Vol 12 No 6, June 2003
1009-1963/2003/12(06)/0599-05

Chinese Physics

© 2003 Chin. Phys. Soc.
and IOP Publishing Ltd

Neutronics studies of solid targets for spallation neutron source using Monte Carlo simulation*

Yin Wen(殷 雯)[a)b)] and Liang Jiu-Qing(梁九卿)[a)]

[a)] *Institute of Theoretical Physics, Shanxi University, Taiyuan* 030006, *China*

[b)] *Institute of Physics, State Key Laboratory of Magnetism, Chinese Academy of Sciences, Beijing* 100080, *China*

(Received 26 February 2003; revised manuscript received 1 April 2003)

Neutronics studies for a solid target have been done with Monte Carlo high-energy particle transport code NMTC/JAM, when the proton beam with high kinetic energy bombards the target. The effect of the main parameters of the target on the neutron flux is discussed to optimize the target, which will be used for the concept design of the target of spallation neutron source. A target with its aspect ratio 1.5:1 or 2:1 gives the highest neutron flux. Tungsten is the most acceptable material from the technical and economical points of view. Beryllium as a moderating reflector can increase the neutron flux effectively.

Keywords: spallation neutron source, neutronics, optimal target
PACC: 2925D, 0650

1. Introduction

Neutron scattering is an important and powerful technique to investigate kinetic structure and dynamics on an atomic scale, complementary to other structural probes such as x-ray diffraction, transmission–electron microscope, etc. This technique was used in a variety of sciences, such as condensed matter physics, materials science, chemistry, polymer science, biology, engineering, etc, in the past 50 years. The importance of neutrons comes from their unique properties: penetrating, uncharged, magnetic moment and wavelengths comparable to interatomic distances in condensed matter.

Reactors have been the major neutron sources, which use the "proved" technique and have a great contribution to the neutron scattering research. However, the highest neutron flux available from a high-flux reactor is saturated since the 1970s. Pulsed spallation neutron source (PSNS) came out in the late 1980s, in which the available neutron flux was gradually getting higher. The time-fly electronic technique makes the neutron flux from PSNS on sample position one or two orders of magnitude higher than that from a high-flux reactor.

It is clear that there still exist many possibilities to improve the performance of PSNS.[1] The most important work is to optimize the source parameters and provide basic data necessary for engineering design. In this paper, the effect of the target on the neutron yield is discussed to determine the optimal material, shape and dimensions of the solid target by using the high-energy particle transport code NMTC/JAM,[2] which provides the primary information for further studies on the target-moderator-reflector system.

2. Calculation model

Spallation refers to a non-elastic nuclear interaction induced by a high-energy particle.[3,4] One important feature of spallation is the production of a large number of secondary particles. In the spallation reaction two-stage processes take place. In the first stage an incident particle such as proton collides with individual nucleons inside the nuclei of the target material and the struck nucleons with enough high energy will cause further collisions, forming a particle cascade called intranuclear cascade. In this stage the emission of various secondary particles, protons, neutrons, pions, etc, occurs. If the energy of these hadrons is higher than 15 MeV and the target is sufficiently thick, additional cascades will proceed by these hadrons. This process is called internuclear cascade or hadronic cascade. The cascades leave excited nu-

*Project supported by the Program of International Cooperation of Science and Technology (Grant No 2002 CB713903) and the National Natural Science Foundation of China (Grant No 10075302).

clei. The second process of the spallation reaction is the evaporation of low-energy (about 0.1–10 MeV) particles from these excited nuclei and the emission of neutrons, protons, deuterons, tritons, ^{3}He and heavier particles.

The high-energy part of the spallation reaction can be calculated by using a Monte Carlo high-energy particle transport code with an appropriate cross section library such as MCNP,[5] HETC/KFA2, SHIELD and NMTC/JAM. In NMTC/JAM the main control subroutine is to transport a source particle to the collision point or the boundary point of the region, losing the energy by ionization for charged particle under a Coulomb field or magnetic field. If the particle reaches the collision point, we check its energy. If the energy is above the cut-off energy, then the nuclear reaction is treated by the other subroutines. As an example, we consider the model for calculating the second stage of spallation: the evaporation of low-energy particles. The evaporation model is based on the Weisskopf–Ewing formula. According to this formula, the decay probability P_j for the emission of a particle j from a parent nucleus i with total kinetic energy in the centre-of-mass system between ε and $\varepsilon + \mathrm{d}\varepsilon$ is

$$P_j(\varepsilon)\mathrm{d}\varepsilon = g_j \sigma_{\mathrm{inv}}(\varepsilon)\frac{\rho_{\mathrm{d}}(E-Q-\varepsilon)}{\rho_i(E)}\varepsilon \mathrm{d}\varepsilon, \qquad (1)$$

where E is the excitation energy of a parent nucleus i with mass A_i and charge Z_i; d denotes a daughter nucleus produced after the emission of particle j; ρ_i and ρ_{d} are level densities of the parent and the daughter nucleus respectively; σ_{inv} is the cross section for the inverse reaction, which is expressed as follows.

For neutrons we have

$$\sigma_{\mathrm{inv}} = \sigma_{\mathrm{g}} c_{\mathrm{n}}(1 + b/\varepsilon). \qquad (2)$$

For charged particles we have

$$\sigma_{\mathrm{inv}} = \sigma_{\mathrm{g}} c_j(1 - V/\varepsilon), \qquad (3)$$

where the geometric cross section $\sigma_{\mathrm{g}} = \pi R_b^2$; c_{n}, c_j and b are the cross section parameters, and the Coulomb barrier $V = kZ_jZ_{\mathrm{d}}e^2/R_{\mathrm{c}}$. The parameter g_j in Eq.(1) is determined by the spin S_j and the mass m_j of the emitted particle j,

$$g_j = (2S_j + 1)m_j/\pi^2\hbar^2. \qquad (4)$$

The Q-value is calculated using the excess mass $M(A, Z)$,

$$Q = M(A_j, Z_j) + M(A_d, Z_d) - M(A_i, Z_i). \qquad (5)$$

The total decay width Γ_j can be calculated by integrating Eq.(1) with respect to the total kinetic energy ε from the Coulomb barrier V up to the maximum possible value $(E - Q)$. For neutrons, the total decay width for the particle emission is expressed as

$$\Gamma_j = \frac{g_j \sigma_{\mathrm{g}} c_{\mathrm{n}}}{\rho_i(E)} \int_V^{E-Q} (\varepsilon + b)\rho_{\mathrm{d}}(E - Q - \varepsilon)\mathrm{d}\varepsilon. \qquad (6)$$

For charged particles we have

$$\Gamma_j = \frac{g_j \sigma_{\mathrm{g}} c_j}{\rho_i(E)} \int_V^{E-Q} (\varepsilon - V)\rho_{\mathrm{d}}(E - Q - \varepsilon)\mathrm{d}\varepsilon. \qquad (7)$$

3. Calculated results

3.1. The effect of proton energy on neutron flux

The experimental values of the neutron yield increase with the energy of the incident proton.[6] However, the optimal proton energy must be determined by taking into account the energy cost required to produce one neutron. As the first step we consider the escaping neutron flux from the upper surface per incident proton energy as a function of proton energy under the same condition of the target.

A rectangular tungsten target with its dimensions 17.32 cm×5.77 cm×40 cm is bombarded by three proton beams whose energies are 1.6, 3.0 and 5.0 GeV respectively. The profile of the incident proton beam is also rectangular with its dimensions 13.86 cm×4.62 cm. The area of the proton beam is about 80% of that of the target. The tally zone extends from the upper surface to a height 1 cm away from the upper surface with its length equal to that of the target.

Figure 1 gives the results of the calculation. When the incident proton energy E_{p}=1.6 GeV, the neutron flux per proton energy is highest. With increasing E_{p} the peak flux decreases and shows a broader distribution. The peak fluxes at 3.0 and 5.0 GeV are approximately 80% and 60% respectively of the value at 1.6 GeV. This is because the proton energy consumed for the pion production increases with E_{p}, especially at above 1.0 GeV. As a result, the energy of the incident proton beam 1.6 GeV has been used throughout the calculation.

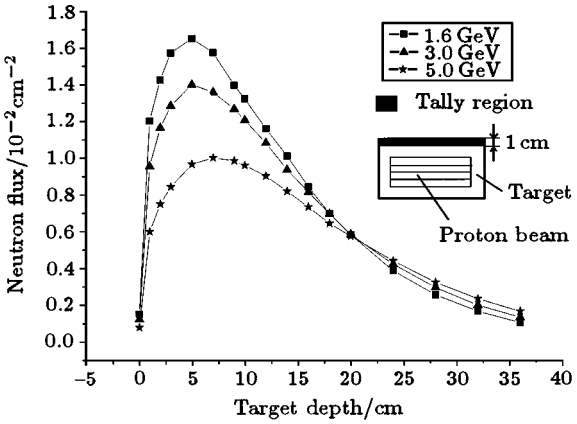


Fig.1. Comparison of calculated neutron fluxes produced by a proton from various incident proton energies.

For every tally position, the relative error does not exceed 5%.

3.2. The effect of materials of the target on neutron flux

Now, we consider which material will be the best for the production of neutron flux. Neutron flux as a function of the material of the target has been calculated. The neutron fluxes from uranium, tungsten, gold and lead are compared with one another. The main parameters of the incident proton beam and the target are the same as those described in section 3.1. The tally zone extends from the upper surface to a height 1 cm away from the upper surface with its length equal to that of the target.

Figure 2 shows the results of the calculation. Lead gives the lowest neutron flux due to its smallest atomic number density. Uranium gives the highest neutron flux because two nuclear reactions (spallation and fission) occur when the proton beam bombards the uranium target; however, the heat produced by this process is also the highest so that this will shorten the lifetime of the target and decrease its mechanical properties. After considering other properties such as strength, corrosion resistance, mechanical resistance and cost, tungsten (W) is the most acceptable material. As a result, tungsten has been used as the material of the target throughout the calculation.

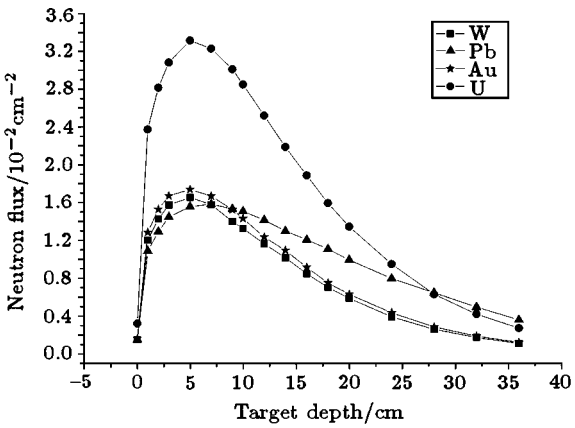


Fig.2. Comparison of calculated neutron fluxes produced by a proton from various target materials.

For every tally position, the relative error does not exceed 2%.

3.3. The effect of the shapes of targets on neutron flux

The neutron flux from a target depends not only on the proton energy, materials of the target but also on the target shape.[7] The effect of target shape on the neutron flux has been discussed by calculating various bare targets. The areas of the targets and proton beams, the tally zones for every shape of targets are kept the same so as to have a fair comparison. The main parameters are given in Table 1. The tally zone extends from the upper surface to a height 10 cm away from the upper surface with its length equal to 5 cm.

Table 1. Proton beam profile, target materials and dimensions.

Proton beam			Target		
Energy	Profile	Cross section/cm	Material	Shape	Dimension/cm
1.6 GeV	Rectangular	8.00×8.00	W	Rectangular	10.00×10.00c40.00
		9.80×6.53			12.25×8.17×40.00
		11.31×5.66			14.14×7.07×40.00
		13.86×4.62			17.32×5.77×40.00
		17.89×3.58			22.36×4.47×40.00

Figure 3 gives the results of the calculation. A flat target with a flat proton beam gives a higher neutron flux than a cylindrical target with a cylindrical beam. The bare rectangular target with its ratio of length to height 1.5:1 or 2: 1 will give the highest neutron flux. Although the target with its ratio of length to

height 3:1 or 5:1 can give more escaping neutrons, the number of the neutrons that can enter the tally zone (the position of moderator) is limited.

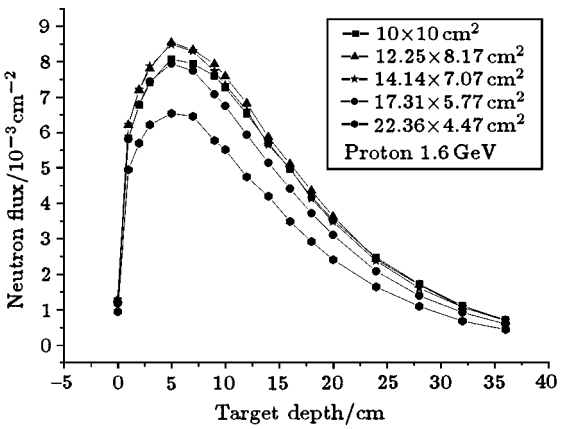


Fig.3. The effect of the shape of the target on neutron flux.

For every position, the tally relative error does not exceed 5%.

3.4. The effect of target thickness on neutron flux

Then we consider the effect of target thickness on neutron flux. The targets with different thicknesses 20, 40 and 60 cm are bombarded by proton beams. The other parameters of the targets and proton beams are the same as those described in section 3.1. The tally zone extends from the upper surface to a height 1 cm away from the upper surface with its length equal to that of the target.

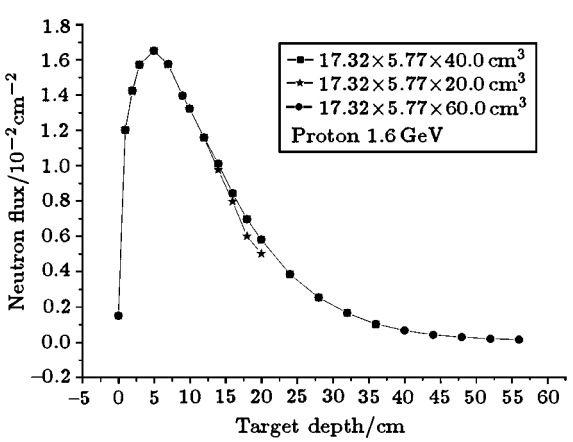


Fig.4. The effect of the thickness of the target on neutron fluxes.

Figure 4 gives the results of the calculation. If the thickness of the target satisfies the condition that nuclear collisions take place before the incident particles reach the end of its range, the thickness of the target will not influence the neutron flux obviously. This gives a flexibility in the target engineering design.

For every position, the tally relative error does not exceed 5%.

3.5. Neutron production in the target-reflector system

In spallation sources neutrons are produced in a target as well as in a reflector.[8] The main processes of the neutron production are spallation reaction induced by energetic hadrons escaping from the target and (n, xn) reactions in the reflector. The reflector materials are classified into two categories: moderating and non-moderating. Beryllium is a typical moderating reflector material, while lead is a typical non-moderating one. There are some merits and demerits in each type. In our work, the effect of a cylindrical beryllium reflector, with its diameter 60 cm and height 100 cm surrounded by a cylindrical iron shield with its diameter 100 cm and height 100 cm, on neutron flux have been calculated. A rectangular target with its dimensions 7.5 cm×5.0 cm×40.0 cm are bombarded by the proton beam with a rectangular profile, whose dimensions are 6.0 cm×4.0 cm. Tally zone extends from the upper surface to a height 10 cm away from the upper surface with its length equal to 5 cm.

Figure 5 gives the difference between a bare target and a target-reflector system, beryllium as a moderating reflector increases the neutron flux effectively. It is not only because beryllium can reflect the leakage neutrons from the target, which do not directly enter the moderator, towards the moderator, but also because the number of neutrons produced in it by spallation is 4%, and by (n,2n) reactions is 18% of the target neutron yield.

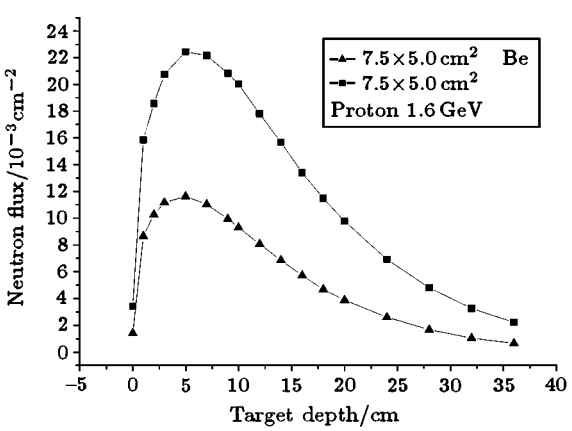


Fig.5. Calculated neutron flux produced by a proton with or without a beryllium reflector.

For every position, the tally relative error does not exceed 5%.

4. Conclusion

Optimizing the parameters of the spallation neutron source can bring about better neutronic performance for neutron scattering and other neutron beam experiments. In this paper our main purpose is to gain the optimal target by neutron flux calculations with Monte Carlo code NMTC/JAM for various targets, and to provide the primary information for further studies on a target-moderator-reflector system.

Acknowledgments

The authors would like to thank Japan Atomic Energy Research Institute for granting the permission to use Monte Carlo code NMTC/JAM and other helps.

References

[1] Russell G J 1990 *ICANS Proc.* (XI) 291
[2] Koji N *et al* 2001 *High Energy Particle Transport Code NMTC/JAM* (Tokai-mura: Japan Atomic Energy Research Institute)
[3] Watanabe N 2002 *Neutronics of Pulsed Spallation Neutron Source* (Tokai-mura: Japan Atomic Energy Research Institute) p 5
[4] Watanabe N 2002 *Neutronics of Pulsed Spallation Neutron Source* (Tokai-mura: Japan Atomic Energy Research Institute) p 8
[5] Mu W B *et al* 2001 *Acta. Phys. Sin.* (in Chinese) **50** 189
[6] Vassil R G 1990 *ICANS Proc.* (XI) 340
[7] Teshugawara M *et al* 1999 *Neutronics Studies of Bare Target for JAERI* 5MW *Pulsed Spallation Neutron Source* (Tokai-mura: Japan Atomic Energy Research Institute)
[8] Kiyanagi Y *et al* 1998 *ICANS Proc.* (XV) 478