III.B.4. Crystal-Lattice Model of Doppler Broadening

The crystal-lattice model (CLM) of Doppler broadening used in SAMMY is based on the DOPUSH model of Naberejnev [DN99, DN99a], which in turn is based on the LEAPR model of NJOY [RM82]. Only the continuous and the discrete modes were developed further in DOPUSH.

(Readers are encouraged to consult the references for a description of the physics; a later revision of the SAMMY manual will include more detail. Alternative descriptions can be found in works by Meister [AM94].)

The algorithm used in SAMMY is virtually identical to the algorithm used in the DOPUSH code, where "identical" implicitly implies "for the examples that were available." No attempt has yet been made by this author to extend the validity of the model beyond ensuring agreement between DOPUSH and SAMMY when run with the same input.

Prior to implementing the DOPUSH CLM into SAMMY, this author created a modified version of DOPUSH (denoted DOPUSHx) which uses the same input and runs in the same manner as DOPUSH but whose coding is streamlined and more readily portable than the original DOPUSH code. Below is an itemization of the changes made for DOPUSHx (and also incorporated into SAMMY).

1. Values of physical and mathematical constants conform to ENDF standards. See Section IX.A of this document.

2. One or two "trivial" errors were corrected [notably, mass-factor self-consistency is ensured by using $(M+m)/M$ not $(M+1)/M$ with M and m in units of amu].

3. Redundant calculations were moved outside the energy loops; many of the intermediate computations required for convolving the phonon distributions are energy independent and do not need to be repeated for each energy. This change resulted in a significant decrease in computer processor unit (cpu) time.

4. More efficient sorting algorithms are employed; in general, FORTRAN operations have been made more efficient.

Changes made from DOPUSHx to SAMMY include the following.

1. Nomenclature has been modified to conform to SAMMY conventions.

2. Savings in cpu time from DOPUSHx to SAMMY are primarily the result of SAMMY's organizational scheme, in which the unbroadened cross sections are first calculated on an energy grid designed to describe the curvature of the cross section with reasonable accuracy, assuming a quadratic interpolation scheme. When the unbroadened cross section is required at a different energy, interpolation is used. In contrast, DOPUSH and DOPUSHx re-calculate the unbroadened cross section whenever it is needed, using algorithms similar to those employed in NJOY. (The cost which SAMMY users must pay for this increased speed

is that the accuracy of integrations cannot be tested during the integration process, as it is in NJOY. SAMMY users are reminded to make such tests themselves in order to have full confidence in their results.)

The examples of input for DOPUSH which were provided by Naberejnev have been organized into SAMMY test case tr124. For those examples that run on all three programs (DOPUSH, SAMMY, & DOPUSHx), the three codes give virtually the same results. The time required for the computations is significantly shorter with the newer codes (details available from the author upon request). This is true even when the number of points in SAMMY's auxiliary grid was increased dramatically (NXTRA was changed from 0 to 99), as a double-check on the accuracy of SAMMY's calculation. Accuracy was not significantly affected by the additional energy points, indicating that SAMMY's original grid is sufficiently dense.

For this release of SAMMY, no attempts have been made to improve or expand upon the model as provided by Naberejnev. One improvement that will likely be made for a subsequent release is the ability to treat the temperature as a search parameter in the fitting procedure.

For a description of the input to SAMMY's CLM, see Section VI.F.5.