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TITLE: **Improvements To The Nuclear Model Code Gnash For Cross Section Calculations At Higher Energies**

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IMPROVEMENTS TO THE NUCLEAR MODEL CODE GNASH FOR CROSS SECTION CALCULATIONS AT HIGHER ENERGIES

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ABSTRACT

The nuclear model code GNASH, which in the past has been used predominantly for incident particle energies below 20 MeV, has been modified extensively for calculations at higher energies. The model extensions and improvements are described in this paper, and their significance is illustrated by comparing calculations with experimental data for incident energies up to 160 MeV.

I. INTRODUCTION

We have made a number of modifications to the nuclear model code GNASH[1] in order to improve the accuracy of calculations at incident particle energies up to 200 MeV. Most important among the changes is the adaptation of the code to permit its use in conjunction with quantum mechanical preequilibrium calculations, implementing (and extending) the theory of Feshbach, Kerman, and Koonin[2] (FKK) in our FKK-GNASH version of the code.[3] We have also incorporated a model for calculating multiple preequilibrium effects, that is, we permit particle-hole states left after the first preequilibrium particle is emitted to further decay by "multiple preequilibrium" emission.[4] We demonstrate below that it is important for certain applications to include multiple preequilibrium effects for secondary neutrons and protons as well as the usual corrections in the primary decay channels. Additionally, we have developed an FKK-based formalism for estimating spin distributions in preequilibrium reactions and have used this result to obtain an easily applicable method for including spin effects in an exciton model.[5]

In this paper we illustrate the significance of the model improvements and include comparisons of calculations with experimental data for several target materials. We apply both GNASH and FKK-GNASH to calculate *(p,xn)* and *(p,xp)* reactions for incident energies to 160 MeV (part of a recent Nuclear Energy Agency code Intercomparison),[6] which allows a comparison of semiclassical and quantum descriptions of preequilibrium emission for high energies. We also investigate angular momentum effects in our new equilibrium and preequilibrium modeling by analyzing two phenomena sensitive to spin distributions: *(n,xnγ)* discrete gamma-ray production for incident neutron energies to 200 MeV, and long-lived isomer production in reactions important for fusion technology.

II. Standard Models in GNASH

The standard GNASH code implements Hauser-Feshbach theory in an open-ended sequence of reaction chains, with full conservation of angular momentum. Transmission coefficients for particles are obtained from optical model calculations and for gamma rays from a generalized Lorentzian giant dipole resonance model. In addition, optical model potentials are used to obtain initial compound nucleus formation cross sections, which then determine the overall normalization of all calculated emission cross sections. Continuum level densities are obtained from phenomenological level density functions, which are matched at lower excitation energies to discrete level data. Both discrete and continuum structure data are utilized in GNASH calculations. Preequilibrium corrections, which become increasingly important at energies above 10 MeV, are made in the original GNASH code using a semiclassical exciton model.[7] For actinide studies, the code contains a detailed fission model, allowing use of up to three uncoupled fission barriers.

III. Model Extensions for Higher Energy Calculations

A number of model improvements have been incorporated in the GNASH code system that enhance its capabilities in calculations for incident energies above ~20 MeV. These include improved level density representations as well as more appropriate direct reaction models and higher energy optical model potentials.[8] In the sections below we describe improved capabilities for calculating preequilibrium reactions in the FKK-GNASH code.

A. FKK-GNASH

With a view toward improved predictive capabilities, the existing semiclassical preequilibrium model in

GNASH has been complemented with an improved quantum mechanical model from FKK preequilibrium theory in our FKK-GNASH code. FKK theory, which has been used successfully to calculate nucleon-induced reactions up to the pion threshold, describes reactions as passing through a series of particle-hole excitations, caused by nucleon-nucleon interactions as the nuclear system evolves towards equilibrium. Preequilibrium emission occurs when particle decay takes place from simple particle-hole stages early in the reaction, and typically results in high-energy and forward-peaked particle emission. In the FKK theory two different types of preequilibrium emission can occur: multistep direct (MSD) and multistep compound (MSC). In FKK-GNASH, we combine the MSD and MSC preequilibrium components with full Hauser-Feshbach calculations, which allows the whole particle and gamma-ray emission spectrum to be calculated in a consistent manner.

The FKK-GNASH code has been used to calculate neutron and proton emission spectra from n + ^{93}Nb reactions[3] and from p + ^{90}Zr and p + ^{208}Pb reactions.[6] The latter calculations are part of a code intercomparison activity by the NEA, which also includes calculations using our standard GNASH code. A comparison of calculated and measured[9] angle-integrated neutron emission spectra for 160-MeV proton reactions on ^{90}Zr is given in Fig. 1, and comparisons of the angular distributions are given in Fig. 2 for emission energies of 80, 100, and 140 MeV. Both the FKK-GNASH and standard GNASH calculations are seen to reasonably reproduce the measured data. Angular effects are incorporated in the standard GNASH results by means of the systematics of Kalbach,[10] which appear to be valid out to back angles. The FKK-GNASH calculations reproduce the angular distribution reliably at angles below ~100° but tend to fall off too rapidly at far back angles.

B. Multiple Preequilibrium

The FKK theory, as originally formulated, only takes into account the preequilibrium emission of one particle (primary preequilibrium emission). The assumption is that this particle carries away so much energy that the remaining excited residual nucleus cannot emit another preequilibrium particle, and instead becomes equilibrated before undergoing compound-nucleus decay. This assumption begins to fail, however, for nucleon energies above a few 10's of MeV, where it becomes possible to emit more than one particle through a preequilibrium mechanism. We refer to this process as multiple preequilibrium and have developed formalisms for computing its effects, both a preliminary version in the context of the exciton model[8] (as shown in Fig. 1) and a preferred model utilizing FKK theory.[4] This latter model makes use of DWBA matrix elements that are already determined in FKK calculations of primary preequilibrium and is therefore straightforward to implement in FKK calculations.

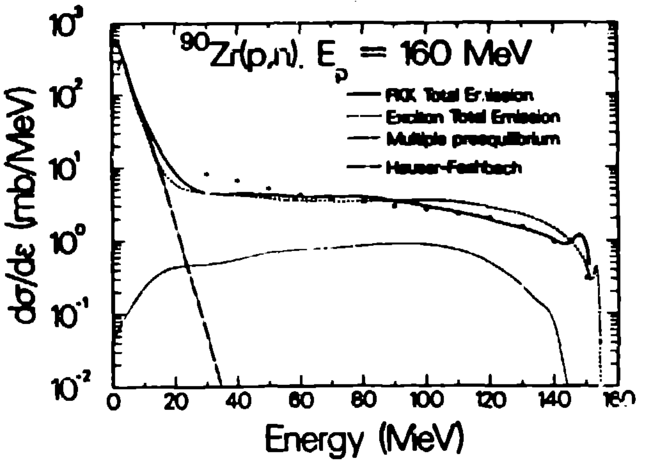

Fig. 1. Comparison of calculated and measured[9] angle-integrated neutron emission spectra from p + ^{90}Zr reactions at a proton energy of 160 MeV.

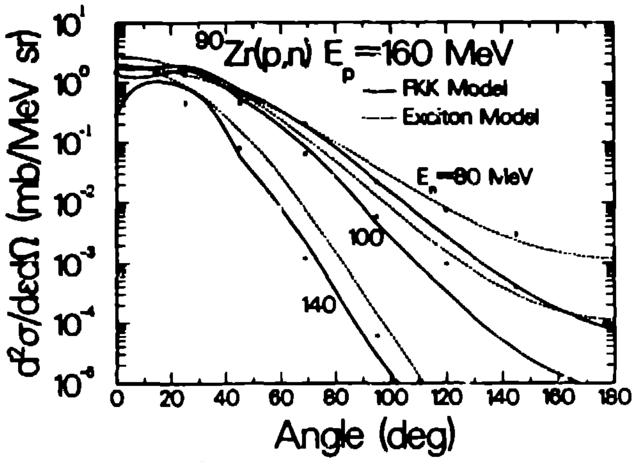

Fig. 2. Measured[9] and calculated angular distributions of neutrons from ^{90}Zr(p,xn) reactions for E_p = 160 MeV at several emission energies.

A clear indication of the importance of including multiple preequilibrium processes in calculations above ~30 MeV can be seen in comparisons of theoretical calculations with high-resolution measurements of gamma-ray excitation functions from (n,xnγ) measurements. Calculations with and without multiple preequilibrium are compared to measurements[11] of the 0.803-MeV gamma-ray from the ^{207}Pb(n,2nγ) reaction in Fig. 3, which results from decay of the 2^+ first excited state of ^{206}Pb to the 0^+ ground state. This type of reaction is particularly sensitive to multiple preequilibrium effects because the additional high-energy component in neutron emission

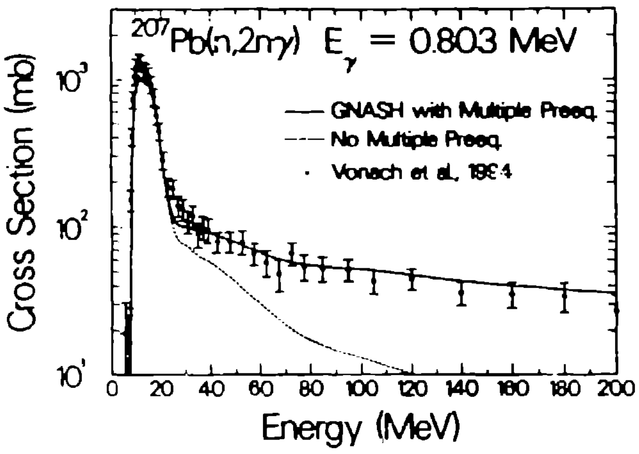

Fig. 3. Calculation of the ^{207}Pb(n,2nγ) cross section with and without multiple preequilibrium compared to experimental data.[11]

from the (n,2n) reaction (relative to the equilibrium process) leads to greatly enhanced (n,2nγ) cross sections at higher incident energies.

We have also demonstrated the importance of multiple-preequilibrium effects by imposing the constraint of unitarity on calculations of p + ^{90}Zr calculations at 80 and 160 MeV.[4] These calculations show that if multiple preequilibrium effects are ignored and experimental ^{90}Zr(p,xp) and (p,xn) data are fit by including only primary preequilibrium, then the sum of the primary preequilibrium cross sections exceeds the reaction cross section at 80 MeV by ~15% and at 160 MeV by ~50%. It should be emphasized that conclusions such as these based on theoretical/experimental comparisons can only be drawn if the calculations include a complete description of all contributing processes.

C. Spin Effects in Preequilibrium

We have developed an MSD formalism within the FKK theory that accounts for nonzero spin in preequilibrium reactions (such a formalism was developed earlier for MSC reactions[12]) and, by considering the relationships between FKK/MSD and exciton theory, also have obtained a new and easily applicable method for including spins in the exciton model.[5] In the FKK/MSD case, we remove the original FKK spin-zero approximation by treating the $1p1h$ states excited in the interaction as absorbing the transferred angular momentum, after which their angular momentum couples with the intrinsic "core" spin of the target. This allows us to use much of the existing MSD calculational formalism while accounting for finite intrinsic spin in a straightforward manner. The extension to the exciton model was motivated by the work of Akkermans and Koning,[13] who observed how the FKK and exciton models relate to each other. The result for the exciton model spin distribution of residual nuclei from a preequilibrium stage N is given by

$$P_N(J) = \frac{(2J+1)}{(2I+1)(2i+1)} \sum_{S_f=0}^{1} \frac{1}{(2S_f+1)} \sum_{S=|I-S_f|}^{I+S_f} \sum_{\ell=|J-S|}^{J+S} R_n(\ell), \quad (1)$$

where $n = p + h = 2N$, where i designates projectile and ejectile spins, I is the target spin, J is the spin of the residual nucleus through coupling with angular momentum ℓ and spin flip S_f, and $R_n(l)$ is a Gaussian angular distribution function

$$R_n(\ell) = \frac{2\ell+1}{2\sqrt{2\pi}\,\sigma_n^3} \exp\left[-\frac{(\ell+\frac{1}{2})^2}{2\sigma_n^2}\right], \quad (2)$$

and $\sigma_n^2 = 0.24nA^{2/3}$ is the spin cut-off.

We have compared the FKK and exciton spin-distribution models by calculating 14-MeV neutron-induced reactions on ^{179}Hf that produce the 25.1-d, 25/2⁻ isomeric state in ^{179}Hf (E_x = 1.11 MeV) and the 31-y, 16⁺ isomer in ^{178}Hf (E_x = 2.45 MeV).[5] We find that the preequilibrium spectra from the two models are quite similar at higher excitation energies, but the FKK spectra is reduced relative to the exciton spectra at lower emission energies. This effect occurs because the multistep contributions in the FKK calculations are significantly smaller than in the exciton case. For example, at 5 MeV residual nucleus energy the FKK 2nd-step is only 3% of the 1st-step, compared to 17% for the exciton case. This, along with the large microscopic DWBA amplitudes we obtain for low ℓ transfers, leads to a FKK spin distribution weighted toward lower spins than in the exciton model case, as is shown in Fig. 4.

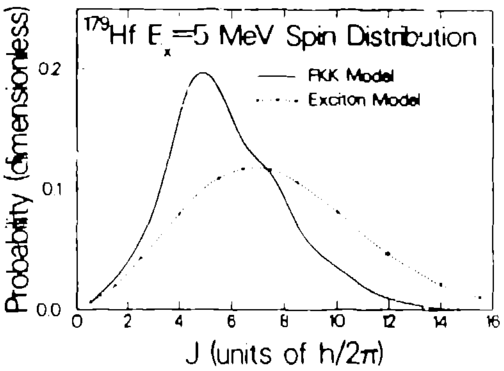

Fig. 4. Comparison of residual spin distribution in ^{179}Hf at an excitation energy of 5 MeV using FKK and exciton preequilibrium models.

The results of the isomer-production calculations from the FKK and exciton models are compared to experimental data[14] in Table 1. The different spin distributions from the two models lead to significantly different isomer cross sections. In fact, however, the uncertainties in the calculation (mainly neutron transmission coefficients and structure data) are sufficiently large that either model leads to results reasonably consistent with the experimental data, although the FKK values are somewhat low. Our new exciton model calculations agree better with the measurements than our earlier ones, which assumed equilibrium spin distributions for both equilibrium and preequilibrium reactions.[15]

Table 1. Theoretical and Experimental 14-MeV Neutron-Induced Cross Sections for the Production of Isomeric States in Hafnium

Reaction	FKK Model	Exciton Model	Experiment[14]
^{179}Hf(n,2n) $\rightarrow^{178m2}$Hf [16$^+$]	2.33 mb	10.82 mb	6.29 ± .35 mb
^{179}Hf(n,n') $\rightarrow^{179m2}$Hf [12.5$^+$]	2.93 mb	15.23 mb	12.8 ± 1.5 mb

IV. Conclusions

The FKK and exciton models that we have developed and incorporated into the GNASH-FKK code have been shown to give a very satisfactory description of preequilibrium reactions out to an incident nucleon energy of 160 MeV. We have summarized a formalism for determining multiple preequilibrium emission that is straightforward to implement in FKK/MSD calculations and have demonstrated the importance of multiple preequilibrium reactions at higher energies. In particular, inclusion of this effect is essential if agreement with measurements of particle emission spectra and flux conservation are to be simultaneously achieved. Finally, we have presented an MSD formalism that accounts for finite spins, and have developed a new and easily applicable method for including spin effects in the exciton model.

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