



## UTILIZATION OF SINGLE CRYSTALS AS FILTERS FOR OBTAINING THERMAL NEUTRON BEAMS

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RESUMO

Um breve estudo sobre a utilização de filtros de nêutrons térmicos é aqui apresentado, utilizando os conceitos fundamentais e as propriedades das secções de choque dos elementos.

A análise dos resultados experimentais já publicados e dos dados fornecidos por Rustad e Nielsen demonstram a vantagem do emprêgo de monocristais de bismuto.

ABSTRACT

A bried study on the utilization of thermal neutrons filters is presented in this paper, utilizing the fundamental concepts and the cross section of the elements.

Based on experimental results already published and on the data given by Rustad and Nielsen, it is shown that there is a great advantage in using bismuth single crystals.

RÉSUMÉ

Une brève étude sur l'utilisation de filtres de neutrons thermiques est présentée ici, en utilisant les concepts fondamentaux et les propriétés de la section efficace des éléments.

En s'appuyant sur des resultats déjà publiés et sur les données fournies par Rustad et Nielsen, on conclut que l'emploi des monocristaux de bismuth est très avantageux.

## I. INTRODUCTION

In thermal neutron nuclear reactions studies there is always some difficulty in obtaining intense neutron beams that are sufficiently free from gamma radiation and from neutrons having higher than the desired energy. This problem has been solved essentially in two ways: either by using a beam reflected by a crystal, or by using a beam transmitted by filters, that is, substances that because of their cross sections, may introduce considerable changes in the velocity distribution of the neutrons transmitted by them.

The use of reflected beams presents as characteristics: a neutron velocity distribution that is practically monochromatic, completely free of gamma radiation coming directly from the pile, and low intensity. Filters present as characteristics a neutron velocity distribution with a strong attenuation in high energies, reduction of the gamma radiation flux and high intensity. We shall study this last solution in the particular case in which single-crystals are used.

## II. THEORY

Let us review the behaviour of the cross sections of the elements:

### A. Cross Section

The total neutron cross section of an element consists essentially of the sum of the cross sections due to absorption, Laue-Bragg scattering, incoherent scattering, thermal scattering and diffuse paramagnetic scattering.

1. Absorption: When the principal interest is obtaining thermal neutron beams by transmission or reflection, substances having low absorption cross section in the thermal

region, are chosen, because, for low energies,  $\sigma_a \propto \frac{1}{v}$ .

2. Laue-Bragg scattering: Neutron properties of optical interference are determined by a cross section of the kind that gives rise to a scattered wave interfering with the incident wave. In the cases where there are no nearby resonances, it is given by  $\sigma = 4 \pi R^2$ , where "R" is the radius of the nucleus.

In the case of scattering by several nuclei, interference among scattered waves, will be present, giving rise to an anisotropy in the reflected beam, which, in the case of a single crystal, will be evident by noticing a beam of a maximum intensity for neutrons having wavelength  $\lambda_0$  given by

$$\lambda_0 = \frac{2}{n} d \sin \theta ,$$

where:

- $\theta$  is the angle between the incident beam and the crystal reflection plane,
- $n$  is the order of reflection, and
- $d$  is the corresponding interplanar spacing.

In this case the crystal cross section for neutrons of wavelength  $\lambda_0$  will be

$$\sigma_{\text{coher}} = \frac{\lambda_0^2 N}{2} \left( |F|^2 \sin^2 \frac{4}{n} \right)_{h,k,l}$$

where:

- $N$  is the number of unit cells per  $\text{cm}^3$  of the crystal,
- $M$  is the number of possible orientation of the unit cell for a given reflection  $h, k, l$ , and

$$F = \sum_j a_j \exp \left[ 2 \pi i (h x_j + k y_j + l z_j) \right]$$

This sum is made over all the atoms of the unit cell,

$a_j$  is the coherent scattering amplitude of a given atom,

$h, k, l$  are the Miller indices of the unit cell, and  $x, y, z$  define the position of a given atom.

3. Incoherent scattering: Incoherent scattering is due to any process that originates waves that are not able to interfere with the incident wave. This kind of scattering is due to variations of the properties of the nucleus with the considered position.

The incoherent scattering may result from the following possibilities:

a) Spin incoherence

If a nucleus of spin  $I$  scatters a neutron, the compound nucleus will have spin  $I \pm 1/2$  and the scattering amplitude will be different for the two cases. It can be shown that

$$\sigma_{\text{coher}} \propto 4\pi (w_+ b_+ + w_- b_-)^2$$
$$\sigma_{\text{incoher}} \propto 4\pi (w_+ w_-) (b_+ - b_-)^2$$

where:

$\sigma_{\text{coher}}$  is the coherent scattering cross section,

$\sigma_{\text{incoher}}$  is the incoherent scattering cross section,

$b_+$  is the scattering amplitude when the spins are parallel

( $b_-$  anti-parallel),

$$w_+ = (I + 1) / (2I + 1)$$

$$w_- = I / (2I + 1)$$

The spin influence can be easily noticed when we compare  $\tau_{\text{total}}$  with  $\sigma_{\text{coher}}$  of nuclei with spin equal zero and different

from zero, there being cases in which  $\sigma_{\text{conher}}$  or  $\sigma_{\text{incoher}} \neq 0$ .

### b) Incoherence due to isotopes

When a sample is constituted by more than one isotopic species, nuclei with different scattering amplitudes will be distributed at random. Consequently, the value of the form factor  $F_{h,k,l}$  must be an average over the possible positions.

$$F_{h,k,l} = \sum_r w_r b_r^2 - \left( \sum_r w_r b_r \right)^2 + 1/N_0 \left( \sum_r w_r b_r \right)^2 \cdot \left| \sum_r \exp \left[ 2 \pi i \left( hx/a_0 + ky/b_0 + lz/c_0 \right) \right] \right|^2,$$

where  $w_r$  is the isotopic abundance.

When the spins are different, in the calculation of the average, the scattering amplitude values  $w_+ b_+$  and  $w_- b_-$  for each isotope must be taken into account.

One can write

$$\overline{F_{h,k,l}} = \left\{ \overline{b_r^2} - (\overline{b_r})^2 \right\} + 1/N_0 (\overline{b_r})^2 \left| \sum_r \exp 2 \pi i \left( hx/a_0 + by/b_0 + lz/c_0 \right) \right|$$

The first term of  $\overline{F_{h,k,l}}$  gives the contribution of the incoherent scattering and the second the coherent scattering.

### c) Incoherence due to inelastic scattering.

When the neutron scattering by nuclei of infinite mass in a crystal, is studied, there is an effect due to spatial periodicity; if however a nucleus of finite mass is under consideration, the collision can be considered as inelastic, and an exchange of energy between the crystal and the neutron takes place. If elastic scattering is considered as a particular case of inelastic scattering, it will be a function of temperature, as it happens in Debye theory,

and the scattering amplitude will be given by  $be^{-W}$ , where

$$W = \frac{6 h^2 \sin^2 \theta}{m_A \bar{k} \Xi \lambda^2} \left( \frac{\Phi(x)}{x} + \frac{1}{4} \right)$$

$h$  ... Planck's constant

$\bar{k}$  ... Boltzmann's constant

$\Xi$  ... Debye temperature

$$\Phi(x) = \frac{1}{x} \int_0^x \frac{\xi d\xi}{e^\xi - 1}$$

$\xi$  ... Nuclear radius ( $\xi = 1.5 \times 10^{-13} A^{1/3}$ )

$m_A$  ... Mass of the atom

This equation is valid for a cubic monoatomic crystal. When this does not happen it is necessary to take an empirical  $W$ , derived from experiment.

For thermal neutron there is change of only one quantum in the collision. This assumption does not hold for very small wavelengths, in which case more than one quantum can be exchanged, similar considerations being valid for very large wavelengths, since then the neutron can only receive energy.

Taking into account this phenomenon, a treatment by Cassels-Finkelstein has been made, showing an agreement of less than 4% with experimental values. In this treatment four kinds of scattering are considered: ordered or disordered elastic scattering and ordered or disordered inelastic scattering. The expressions that give the mode of variation for the different kinds of scattering are given as a function of awkward integrals, that must be calculated for each particular case. They can be expressed, however in an approximate manner as

$$E_{el}(\text{disord}) = \frac{v_{inc}}{4 k^2 Y} \left( 1 - e^{-4k^2 Y} \right),$$

where

$$Y = \frac{3 n^2}{4 \pi^2 m_A k E} \left( \frac{\rho(x)}{x} + \frac{1}{4} \right)$$

$E_{el} (disord)$  . . . disordered elastic scattering cross section integrated over all the space.

For short wavelengths we can write:

$$E_{el} (ord) + E_{el} (disord) = \frac{\sigma}{4 k^2 Y} (1 - e^{-4k^2 Y}),$$

and finally for the disordered and ordered inelastic scattering:

$$\sigma_{inc} = \sigma_{scat} \left\{ 1 - \frac{\lambda^2}{W} \left[ 1 - e^{-W/\lambda^2} \right] \right\}.$$

d) Incoherence due to magnetic moment.

Since the neutron has magnetic moment, there will be incoherent scattering owed to its interaction with the magnetic moments of the atoms.

### III. KINDS OF FILTERS

The filters used can be classified into two kinds: those that present resonances - and thus take out neutrons of some energies from the incident distribution, and those for which optical properties of the neutrons can be applied. The first ones present, generally, a high absorption cross section in the thermal energy region, which is undesirable. Only filters of the second kind will be considered in the following discussion.

#### A. Crystals

It has been shown in section II.A.2 that, when there is

spatial periodicity in the distribution of atoms, that is, in the case of crystals, the coherent scattering cross section presents a resonance whose width depends on the crystal perfection, that is, on the absence of mosaic structure.

1. Coherent scattering. In a single crystal, only neutrons of wavelength  $\lambda_0$ , given by Bragg's law, are reflected. In a polycrystal the cross section varies in such a way that

$$\text{for } \lambda \begin{cases} > \lambda_n \\ < \lambda_n \end{cases} \quad \begin{aligned} \sigma_{\text{coher}} &= 0 \\ \sigma_{\text{coher}} &= \sum_{h,k,l} \sigma_{h,k,l} \end{aligned}$$

where  $\lambda_n = 2 d_n$  and  $d_n$  is the largest interplanar spacing in the crystal.

This behaviour explains the appearance of Bragg's cut-off in the transmission and for the same reason polycrystals are used as filters for transmission of neutron of wavelength

$$\lambda > \lambda_n .$$

Single crystals are mostly used for selecting neutrons of wavelength  $\lambda_0$  given by Bragg's law. It is important to study the velocity distribution for neutrons transmitted by the single crystal. If a perfect single crystal is considered having an incoherent scattering, an absorption cross section, and a diffuse magnetic scattering that are negligible, it will have a low cross section for slow neutron as compared with the cross section for resonance and fast neutrons and it can be used as a filter for slow neutrons. Its cross section for low energies consists only of Bragg scattering and thermal diffuse scattering. The first scattering has negligible influence in the spectrum transmitted by the perfect crystal, because as it has already been said, it takes out around 50% of the neutrons that have a well defined energy. The

second component is a function of the wavelength and of the temperature, approaching zero when the temperature diminishes and when the wavelength grows up, and it approaches the free atom cross section, for short wavelengths.

The cross section, thus, follows the law

$$\sigma_{\text{incoher}} = \sigma = \sigma_{\text{sc}} \left\{ 1 - \frac{\lambda^2}{2B} \left[ 1 - \exp(-2B/\lambda^2) \right] \right\},$$

because one of the imposed conditions is a small  $\sigma_{\text{inc}} / \sigma_{\text{sc}}$ , approximate values can be used for  $\sigma = B \sigma_{\text{sc}} / \lambda^2$ , that diminishes continuously with the energy.

One should have always in mind that for sufficiently large wavelengths the cross section increases in the majority of cases proportionally to the wavelength, which is due to scattering processes in which the neutron gains energy; this effect can be minimized by reducing the temperature of the single crystal.

This behaviour makes the temperature of the velocity distribution of the transmitted neutrons lower than that which corresponds to the incident neutron beam.

## V. CONCLUSION

The conclusion is that, in order to obtain a filter as above described, one needs:

- a) a perfect single crystal,
- b) with low incoherent scattering and magnetic scattering cross section, and
- c) high cross section resonance and fast neutrons.

The single crystals that are mostly used are of quartz and bismuth, that transmit preferably thermal neutrons, eliminating fast neutrons.

Bismuth present the advantage of attenuating very much the intensity of the gamma ray beam, but results of experimental

work reported by Rustad (Rustad-63) have shown that, in the single crystals used, the appearance of several Bragg peaks indicates that more perfect single crystals are needed. That does not happen in the case of quartz, because single crystals of high perfection are found in nature.

Some results obtained by Rustad in the Brookhaven National Laboratory and by Nielsen in Danish Atom Commission are presented here and confirm our discussion that, if very perfect bismuth crystals are available, they are more convenient than the use of other techniques.

#### VI. ACKNOWLEDGEMENTS

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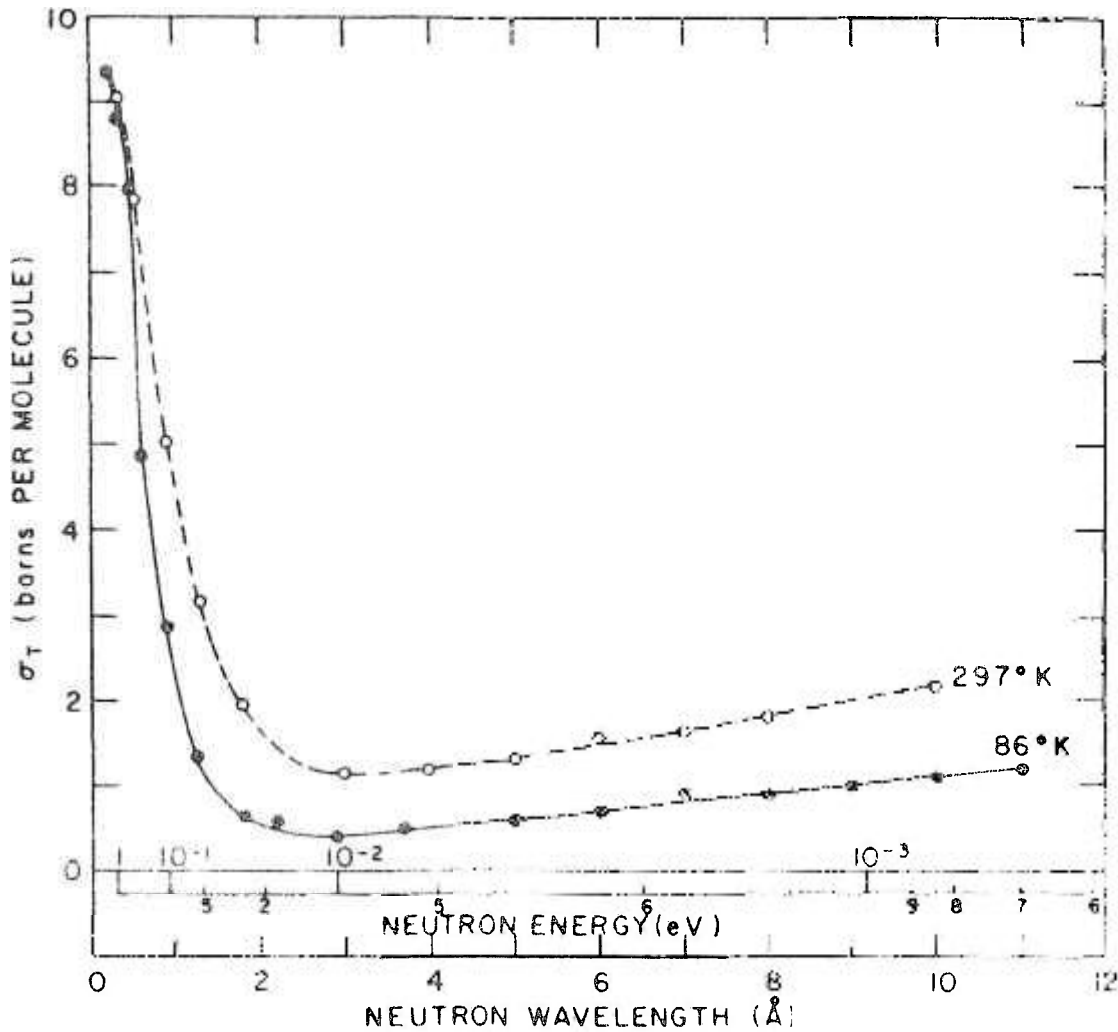


Figura 1

Quartz Single Crystal Filters for Attenuating Epithermal Neutrons and Gamma Rays - Rustad and Nielsen -

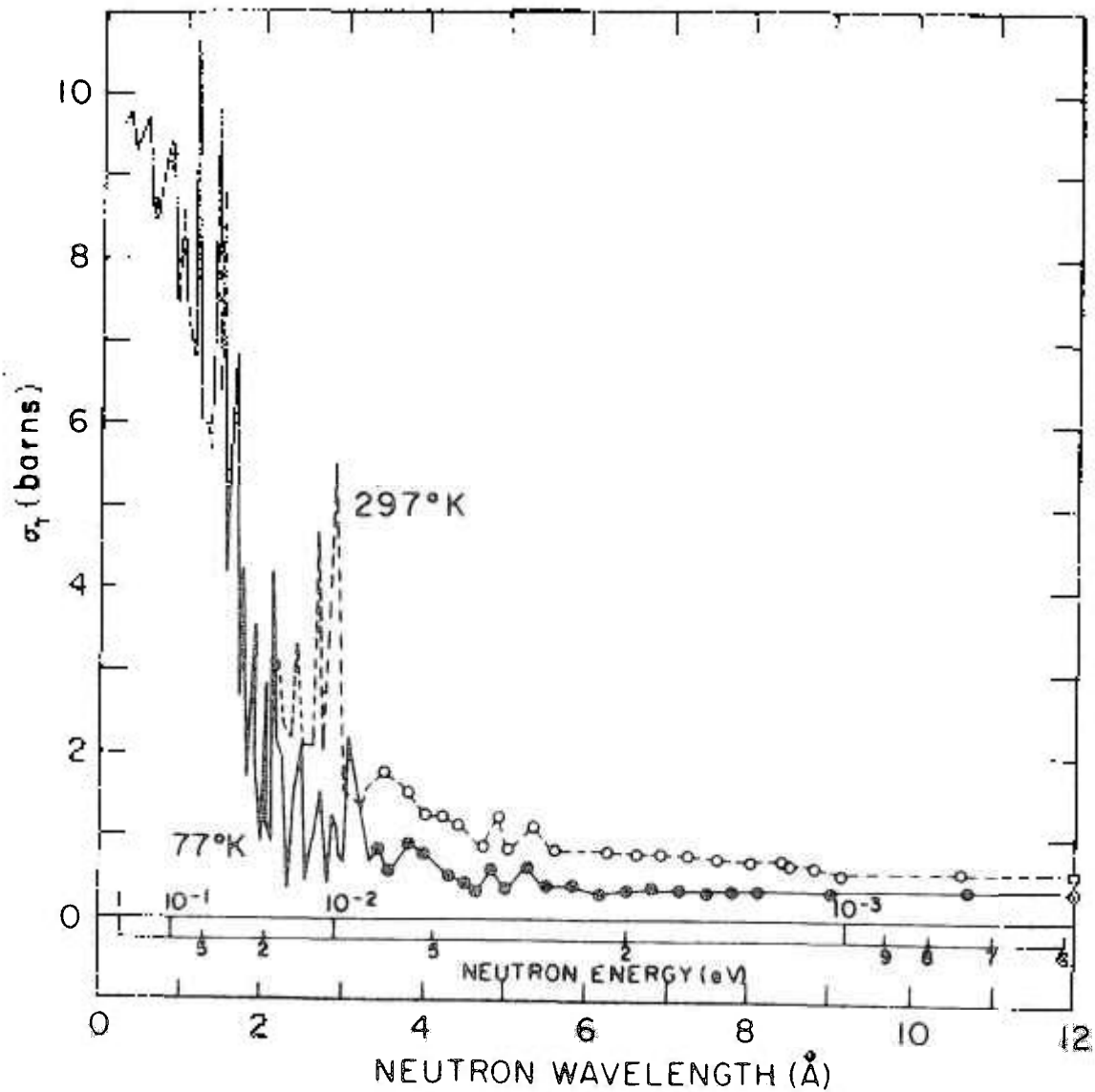


Figura 2

Bismuth Single Crystal Filters for Attenuating Epithermal Neutrons and Gamma Rays - Rustad and Nielsen -

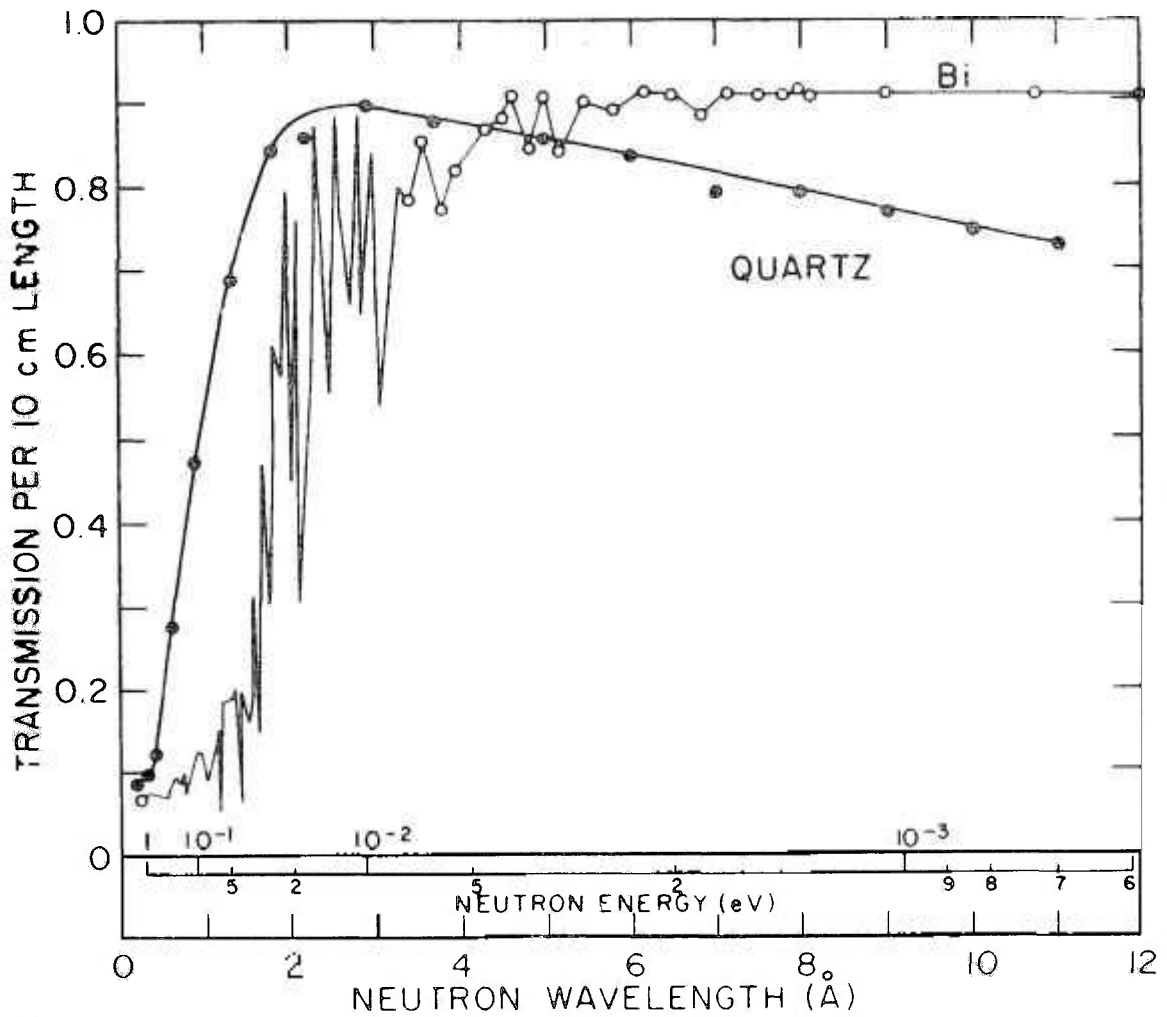


Figure 3

Single Crystal Filters for Attenuating Epithermal Neutrons  
and Gamma Rays

- Rustad and Nielsen -

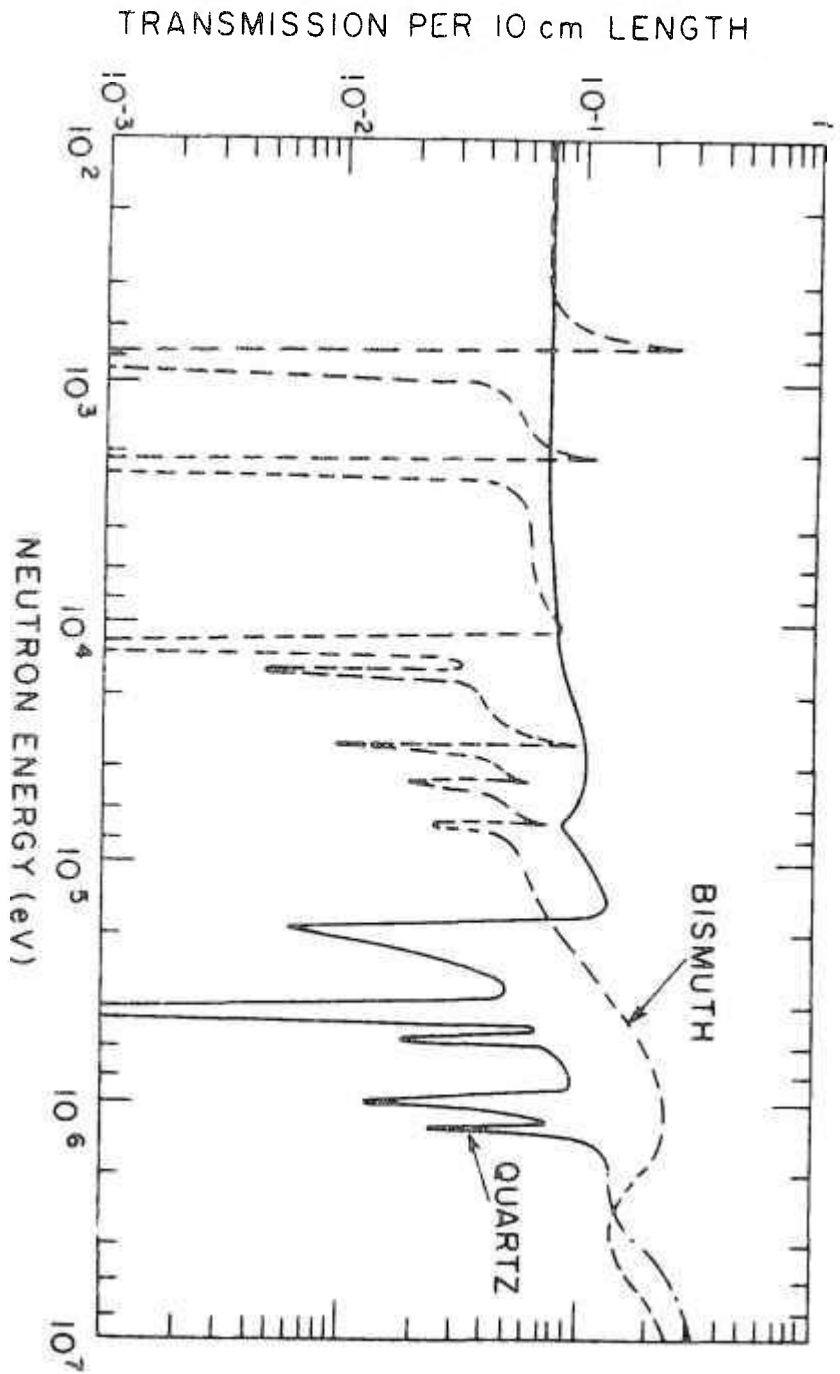


Figure 4

Single Crystal Filters for Attenuating Epithermal Neutrons  
and Gamma Rays - Rustad and Nielsen -

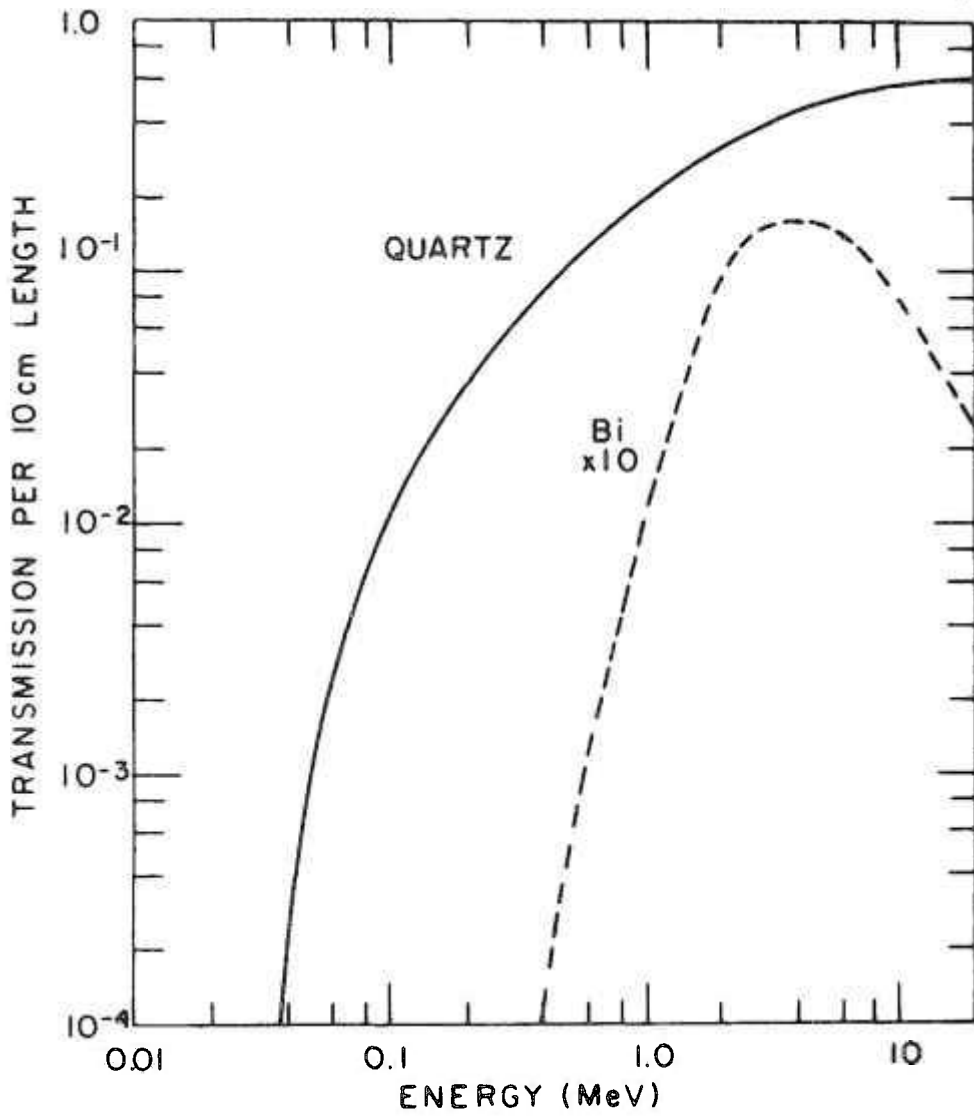


Figure 5

Single Crystal Filters for Attenuating Epithermal Neutron  
and Gamma Rays - Rustad and Nielsen -