Investigation on Thermal Neutron Scattering for Al_20_3 Filter in Support of PGNAA in Xian Pulsed Reactor

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Abstract

Thermal neutron filters in reactor port are routinely used for spectral shaping in neutron beam applications, which can reduce epi-thermal and fast neutron components. Sapphire (Al_2O_3) is usually employed as filters in facilities with thermal neutron beams. However, thermal neutron scattering libraries for Al_2O_3 are lacked in the original ENDF at present. Then simulation code (e.g., MCNP) can only deal with Al_2O_3 with standard free gas model, which cannot appropriately account for the physics of the interaction of the thermal neutrons. In this paper, based on the ab initio method of quantum mechanics, the phonon density of states in Al and O in Al_2O_3 were calculated using VASP and PHONON code. NJOY code has been used to generate ACE format data of Al and O in Al_2O_3 thermal neutron scattering cross sections at different temperatures, which were also validated with available experimental data. The generated cross sections allowed us to study the quality of this filter. Furthermore, the study of the influence to PGNAA design in Xi'an Pulsed Reactor of neutron scattering law data in Al_2O_3 also indicated that the use of selected S(α,β) data could lead to an improvement in thermal neutron scattering simulation of thermal neutron behavior. Different thickness and scattering model of Al_2O_3 filter was analyzed. Neutron group flux and Gamma flux distribution along the XAPR radial 1# port was compared. Results indicated that compared with free gas model, thermal neutron scattering cross sections with an accurate phonon model could capture the phenomenon of neutron Al_2O_3 filtration and enhanced thermal neutron fraction remarkably. A reliable thermal neutron scattering cross section library of Al_2O_3 for thermal scattering calculations was created in this paper, which laid a technical foundation for the PGNAA application in Xi'an Pulsed Reactor of radial 1# port using Al_2O_3 as its thermal neutron filter.