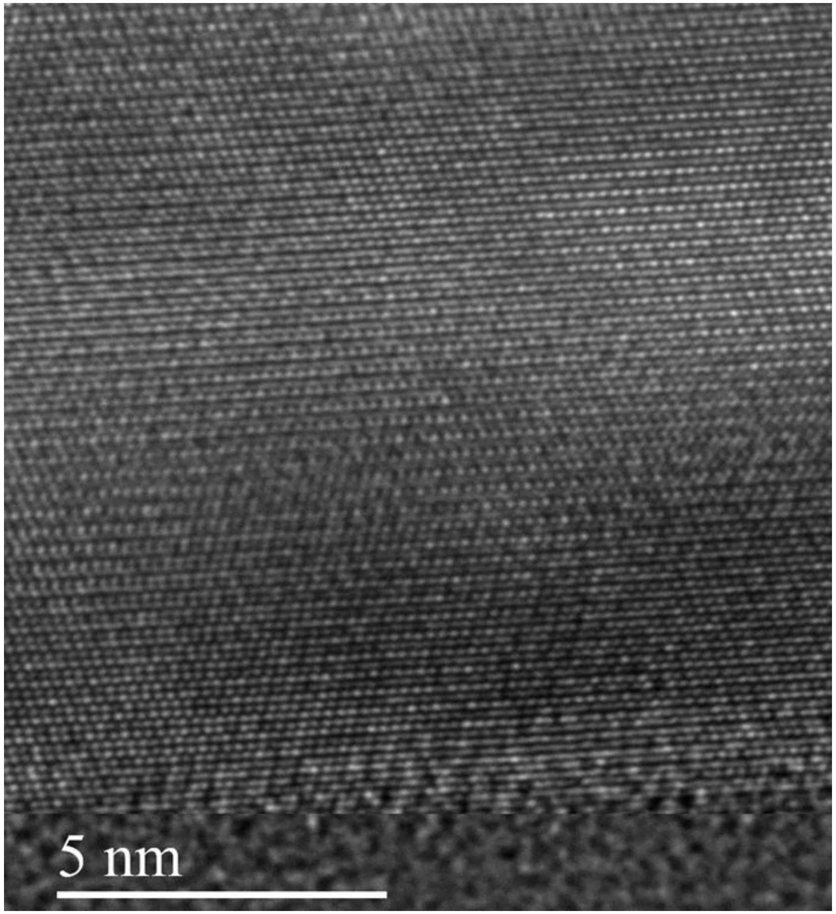
Simulation (TRIM&TCAS) results, G. Lindstroem, 24th RD50 workshop, Bucharest, 2014.

After relaxation of cascade defect & recombination of I-V pairs the rest of the vacancies and interstitials remain separated in space.

Si irradiated by high energy hadrons - *imaging*

An expert decision: The radiation induced cluster internal structure has never been observed directly. [R.S.Newman, private communication, 1977] (The oxygen clusters imagined very well.)

Our attempts to do it by HRTEM (**JEOL ARM200CF**) were not successful, probably due to the sample thinning technique induced cluster transform similar to annealing.



RD50 Romanian group (Ioana et al) was more successful but still more data are necessary for a real cluster properties simulation

Therefore it is necessary to use indirect means to confirm the details of the model.

The diffraction means permits to investigate **the change of structure and disorder.**

Diffraction means

X-rays cannot be applied because they introduce additional defects.

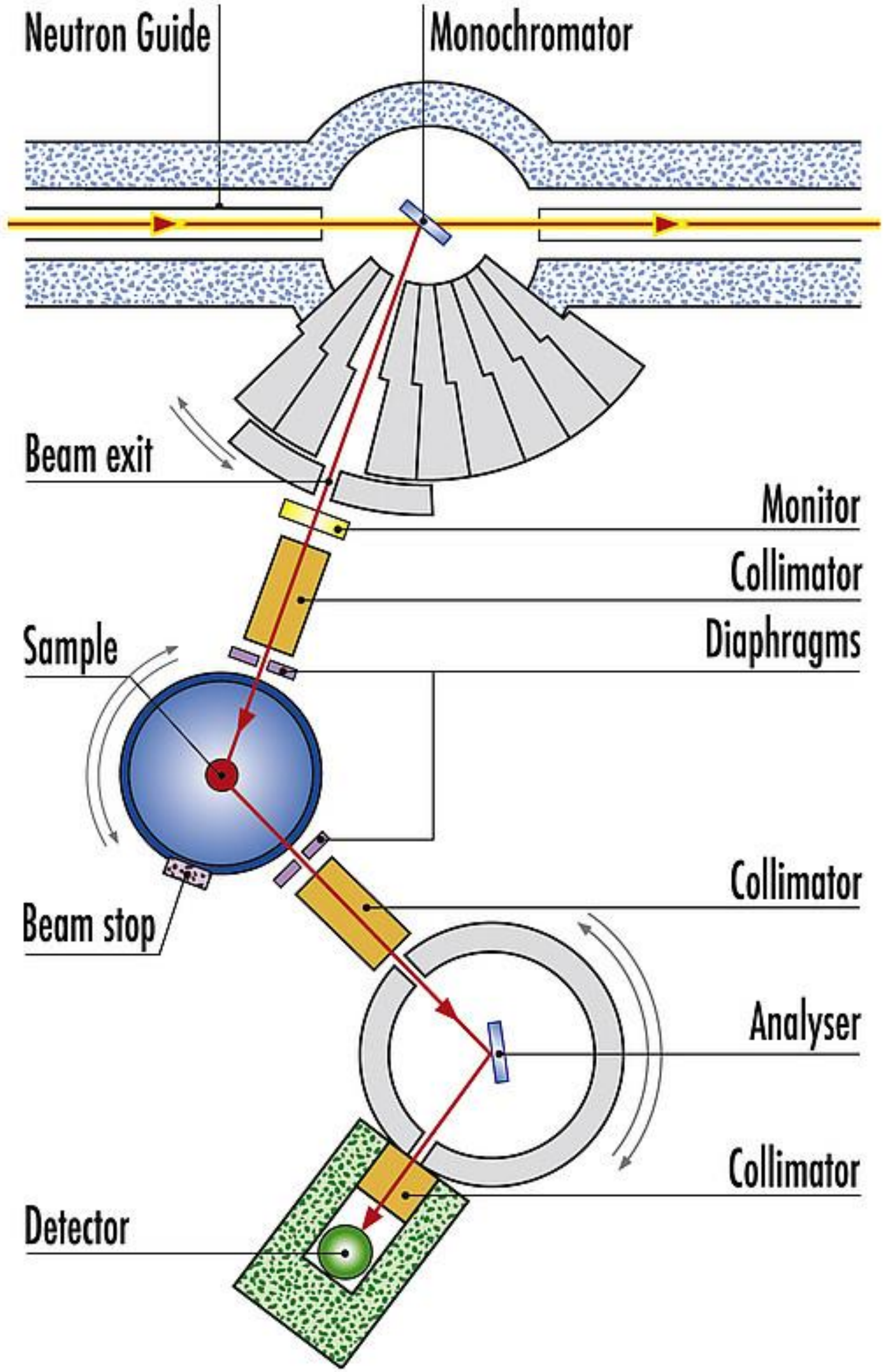
A low energy neutron wavelength is at the same range as the X-rays, neutrons based diffraction technique is non-destructive, therefore it is attractive and promising to analyze hadron generated clusters.

What is known about the clusters in Si by the neutron diffraction technique?

Analysis of neutron irradiated Si properties showed that at least up to 2e 17 cm^{-2} fluence the defects distribution is non-homogeneous, it exists the clusters.

It was given a size of clusters in Si, irradiated by fast neutrons, obtained by SANS. It was found **the clusters scattering length 15 nm and 5 nm.** The 15 nm clusters annealed up to 110 C, and the 15 nm clusters disappear at 600 C. [R.E.Beddoe et al, Inst. Phys. Conf. Ser. No.46: Chapter 3, p.258-266 (1979)].

The oxygen clusters in FZ Si are larger (29 nm) than in the Czochralski-grown crystals (16 nm), but the number of oxygen atoms in precipitates is 10 times lower [R.E.Beddoe et al, Philosophical Magazine A , Vol.48, No. 6, 935-952 (1983)].



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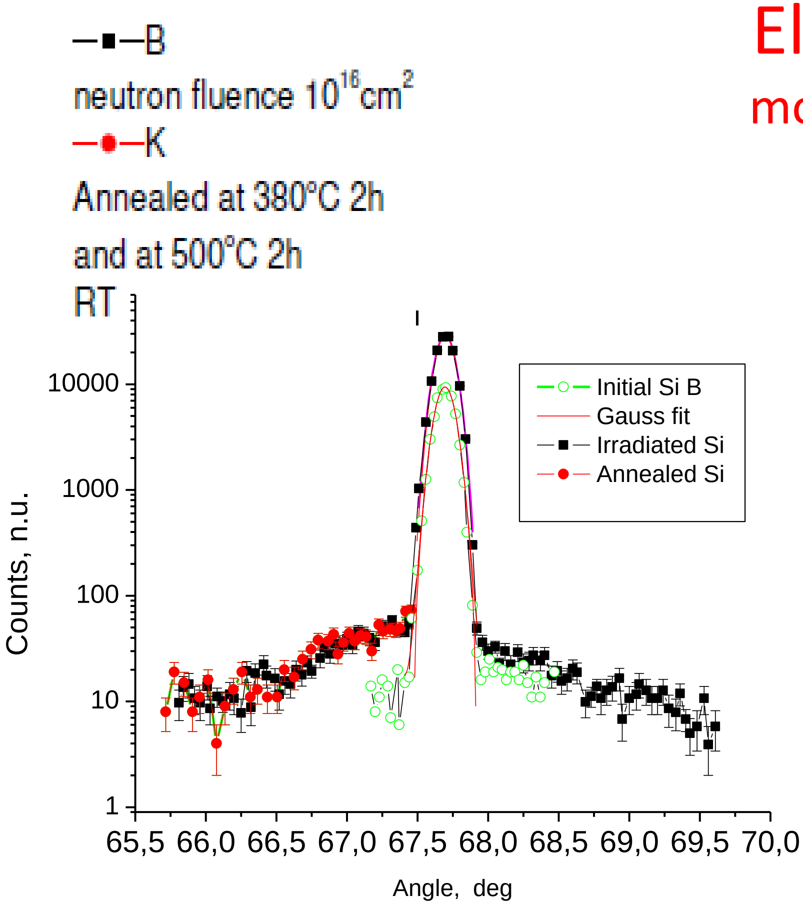
- The Si single crystals, the same type as user for the detectors at LHC, were irradiated in TRIGA nuclear reactor to the neutron fluence 10^{16} cm $^{-2}$.
- **A challenge:** the clusters fills unknown part of the sample volume, maybe in between 0,01-2%
- Instrument was used with incident and scattered wave vectors of 2.662Å.
- The neutron scattering was measured in the FZ Si samples at room temperature:
  - 1.before irradiation,
  - 2.after irradiation,
  - 3. after annealing at high temperature (2 h @380 C & 2 h @500 C).

Experimental data



Elastic scattering was approximated by Gauss model after removal the diffuse and incoherent part in the scattering intensity-angle dependence.

A width of the Gauss:
in non-irradiated sample is 0.13546±0.00011 deg,
after the irradiation - 0.13679±0.00026 deg,
in annealed sample - 0.13301±0.00046 deg

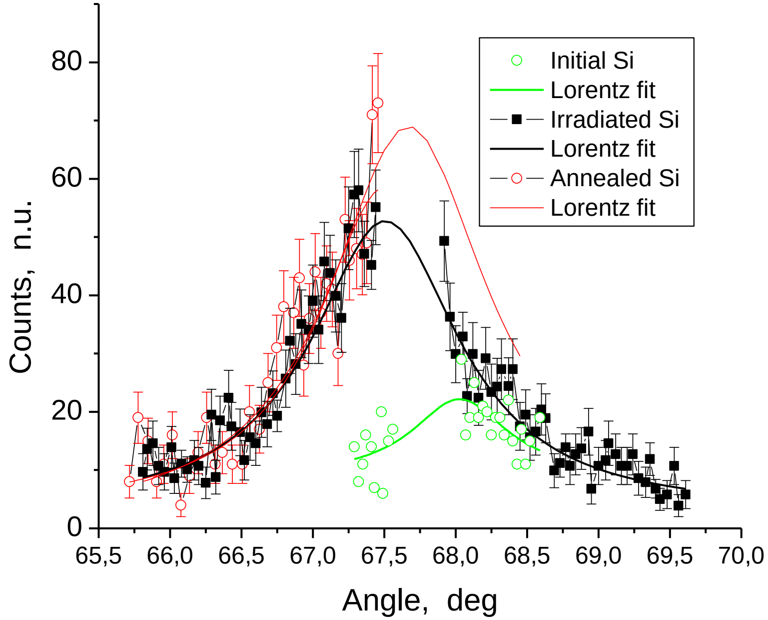
Irradiation created a different disorder in comparison with initial.

Annealing decreased the peak's width, i.e., a disordered region was reduced that confirmed as a known dependence.

Annealed sample became better quality than the initial crystal !?

Diffuse scattering

- The diffuse scattering spectra, which are 1000 times weaker than in the elastic scattering region, analyzed after removal of elastic part of the scattered signal (using the Gaussian approximation).



The diffuse scattering in the initial crystal showed existence of, probably, oxygen clusters.

The diffuse scattering maximum shifted to less angles by 0,2 degree in the irradiated sample, and it shows the existence of the Si lattice deformation, probably inside the cluster volume.

Annealing shifted the Lorentz peak to the value corresponding the elastic scattering maximum, and it observed an increase of HW by less than 0,1 deg, and it is in a range of errors.

It could be explained by a proposal of the cluster transform into other random distributed defects.

Conclusions and Future

- The results confirmed the existence of the proposed model requirements.
- There is a plan to perform measurement with better resolution.

Proposal: 1-10-43 **Title:** Radiation induced defect clusters in Silicium cristal

Main proposer: VAITKUS Juozas **Proposers:**

Name	Laboratory	Country
VAITKUS Juozas	VILNIUS UNIVERSITY	LT
BOEHM Martin	ILL, GRENOBLE	ILL
PIRLING Thilo	ILL, GRENOBLE	ILL
LEMEE Marie Helene	ILL, GRENOBLE	ILL

The ILL User Club

- At more near future: a simulation of recombination of carriers inside the cluster, i.e., an analysis of electron transport in the cluster.

- The first steps - **a next talk.**

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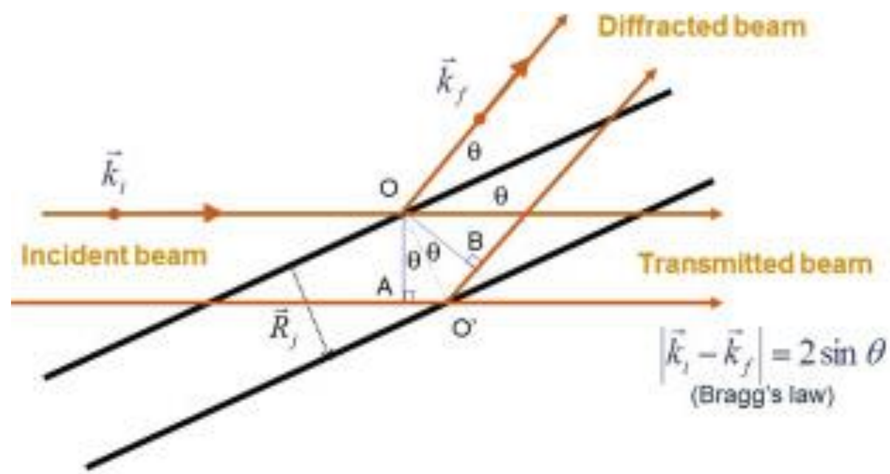
This research was performed in a framework CERN RD50

THANK YOU
FOR YOUR ATTENTION!

Neutron diffraction

- Elastic scattering, or diffraction, describes a process in which the incident and the scattered neutrons have the same energy.
- The scattering angle θ (as defined in Fig.) gives information, through Bragg's law, on the periodicity of the atomic arrangement (i.e. crystal unit cell parameters).
- The intensity of the Bragg peaks is related to the cell symmetry and atomic positions within the crystal unit cell.



Schematic representation of the Bragg law in diffraction.
2dhkl sin θ = λ, relating the diffraction angle θ, the beam wavelength λ, and the space between lattice planes (in thick dark lines) dhkl.

A simple diagram of the set-up used for measuring the crystal rocking curve $R(\theta - \theta B)$ is shown in Fig. : the detector was kept at a scattering angle equal to 2 θB and the crystal was rotated around the exact Bragg position. I

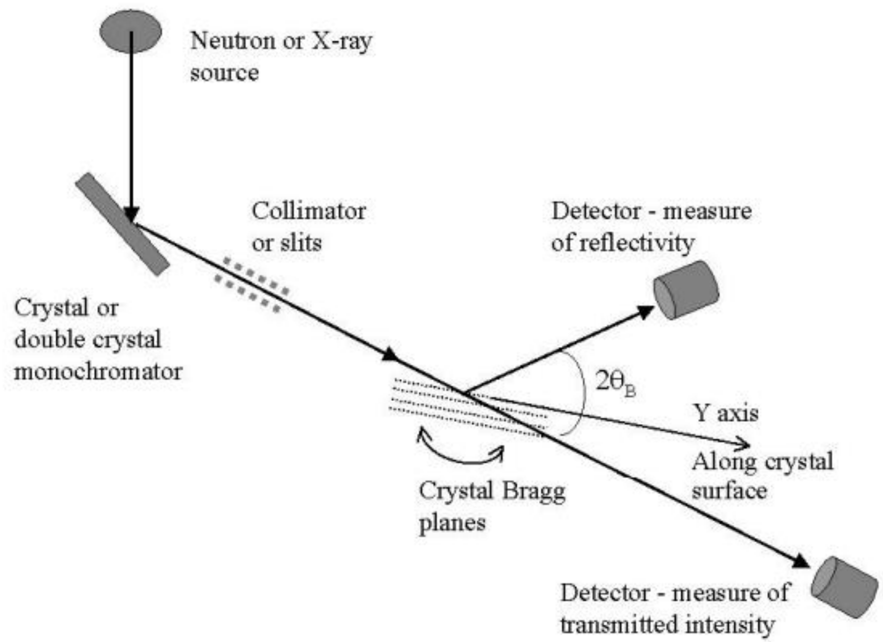
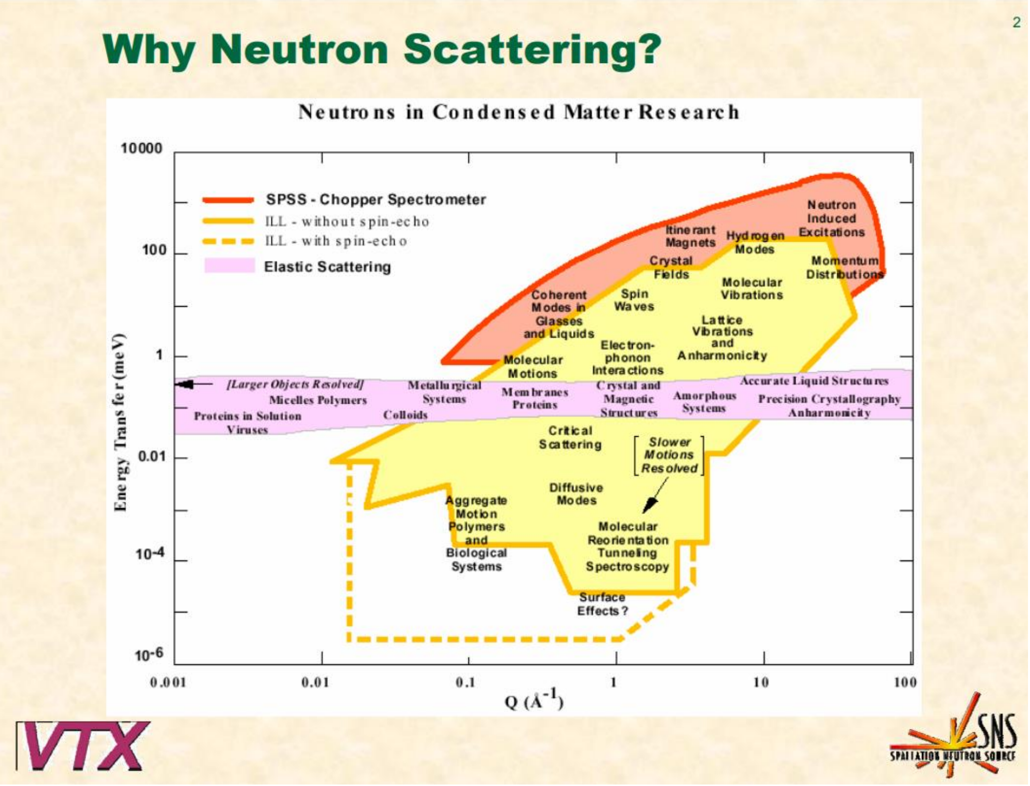
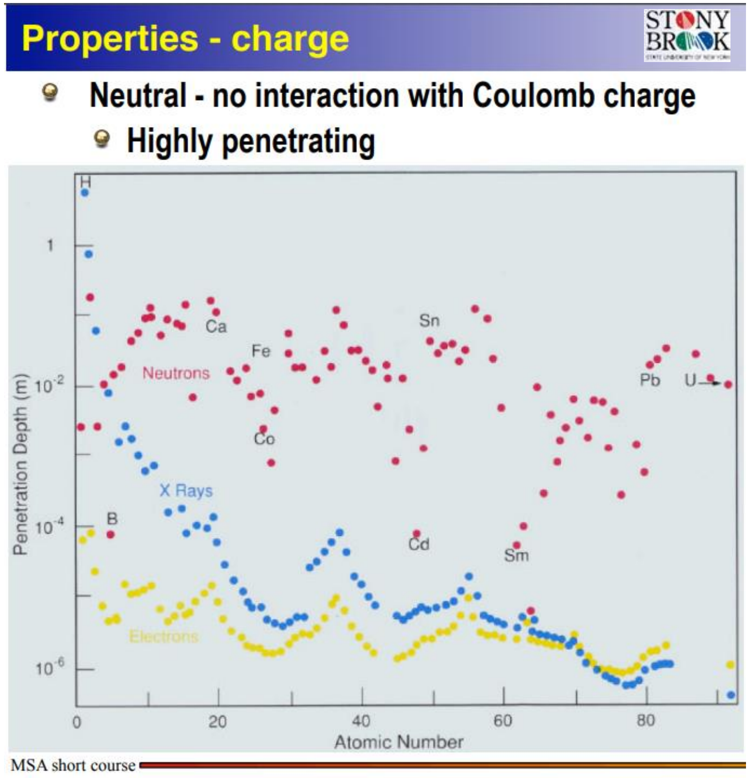


Figure 5.1: *Schematic diagram of the geometry used for recording curves of reflected or transmitted intensity. The Y axis is parallel to the crystal surface.*

Single-Crystal Neutron Diffraction: Present and Future Applications

Christina Hoffmann (SNS)





- Neutrons interact with matter in a variety of ways which make neutron diffraction both similar to and yet different from X-ray diffraction.
- Because X-ray diffraction results from scattering by the electrons, atoms of similar atomic number exhibit very similar scattering and it is hard to distinguish between them by X-ray diffraction. In contrast, neutron scattering depends upon the nature of the scattering nuclide and, as a consequence, atoms of similar atomic number often have quite different neutron scattering lengths *(because the neutron has a magnetic moment, it also is scattered by interaction with any magnetic moments found within a material; the resulting coherent scattering, the magnetic scattering, is superimposed upon the nuclear scattering in any magnetic material).*

Diffuse Scattering

- Deviations from average structure
- e.g. disordered materials

− thermally induced disorder

− disorder resulting from defect impurities