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International Conference on Physics of Reactors 2020

Structure-Dependent Doppler Broadening Using a Generalized Thermal Scattering Law

The thermal scattering law (TSL), i.e. S(α,β), represents the momentum and energy exchange phase space for a material. The incoherent and coherent components of the TSL correlate an atom's trajectory with itself and/or with other atoms in the lattice structure. This structural information is especially important for low energies where the wavelength of neutrons is on the order of the lattice interatomic spacing. Both thermal neutron scattering as well as low energy resonance broadening involve processes where incoming neutron responses are lattice dependent. Traditionally, Doppler broadening for absorption resonances approximates these interactions by assuming a Maxwell-Boltzmann distribution for the neutron velocity. For high energies and high temperatures, this approximation is reasonable. However, for low temperatures or low energies, the lattice structure binding effects will influence the velocity distribution. Using the TSL to determine the Doppler broadening directly introduces the material structure into the calculation to most accurately capture the momentum and energy space. Typically, the TSL is derived assuming cubic lattice symmetry. This approximation collapses the directional lattice information, including the polarization vectors and associated energies, into an energy dependent function called the density of states. The cubic approximation, while valid for highly symmetric and uniformly bonded materials, is insufficient to capture the true structure. In this work, generalized formulation for the exact, lattice-dependent TSL has been implemented within the Full Law Analysis Scattering System Hub using polarization vectors and associated energies as fundamental input. These capabilities are utilized to perform the generalized-structure Doppler broadening analysis for UO_2.