DETERMINATION OF INCOHERENT NEUTRON SCATTERING CROSS SECTION IN ZIRCONIUM ELEMENT BY MCNP4C CODE

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Neutron crystallography is an efficient investigation method for determination the structure of materials, but neutron sources are very rare and expensive to build and to maintain. The strongest neutron source is nuclear reactor, but its expense is billions of dollars to build and operate. High cost was a major factor in the cancellation of the advanced neutron source project. For obviation this difficulty, have been designed computer methods. These methods have been employed for determination of materials characteristics, but very limitations exist for neutron crystallography in methods of computer based. In this paper shown, neutron diffraction and neutron scattering with a proper design method of computer based can be used for overcome some of these limitations. In this context, is studied the feasibility of computer method by MCNP4C code for determination of coherent and incoherent neutron scattering cross section for natural zirconium and also, neutrons diffraction.

1. Introduction

The thermal neutron scattering cross section is usually divided into three different parts:

-Inelastic: Important for all materials and described by the scattering law S (α,β).

-Coherent elastic: Important for crystalline solids like graphite, beryllium or UO_2.

-Incoherent elastic: Important for hydrogenous solids like polyethylene or light water and zirconium.

Thus, for research of incoherent neutron scattering cross section, we select zirconium element. In nuclear reactors one of the most practical elements is zirconium. Zirconium is widely used in core reactor. All channels, spacer grids, and clad materials (as fuel rod cladding), are made up of zirconium alloy in order to save neutron economy [7].

In this paper simulated Pressurized Water Reactor (PWR) and neutron diffraction in crystallography section. Finally, coherent and incoherent cross sections of zirconium element by thermal neutrons are obtained, by means of MCNP4C code.

MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems.

The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first- and second-degree surfaces and fourth-degree elliptical tori. In MCNP4C code, the neutron energy regime is from 10^{-11} MeV to 20 MeV, consequently (existence of thermal neutrons in these limits) it is possible to simulate neutron diffraction and Bragg's law [1-4].

2. The model preparation for calculation of MCNP4C code

We can employ two designs for our investigation. A schematic diagram of the equipment used in studying neutron diffraction effects is given in figure 1 (A, B).

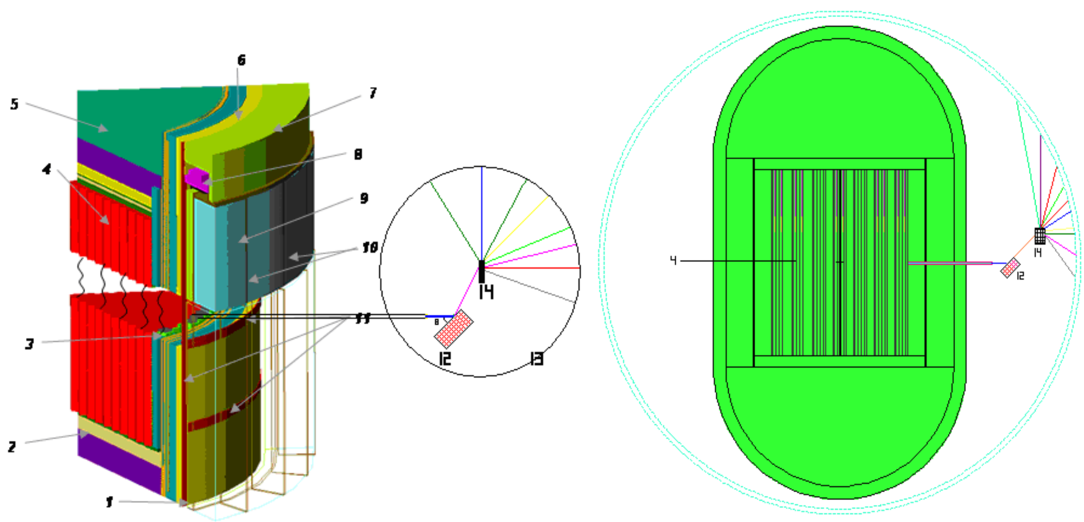

Fig.1: Two designs for investigation of neutron scattering and neutron diffraction.
1-Thermal insulation; 2-down reflector; 3- Core baffle; 4- Reactor core; 5- Up reflector; 6-Reactor pressure vessel; 7- Shielding; 8- Thrust truss; 9- Water tank; 10- Tank edge; 11- Registration areas; 12- Crystal monochromator; 13- Metallic sphere; 14- Zirconium.

Reactor core consists of 163 hexagonal fuel assemblies with U^{235} enrichment between 1.6 and 4.02 %.Fuel assemblies are in hexagonal shape and consist of 311 pin-type fuel rods. Fuel rods are arranged in a triangular array with 12.75 mm pitch. Every fuel rod is constrained in the correct position by the presence of 15 spacer grids made up of Zr + %1Nb. There are 20 special channels in the fuel assemblies. The central channel serves as a structural element of the fuel assembly framework. One channel shifted with respect to the center is used to house the in-core instrumentation systems. Eighteen channels are the guide ones wherein the control rods are moving and the burnable absorber rods are installed as well. All channels and spacer grids are made up of zirconium alloy in order to save neutron economy. Arrangements of fuel rods over the sections of the fuel assembly types are shown in figure 2.

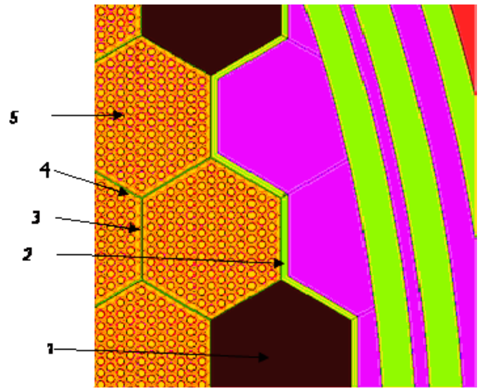

Fig.2: Reactor core configuration. 1- Measurement tube 2- Core baffle 3- Cladding fuel Assembly 4-Water in reactor core. 5- Fuel rod.

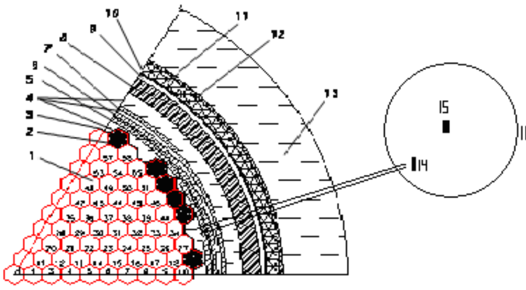

Fig.3: Configuration of reactor core and crystallography section. 1- Reactor core; 2- Cladding fuel Assembly; 3- Core baffle; 4- Water; 5- Basket; 6- Core barrel; 7- Shield; 8- Pressure vessel; 9- air gap; 10- Cladding; 11-Thermal insulation; 12- Tank wall; 13- Biological shield; 14- Crystal monochromator; 15- Metallic sphere.

A collimated beam of thermal neutrons is passed out through the radiation shielding in reactor and falls upon a single crystal monochromator of sodium given in figure 3. This crystal is oriented so as to Bragg-reflect neutrons of wavelength 1.08 Å (energy 0.069 eV). After collimation through slits of size 1 cm by 3.5 cm, the monochromatic beam strikes a flat plate of the crystalline solid of zirconium under study that zirconium located inside metallic sphere in near of reactor pressure vessel (the diffracted neutrons count-rate is measured in a detector that here accomplished by this metallic sphere, figures 1,3). The neutron current in the primary monochromatic beam is about 200000 neutrons and in the diffraction peaks about 155000 neutrons [5, 7-16].

3. The results of calculations and their analysis

Relation of total scattering cross section (σtot) with coherent scattering cross section (σ_{coh}) and incoherent scattering cross section (σ_{inc}) are:

$$\sigma_{inc} = \sigma_{tot} - \sigma_{coh} \tag{1}$$

Therefore, at first we obtain coherent scattering cross section (σ_{coh}), thereafter total scattering cross section (σ_{tot}) and finally incoherent scattering cross section (σ_{inc}).

A) Method of calculation of coherent scattering cross section (σ_{coh})

We now calculate by MCNP4C code the intensity of the Bragg peak of standard method, originally devised for the scattering of neutrons, namely rotating and oscillating crystal method (rotation of crystal) [6,21].in this method of measuring a Bragg peak, a monochromatic beam of neutrons is incident on a crystal that can be rotated.

From the intensity of the diffraction peaks, it is possible to calculate coherent cross section by use of equation [11]:

$$F_{hkl}^2 = \frac{P_{hkl}}{P_0}\cdot\frac{4\pi r}{\lambda^3\cdot L\cdot h}\cdot\frac{\sin^2 2\theta}{e^{-\mu h\sec\theta}}\cdot\frac{1}{j_{hkl}\cdot M^2}\ , \tag{2}$$

where F_{hkl} structure factor; P_{hkl} and P_0 are the peak and incident beam intensities; λ the neutron wavelength; L and h the width and thickness of the specimen; M the number of molecules per cubic centimeter; μ the absorption (linear) coefficient; j the multiplicity factor for the planes in question; r distance of specimen from outlet thermal neutrons of gap; and θ the angle between the plane and beam.

In case of single-atom samples, like natural zirconium (Zr), scattering amplitude (f_0) is determined by use of formula [18]:

$$F_{hkl} = R_{hkl} . f_0\ , \tag{3}$$

were R_{hkl} is geometrical part of structure factor.

With use of f_0, it is possible to calculate coherent cross section by use of equation:

$$\sigma_{coh} = 4\pi(f_0)^2\ , \tag{4}$$

In figure 4 is shown neutron diffraction pattern taken for a crystal sample of natural zirconium (Zr) [17-20].

After calculations, value of coherent neutron scattering cross section (σ_{coh}) of natural zirconium obtained 6.41 barns.

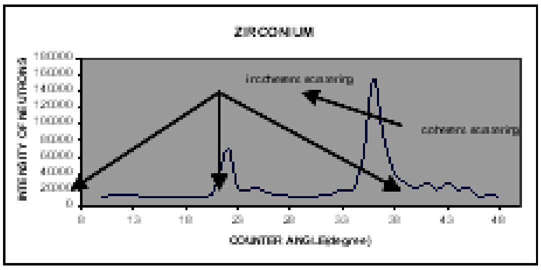

Fig .4. Neutron diffraction pattern taken for natural zirconium.

B) Method of calculation of total scattering cross section (σ_{tot})

For calculation of total scattering cross section (σ_{tot}), we can use of elements cross sections in MCNP code. MCNP has plotting capabilities. MCPLOT command, plots tally results produced by MCNP and cross section data used by MCNP.

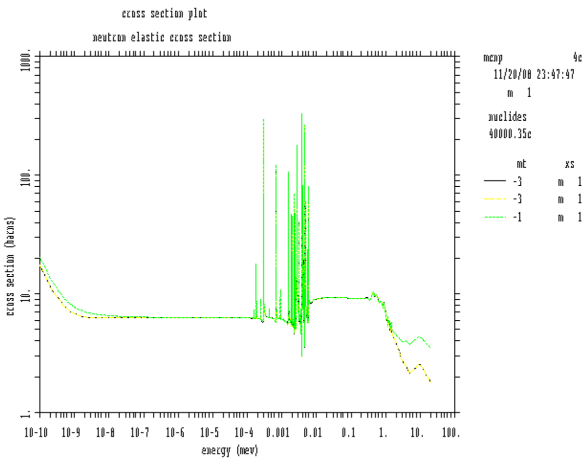

Fig. 5. Neutron total cross section and total scattering cross section for natural zirconium.

It can draw ordinary two-dimensional x-y plots, contour tally plots, More than one curve can be plotted on a single x-y plot. For natural zirconium, neutron total cross section and elastic scattering cross section are shown in fig.5. The neutron energy regime is from 10^{-10} MeV to 20 MeV. From this figure and use of effective scattering cross section in the laboratory system for neutrons in MCNP code, value of total neutron scattering cross section (σ_{tot}) in range of thermal neutrons for natural zirconium obtained 6.47 barns [1-4].

C) Definition of incoherent scattering cross section (σ_{inc})

We now calculate value of incoherent neutron scattering cross section (σ_{inc}) by use of formula: $\sigma_{inc} = \sigma_{tot} - \sigma_{coh}$, which has obtained 0.06 barns.

In table.1 is shown comparison of obtained results with experiment results [18, 22].

Table 1

Cross section (b)	Coherent scattering	Incoherent scattering	Total scattering
Laboratory	6.44	0.02	6.46
MCNP4C	6.41	0.06	6.47

4. Conclusion.

As one can see from this discussion, the computer simulation technique as MCNP4C code has enabled the determination of coherent and incoherent neutron scattering cross section. The power of this method can be further will be enhanced by proper combination of several methods from several computer simulation techniques to eliminate the ambiguities in complex crystals structure.

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MCNP4S KODU VASİTƏSİLƏ NEYTRONLARIN SİRKONİUM ELEMENTİNDƏN QEYRİ-KOHERENT SƏPİLMƏSİNİN EFFEKTİV KƏSİYİNİN TƏYİNİ

Materialların strukturlarının təyinində neytron kristalloqrafiyası effektiv metodlardan biridir. Lakin neytron mənbələrinin qurulub və istisması olduqca baha başa gəlir. Ən güclü neytron mənbəyi reaktordur ki, onun da qiyməti milyard dollardır. Bütün bunlar materialların xarakteristikalarının təyini üçün kompüter metodlarının işlənib hazırlanmasına səbəb olmuşdur. Kompüter metodlarında da neytron kristalloqrafiyası üçün müəyyən məhdudiyyətlər vardır. Baxılan işdə müvafiq kompüter metodları və MCNP4S kodu vasitəsilə neytronların difraksiya səpilmələrinin tədqiqindəki məhdudiyyətlərin aradan qaldırılması göstərilmişdir. MCNP4S kodu vasitəsilə neytronların sirkoniumdan qeyri-koherent səpilməsinin effektiv kəsiyi təyin edilmişdir.

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ОПРЕДЕЛЕНИЕ СЕЧЕНИЯ НЕКОГЕРЕНТНОГО РАССЕЯНИЯ НЕЙТРОНОВ НА ЦИРКОНИИ КОДОМ MCNP4C

Нейтронная кристаллография является эффективным методом для определения структуры материалов. Но строительство и содержание нейтронных источников очень дорогие. Самый мощный нейтронный источник - ядерный реактор, но его расходы составляют миллиарды долларов. Высокая стоимость была главным фактором для разработки компьютерных методов для определения характеристики материалов. В компьютерных методах тоже существуют ограничения для нейтронной кристаллографии. В данной работе показано, что с помощью компьютерного метода и кода MCNP4C можно устранить эти ограничения для исследования дифракционного рассеяния нейтронов. Кодом MCNP4C определяются сечения некогерентного рассеяния нейтронов на цирконии**.**

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