Investigation of Thermal Neutron Scattering Data Evaluation for H in ZrHx

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Abstract: Traditional evaluation process in the past was usually done by using differential experimental data which was then complemented with nuclear model calculations. This trend is fast changing due to the increase in computational power and tremendous improvements in nuclear reaction models over the last decade. The behavior with the energy of the neutron cross sections of hydrogen in ZrH_x depends on the Thermal Scattering Laws tabulated in terms of S(α,β). However, uncertainties on the corresponding S(α,β) were never reported. And till now no recommended procedure exists for computing covariance of TSLs available in the international evaluated nuclear data libraries. In the previous work, based on differential experimental nuclear data, the phonon model parameters related to a semi-empirical phonon model were adjusted by the uniform Monte Carlo method. The covariance of TSLs for H in ZrH_x was generated ignoring the integral experiments’ result. Considering that Monte Carlo method consumes much time in data assimilation, this work presents another deterministic nuclear data adjustment methodology to produce such a covariance matrix-associated to the same phonon model using both differential and integral experiments, in which Generalized Non-Least Square (GNLS) method was used to adjust the phonon model parameters on evaluated data and generate covariance matrices between the phonon model parameters. It can be observed that after data adjustment, the error and uncertainty of the differential cross-section data and integral data are both reduced.

中文摘要：过去的传统评价过程通常是利用微分实验数据，然后再加上核模型计算完成。在过去的十年中，由于计算机模拟水平的增加和核反应模型的巨大改进，这一趋势正在迅速改变。ZrHx中H的热中子散射截面的能量行为取决于用 S（α，β）表示的热散射律。然而，对相应的 S（α，β）的不确定性从未被报道过。到目前为止，还没有推荐的程序可用于计算国际评价核数据库中的S（α，β）的协方差。在以前的工作中，基于微分实验核数据，用统一的蒙特卡罗方法对半经验声子模型的声子参数进行了调整，在不考虑积分实验结果的情况下，生成了 ZrHx中H的S（α，β）协方差。考虑到蒙特卡罗方法在数据同化方面花费了大量时间，本文提出了另一种确定论的核数据调整方法，利用微分和积分实验相结合的方法，基于广义非最小二乘法（GNLS）对热中子散射数据上的声子模型参数进行调整，并在模型参数之间生成协方差矩阵。从结果中国可以观察到，经过数据调整后，微分截面数据和积分数据的误差和不确定度都减小了。