STATUS OF THEORIES FOR CALCULATIONS OF PRODUCTION CROSS SECTIONS OF LONG-LIVED RADIONUCLIDES

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INTRODUCTION

The theories discussed in this paper are confined to those currently being used or considered for the calculation of activation cross sections. The theories are the same regardless of whether the activation product is long lived or short lived. However, the cross sections for the generation of long-lived radionuclides are more difficult or expensive to measure, hence there are fewer data available and the requirement on the predictive capability of the theories used is more stringent.

It is clear from other papers presented in this meeting and the adjoining NEANDC specialists' meeting on activation cross sections that the nuclear theories of interest to this group are those used or needed in modern Hauser-Feshbach (H-F) codes with pre-equilibrium correction and gamma-ray cascades. The H-F formalism is indispensible due to the sensitivity of the calculated results, especially isomeric ratios, to the spins and parities of the discrete levels as well as to the spin distributions in the total and exciton level densities.

Topics included in this paper are the optical model, gamma-ray strength function, total and exciton level-density theories, and the pre-compound model. In each subject, we describe the most commonly used theories first, followed by relatively new developments that are used in at least one model code or the promising theories that do not appear to require a large effort for incorporation into existing H-F codes.

OPTICAL MODEL

The transmission coefficients for the incident and outgoing particles calculated by the optical model are basic ingredients in the H-F formalism. The spherical optical model can calculate such coefficients rather quickly, and most H-F codes now contain an in-house spherical optical model code with built-in global optical model parameters as options. Because the computer cost is still quite large for deformed optical model or coupled-channel calculations, it is more economical to separate the calculation of the transmission coefficients from the rest of the H-F calculations.

For quick calculation of activation cross sections, one would use the global optical model parameters. For more sophisticated analysis, one adjusts the parameters to fit as many experimental data as possible, particularly the total cross sections, s-wave strength function, differential elastic, (p,n), and (α,n) cross sections. Even so, one still encounters troubles such as the 1-MeV minimum in the total cross sections, as discussed below.

The dispersion relations connecting the real and imaginary parts of the optical potential remove many of the anomalies that arise when the spherical optical model is used to analyze accurate neutron data[1]. Of primary concern to the calculation of activation cross sections is the well known fact that the global optical potentials all over-estimate the neutron total cross sections in the region of the minimum around 1 MeV and the calculated

(n,n') and (n,2n) cross sections just above threshold. It is now known that a consistent dispersion analysis gives smaller values of the total cross sections near the 1-MeV minimum in agreement with the experimental data[1,2,3]. Since the dispersion relations also represent the coupling of the elastic and inelastic channels, a consistent dispersion analysis of total cross sections and differential elastic scattering data would also lead to improved reliability and extrapolability in the calculated (n,n') and (n,2n) cross sections as well.

GAMMA-RAY STRENGTH FUNCTION

Theories of gamma-ray strength functions are important for the correct prediction of (n,γ) cross sections where normalization to experimental data is impossible, and for the calculation of (n,z) cross sections above (n,zn) threshold. The giant dipole theory of Brink-Axel[4] is commonly used for E1 and the Blatt-Weisskopf estimates for M1, E2, etc. The predictability of this approach is no better than a factor of two even in the presence of reliable (γ, n) data for the giant dipole resonance. A common remedy is to normalize calculated $\langle\Gamma_{\gamma 0}\rangle/D_0$ values to measured data. Better approaches are emerging to improve the reliability of the calculation in the absence of data, as described below.

Kopecky and Uhl[5] applied the depressed giant dipole model and Gardner and Gardner[6] the energy-dependent Breit-Wigner model to the calculation of (n,γ) cross sections, isomeric ratios, and gamma-ray production spectra. These models give smaller gamma-ray strength functions around 7 MeV than result from using the giant dipole resonance and are in better agreement with the experimental data. These models are easy to implement and may soon be widely adopted in model codes. There is evidence[5,6] that the M1 strength function can be related to a giant resonance around 8 MeV with a width of about 4 MeV.

LEVEL-DENSITY THEORIES

Both the total and exciton level-density formulas are used in modern H-F codes. A common practice is to use the two-Fermion total level-density formula (the Fermi gas formula as in Gilbert and Cameron[7]) for the Hauser-Feshbach part of the calculation and the one-Fermion exciton level-density formula for the precompound part and normalize the sum of the latter to the former at each excitation energy to force consistency. This has been pointed out[8] to be incorrect because the exciton-number dependences in the one- and two-Fermion exciton level-density formulas are also different. It was pointed out that the normalization practice would lead to a harder emission spectrum that may agree with experimental data but in reality only masks the collective component.

Another problem in making a precompound correction to the H-F calculation is the consistency between the total and exciton level densities. It is well known that the total level-density formula has a constant-pairing-energy correction while the pairing correction in the exciton level-density formula depends on both energy and exciton number. An advanced but simple formula for the latter has been developed[9,10,11] and its use in H-F codes is spreading.

Calculations (for example, see Ref. 12) of exciton level densities from realistic single-particle states naturally account for the pairing and shell effects. In particular, such calculations show large differences between the particle and hole excitations and strong isotopic and isotonic effects. A simple method[12] for estimating such effects in the exciton state-density formula has been proposed and is expected to be used soon.

PRE-COMPOUND MODEL

All calculations of activation cross sections presented in this meeting included pre-equilibrium effects. The current approach in H-F codes is to combine the pre-equilibrium results, calculated without angular momentum conservation, with the H-F part that conserves angular momentum. There are several ongoing efforts (for example, see Ref. 13) to make the two parts of the calculation as consistent as possible. Angular momentum conservation in the pre-equilibrium model automatically accounts for the enhanced surface emission and may lead to improved accuracy in the calculated isomeric-ratios. Alpha-cluster formation is also known to be sensitive to angular momentum effects.[14]

CONCLUSION

It is clear that the H-F codes used for the calculation of cross sections are still being improved and meetings such as the present one provide an opportunity for worldwide interaction between the basic and applied physics communities. Many interesting problems in nuclear theories and their implementation in H-F codes exist and call for action. Since the need for activation cross-section data cannot wait for better theories and codes, what we tend to do at present is to over-stretch the model parameters to fit the available data, hence the predictability of the present generation of model codes remains unsatisfactory – probably around a factor of two. When improvements discussed in this paper are implemented, the ability of the codes to predict activation cross sections will improve.

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