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ITS Version 3.0: Powerful, User-friendly Software for Radiation Modelling

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Abstract

ITS (the Integrated Tiger Series) is a powerful, but user-friendly, software package permitting state-of-the-art modelling of electron and/or photon radiation effects. The programs provide Monte Carlo solution of linear time-independent coupled electron/photon radiation transport problems, with or without the presence of macroscopic electric and magnetic fields. The ITS system combines operational simplicity and physical accuracy in order to provide experimentalists and theorists alike with a method for the routine but rigorous solution of sophisticated radiation transport problems.

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Introduction

Since numerical experiments tend to be cheaper than physical ones, computer modelling of applications of electron beams can be very advantageous provided that the software is sufficiently easy to use, sufficiently flexible to model the important parts of the hardware, and sufficiently accurate for confidence in the results. Such modelling could be used, for example, in personnel hazard assessment when designing an accelerator or in process optimization

Overview of the Monte Carlo Method

Since ITS is a Monte Carlo code, there are a few aspects of the Monte Carlo method of which users must be aware. It has a reputation for being very accurate, but also very time-consuming. As affordable fast computers are becoming commonplace, the time concern is no longer as great as it once was.

The method is based on statistical averaging of individual trials to estimate the desired numerical answer. A specific trial is constructed by using random numbers to sample from appropriate probability distribution functions such as those that describe the motion of an electron moving in a given material at a specified energy, the generation of secondary particles, and the motion of these particles and any further cascade.

Due to the statistical nature of the results, any quantity of interest calculated by the code must have attached to it another quantity which represents the estimated statistical accuracy, typically expressed in terms of a standard deviation. It is important to keep the code's estimate of the standard deviation a small fraction of the calculated quantity of interest. As this estimated fraction becomes larger, the statistical confidence in the calculated quantity of interest decreases. When this estimated fraction becomes large (greater than, say, 10%), the estimated fraction itself is unreliable and may be larger than what is indicated.

The U.S. national laboratories have developed powerful computer programs to solve such problems to help accomplish their missions. Since these codes have been supported by tax dollars, the unclassified programs are made generally available when it seems they may have other applications. The Integrated TIGER Series (ITS) (Ref. 1) is one of these computer packages. The "integration" was performed to make it easier to maintain and easier for the user (and developer) to tailor the code to specific applications. The U. S. distribution site is the Radiation Shielding Information Center located at Oak Ridge National Laboratories. Oak Ridge also puts out a monthly newsletter which notifies users of any updates or revisions.

As a result, ITS enjoys a large, world-wide user base. It has been employed, for example, in the assessment of personnel radiation hazards, the disposal and cleanup of radioactive waste, the pasteurization (e.g., elimination of pathogens in red meat) and disinfestation of foodstuffs, the radiation vulnerability of satellite systems, electron-beam joining, the sterilization of hospital waste, radiation treatment planning, and the safety of nuclear power reactors.

Another important aspect of electron/photon Monte Carlo is that the transport of photons is both faster and more accurate than that of electrons. The photons have a relatively large mean free path which means they typically pass through the material geometry of interest with few interactions (scattering events). The simulation can follow the photons from interaction site to interaction site accurately and efficiently. The electrons, however, are constantly interacting, changing direction and losing energy. It is completely impractical to follow the electrons from interaction point to interaction point. Therefore, the electrons are pushed a predetermined distance. The simulation then tries to account for the cumulative effect of all the multiple interactions which took place over this "step" length (this is what is meant by a "condensed history" method). Even these steps are much smaller than mean free paths of photons of comparable energy. Hence, photons are less expensive to transport than electrons.

Overview of the ITS Package

There are four essential elements of the ITS system:

1. XDATA: the atomic data file

2. XGEN: the program file for generating cross sections
3. ITS: the Monte Carlo program file
4. UPEML: the update processor

The atomic data file contains the data for generating cross sections for arbitrary mixtures or compounds of the first 100 elements. The two program files contain multiple machine versions of the multiple codes (see Table 1 and explanation below for the Monte Carlo program file), integrated in such a way as to take advantage of common coding. Their corresponding binary program libraries are input to the update processor which selects a particular code for a particular machine and makes any modifications requested by the user. The output of the processor in this case is Fortran code that is ready for compilation.

Table 1 shows the eight member codes of the ITS Monte Carlo program file. From top to bottom, the member codes are grouped by rows and will be referred to as the TIGER codes (1-D), the CYLTRAN codes (2-D material geometry with 3-D transport), and the ACCEPT codes (full 3-D), respectively. From left to right, the codes grouped by column will be referred to as the standard codes, the P codes, and the M codes, respectively. All member codes allow transport over the range of 1.0 GeV to 1.0 keV.

Fluorescence and Auger processes in the standard codes are only allowed for the K shell of the highest atomic element in a given material. For some applications, for example, the calculation of energy spectra of low-energy escaping particles, it is desirable to have a more detailed model of the low-energy transport. In the P codes, a more elaborate ionization/relaxation model from the SANDYL (Ref. 2) code was added to the standard codes.

In the M codes, the collisional transport of the standard codes is combined with the transport in macroscopic electric and magnetic fields of arbitrary spatial dependence. This could be used, for example, to model a magnetic field applied in an experiment to turn back electrons which would otherwise have escaped or in simulating a magnetic spectrometer.

To run the programs in the ITS package, the flow of input and output must be understood. Apart from the atomic data file, which is read by the cross-section generator, and the cross-section output file produced by the generator which is read by the Monte Carlo, there are two other types of input required for running either the cross-section generator code or the Monte Carlo code. First, there is the set of instructions to the processor that tells it how to produce a compile-ready Fortran code from either of the program libraries. This input involves a simple syntax for defining code (e.g., TIGER), machine (e.g., IBM), and a few other options. An equally simple syntax allows the user the option to modify the source code via deletions, insertions, and replacements of Fortran code, or simply use the code as a "black box" with no modifications. The second type of input is that required by the resulting executable code. For example, the problem materials and energy range must be specified for the cross-section generator code, and the problem geometry and the source distribution must be defined for the Monte Carlo code.

The default output consists of:

1. Energy and number escape fractions (leakage) for electrons, unscattered primary photons, and scattered photons
2. Charge and energy deposition profiles
3. An explicit statement of energy conservation

In addition to the default output, a number of optional outputs may be selected. These are:

1. Escape fractions that are differential in energy and/or angle for electrons, scattered continuum photons, and line radiation
2. Volume averaged fluxes that are differential in energy and/or angle for electrons, scattered continuum photons, and line radiation for selected regions of the problem geometry
3. A pseudo-pulse-height distribution for a selected region of the problem geometry - for example, the region corresponding to active detector elements
4. Geometry and trajectory plots (for CYLTRAN and ACCEPT)

A more detailed description of the structure and operation of the ITS system can be found in Ref. 1 or Chapter 10 of Ref. 3.

Discussion: Strategies

New users are encouraged to keep their geometry descriptions as simple as possible. Real experiments are performed in the three-dimensional world, but new users are urged to consider how the actual geometry may be simplified for modelling purposes. The input required to describe the TIGER geometry is quite straight-forward: simply specify the material, number of subzones, and layer thickness in centimeters. The CYLTRAN geometry input requires the specification of axial and radial boundaries which is still fairly clear.

The input needed to describe arbitrary three-dimensional geometries requires some care and practice on the user's part. The ability to visualize the specified geometry is essential for verifying the setup of three-dimensional simulations. Appendix I of Ref. 1 describes how a user may interface the called Fortran subroutines within ITS with their local plotting package. Some users employ a geometry-modelling code system such as SABRINA (Ref. 4) to view their constructed geometry. Another user has written a translator (Ref. 5) between a commercial CAD/CAM program (AUTOCAD) and ACCEPT for creating and/or displaying the specified geometry.

The ACCEPT code of ITS uses "combinatorial geometry" (see section 17.3 of Ref. 3) for its three-dimensional input. In combinatorial geometry, geometrical regions are described as various logical combinations of a set of primitive body types (such as spheres, boxes, arbitrary polyhedra, ellipsoids, rectangular right cylinders, and truncated right cones). Logical combinations mean intersections (by an implied "AND"), unions (by an explicit "OR"), and negations. For example, the zone description " +1 -2" means that part of body 1 which is not in body 2. This is one way to describe a cylindrical shell, if bodies 1 and 2 were cylinders. Common errors in coding up the geometry occur when the user is focused on an important part of the geometry but forgets that all space within the escape zone needs to be specified. It is important that there are no gaps between specified zones, hence users are encouraged to try to plot various projections of their geometry to verify what they specified was what they intended. The escape zone is a region which completely surrounds the simulated universe exists. When a particle enters the escape zone, the code considers it has escaped and will no longer continue to track it.

New users are also encouraged to simplify their output requests. For example, requesting very fine resolution for a spatial profile will require many more histories to be run

Users should also be aware, but cautioned about the use, of biasing options available in ITS. For example, to perform a personnel radiation hazard assessment of an accelerator, it may be desired to calculate the energy spectrum of escaping photons produced by the electron beam. However, bremsstrahlung production is a very inefficient process, so an impractical number of histories would need to be run for the simulation. By using the biasing option of artificially increasing the production of bremsstrahlung photons, the user can achieve the desired results far more efficiently. The code will produce many more photons (thereby obtaining more scores to achieve better statistics) but will weight each by the appropriate fraction so that the correct average result will be calculated. This option works well for calculating photon leakage, but can lead to statistically poor results for other quantities of interest. Appendix H of Ref. 1 discusses other biasing options available in ITS. The user should be warned that overbiasing can lead to misleading results.

Calculations should be verified and possibly benchmarked whenever possible. This gives the user confidence that the code is being properly utilized and the simulation is accurately modelled.

Experimental Benchmarks

In this section we present selected experimental benchmarks of the ITS codes. A more comprehensive survey of ITS experimental benchmarks and engineering applications can be found in Chapter 11 of Ref. 3.

Using a Van de Graaff source, Lockwood et al. in Ref. 6 measured electron energy and charge backscatter for a broad matrix of materials (Be through U), source energies (from about 30 keV to 1 MeV), and incident angles (from 0 to 75 degrees) and compared the results with predictions of the TIGER code. Figure 1 shows a comparison of TIGER predictions to measured energy backscatter fraction from several materials for a 300-keV electron source at 0° and 60° incidence. Figure 2 shows a a similar comparison for the fractional number of electrons backscattered. In general, agreement is very good.

Lockwood et al. in Ref. 7 also measured electron energy deposition profiles for a more selective matrix of materials (Be through U), source energies (from 300 keV to 1.0 MeV), and incident angles (0, 30 and 60 degrees). Figure 3 shows a comparison of results from a TIGER calculation with measurements for a 300-keV electron source on aluminum at normal incidence. Figure 4 shows a similar comparison for a source at 60° incidence. Figure 5 compares calculations and measurement for a 300-keV electron source on tantalum at normal incidence. There does seem to be a systematic overprediction near the peak, particularly for lower energies in higher atomic number targets. Figure 6 shows a similar comparison for a 1.0 MeV electron source at 60° on tantalum where the agreement is again very good.

Frederickson and Woolf in Ref. 8 measured charge-deposition profiles in an electrically conductive polymer irradiated by monoenergetic electron beams at energies ranging from 400 keV to 1.4 MeV. Figure 7 compares results of TIGER calculations with their measurements. There is a systematic tendency to overpredict the peak and to slightly underpredict the width.

Miller in Ref. 9 used the CYLTRANP code (but there was no reason to use the P-codes in this case!) to simulate the measurements of Farley et al. in Ref. 10 of the two-dimensional energy deposition by a 500-MeV electron beam in layered targets using

Conclusions

Very powerful software such as the ITS system is available for use in simulating radiation effects of electron or photon sources. The software is flexible enough to allow detailed descriptions of arbitrary geometries or quicker calculations through one-dimensional layers, and permits the user to tailor the code for specific applications such as describing a line source as opposed to a point in space or a flat disk. ITS has been benchmarked against a variety of experiments and is employed in a multitude of applications world-wide.

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Keywords:

Monte Carlo, Simulation, ITS, TIGER, CYLTRAN, ACCEPT, Modelling.

TABLE 1. Monte Carlo Member Codes of ITS

GEOMETRY	STANDARD CODES	ENHANCED PHYSICS	MACROSCOPIC FIELDS
1-D	TIGER	TIGERP	
2-D/3-D	CYLTRAN	CYLTRANP	CYLTRANM
3-D	ACCEPT	ACCEPTP	ACCEPTM

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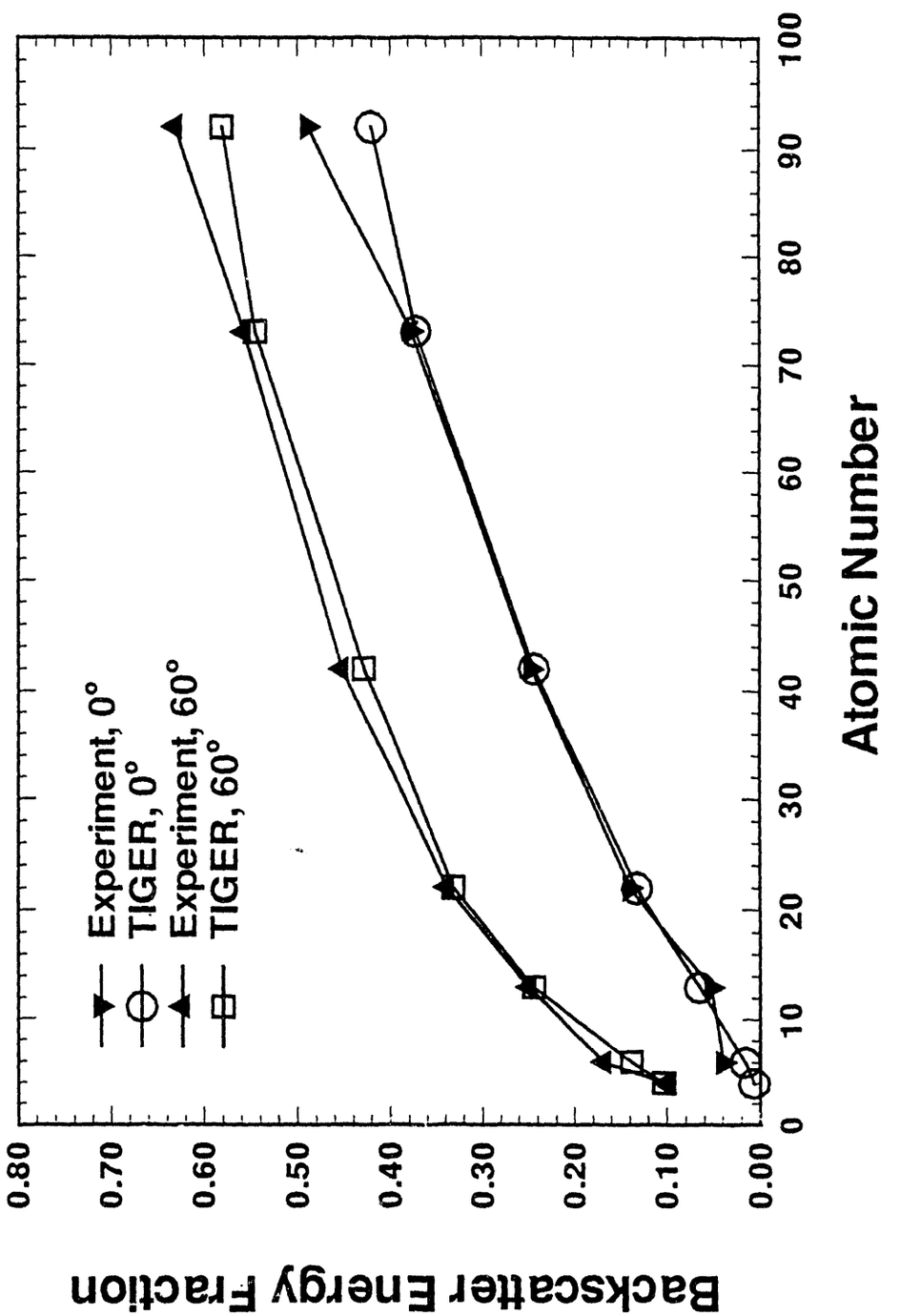

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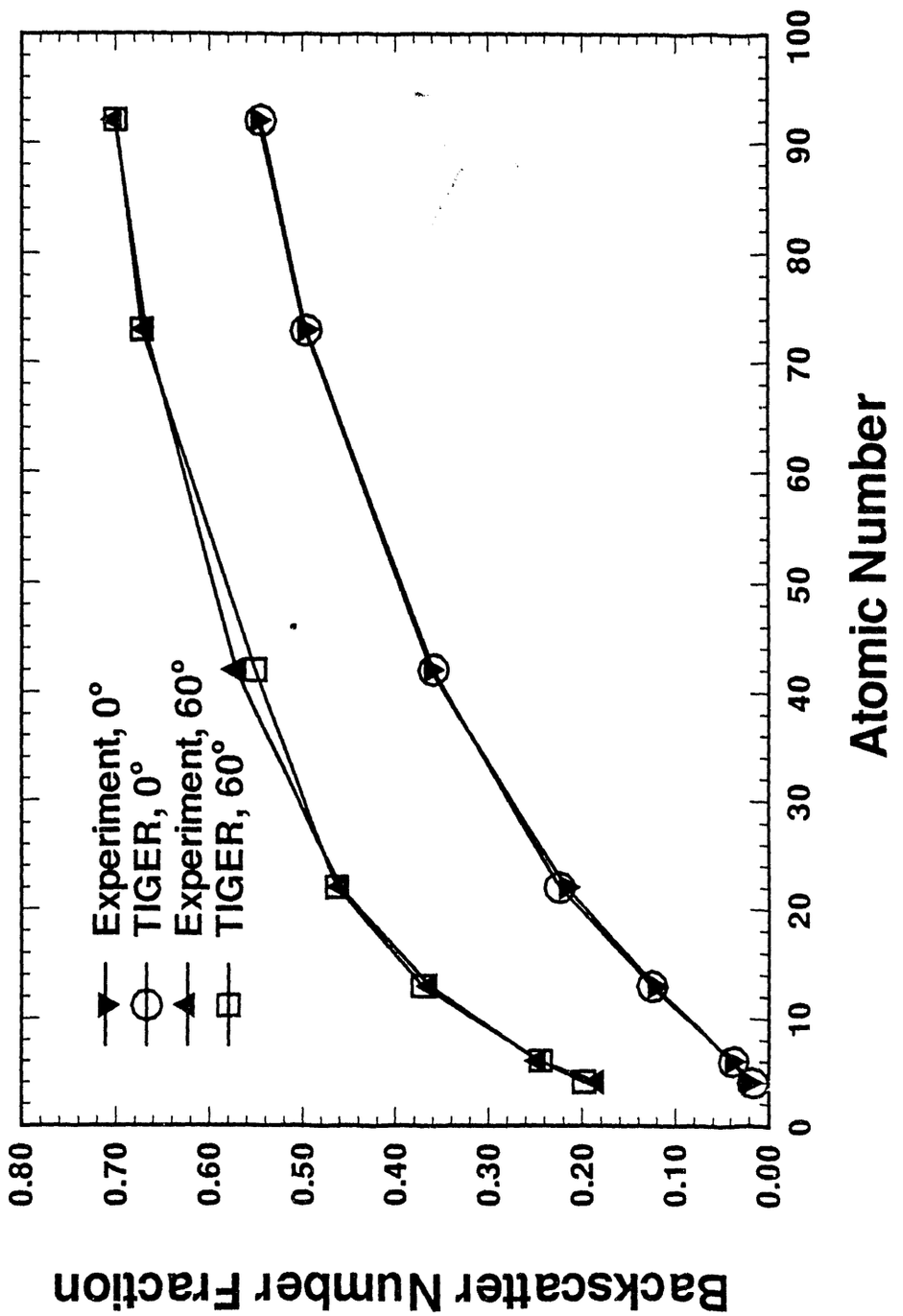

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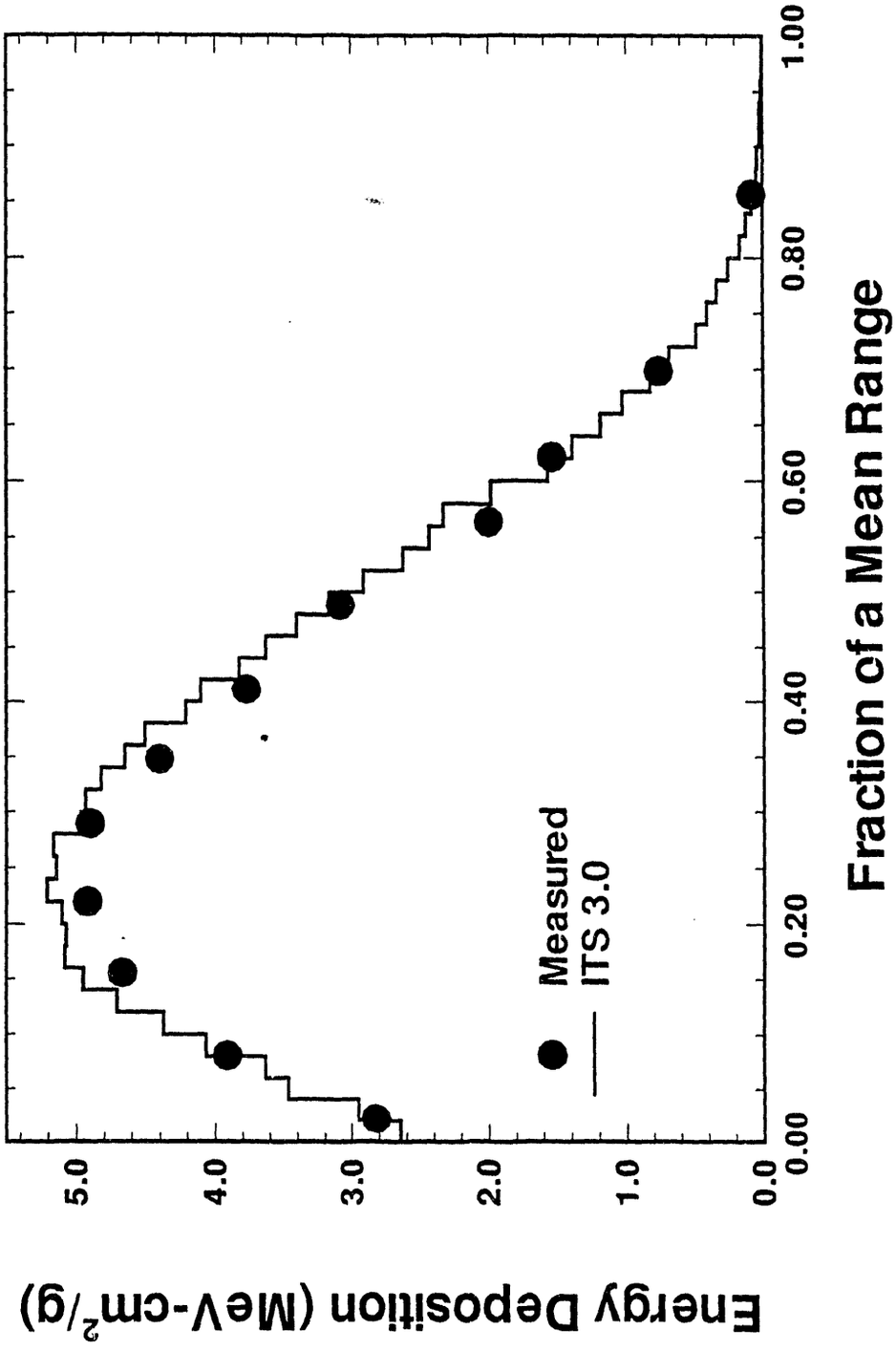

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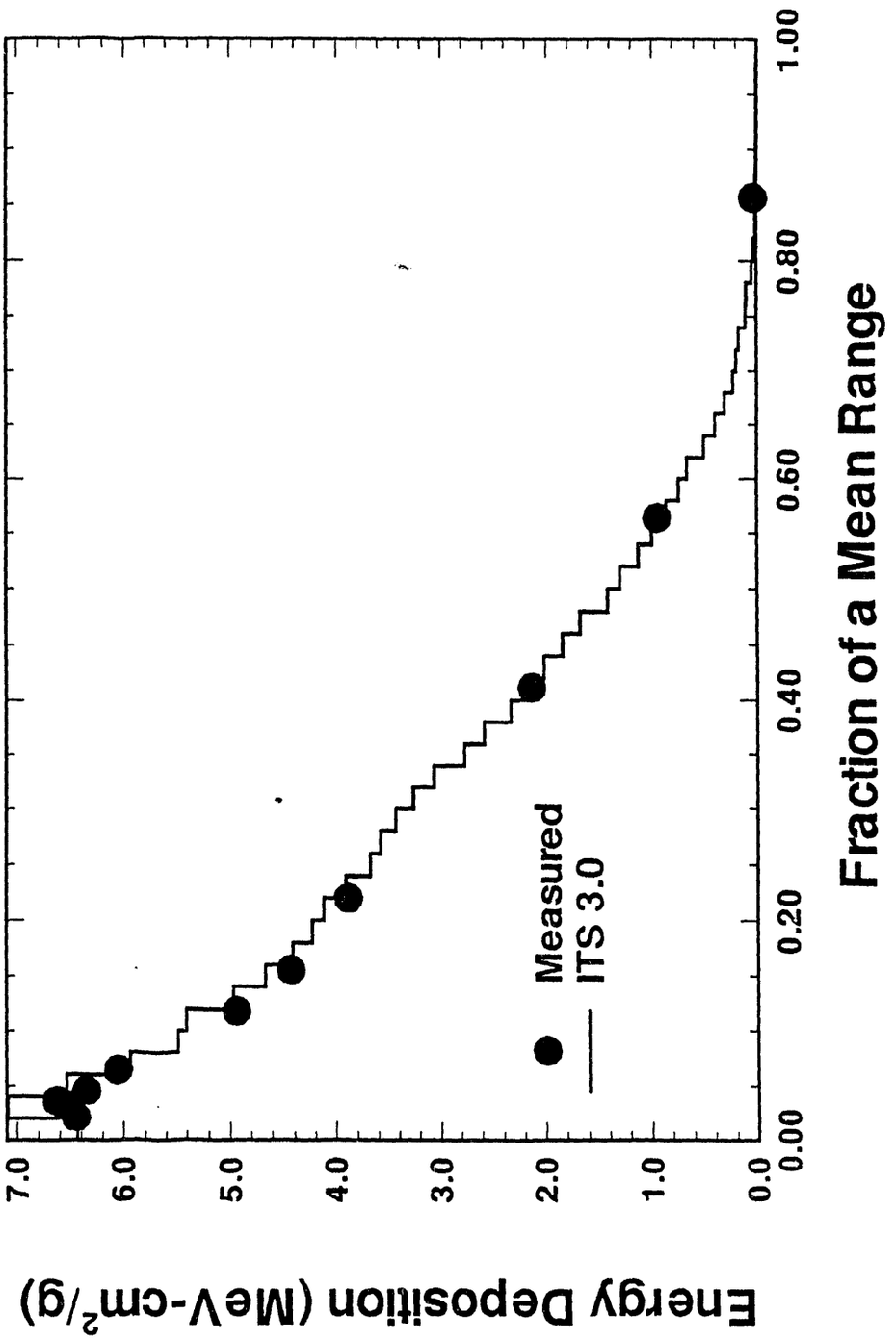

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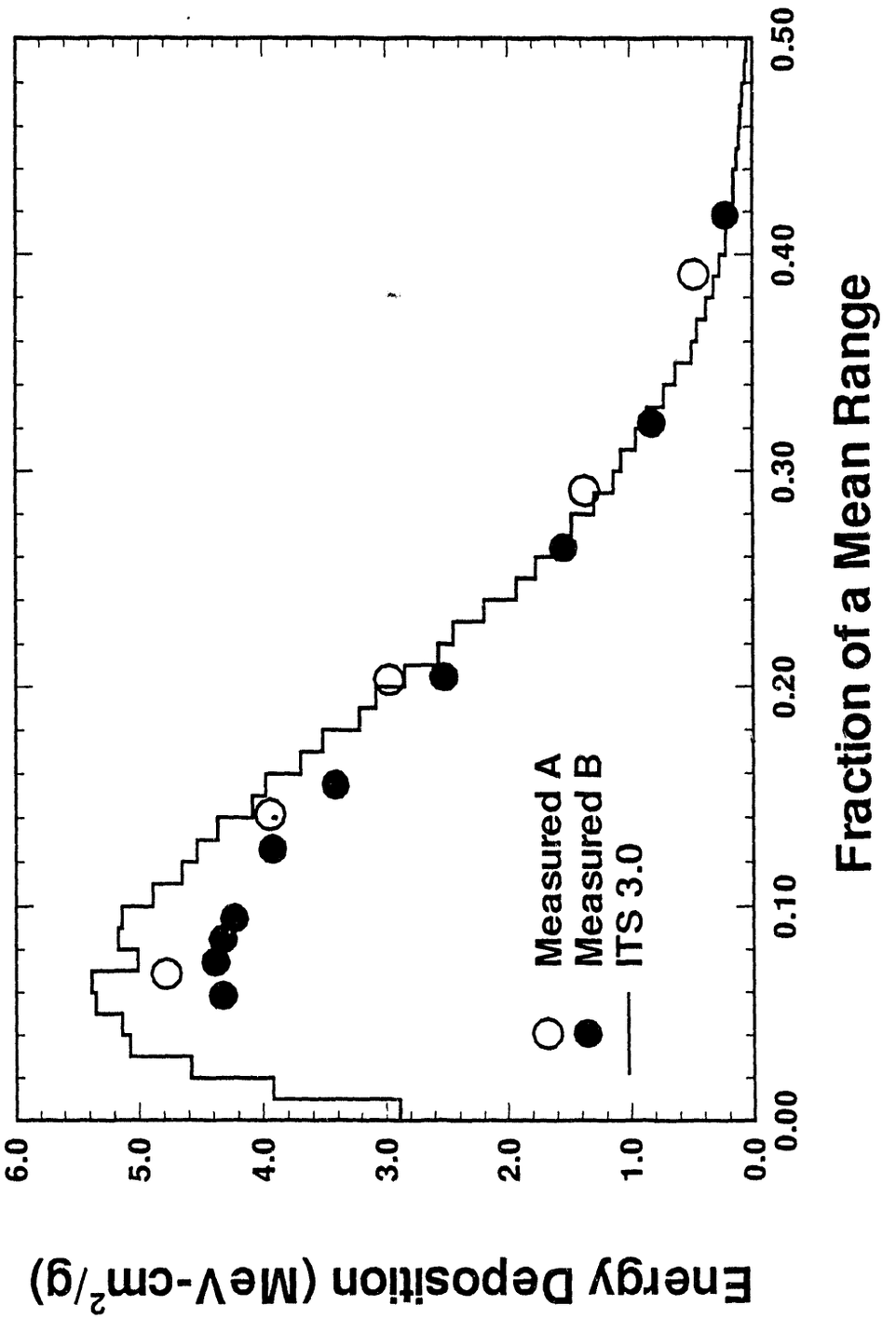

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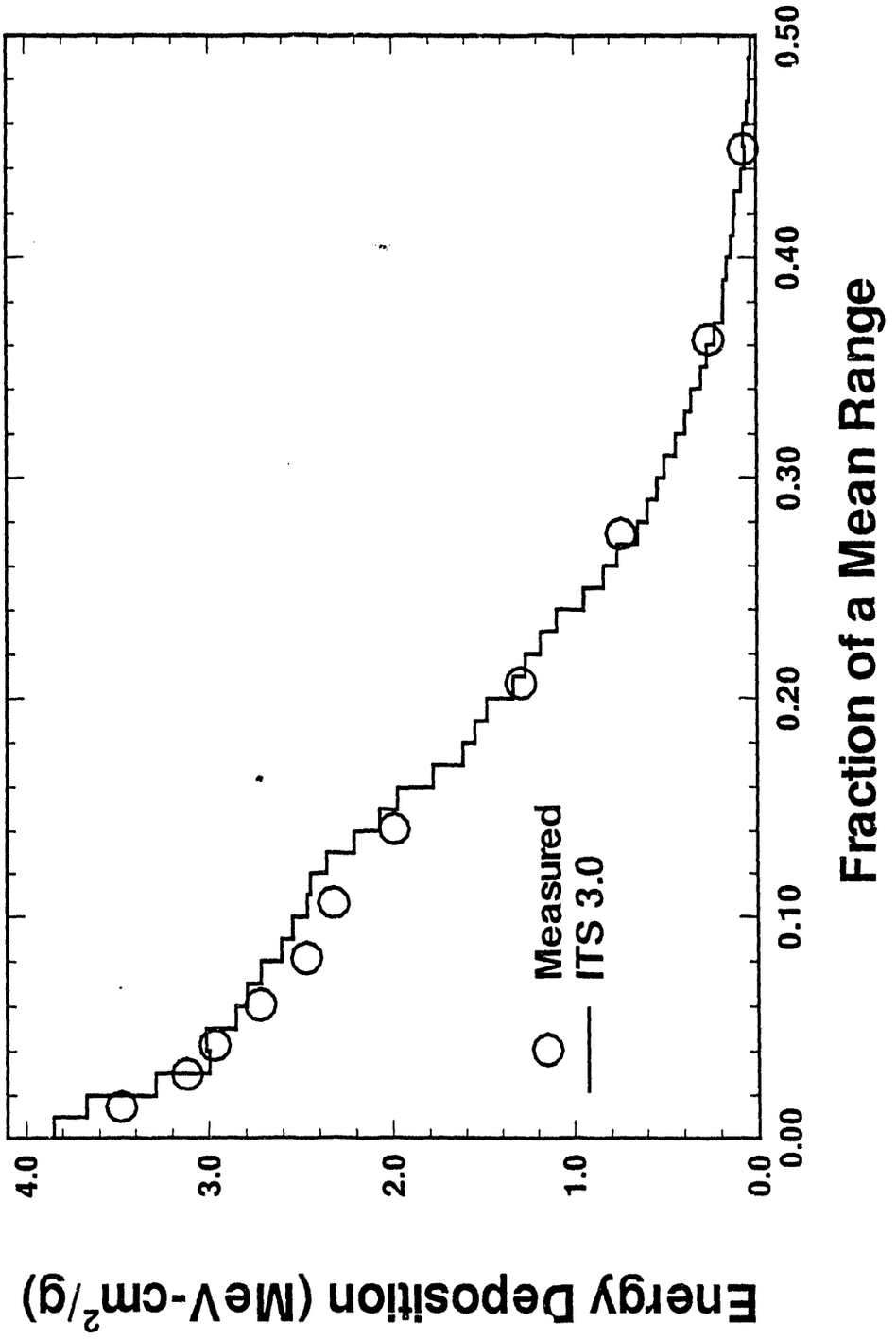

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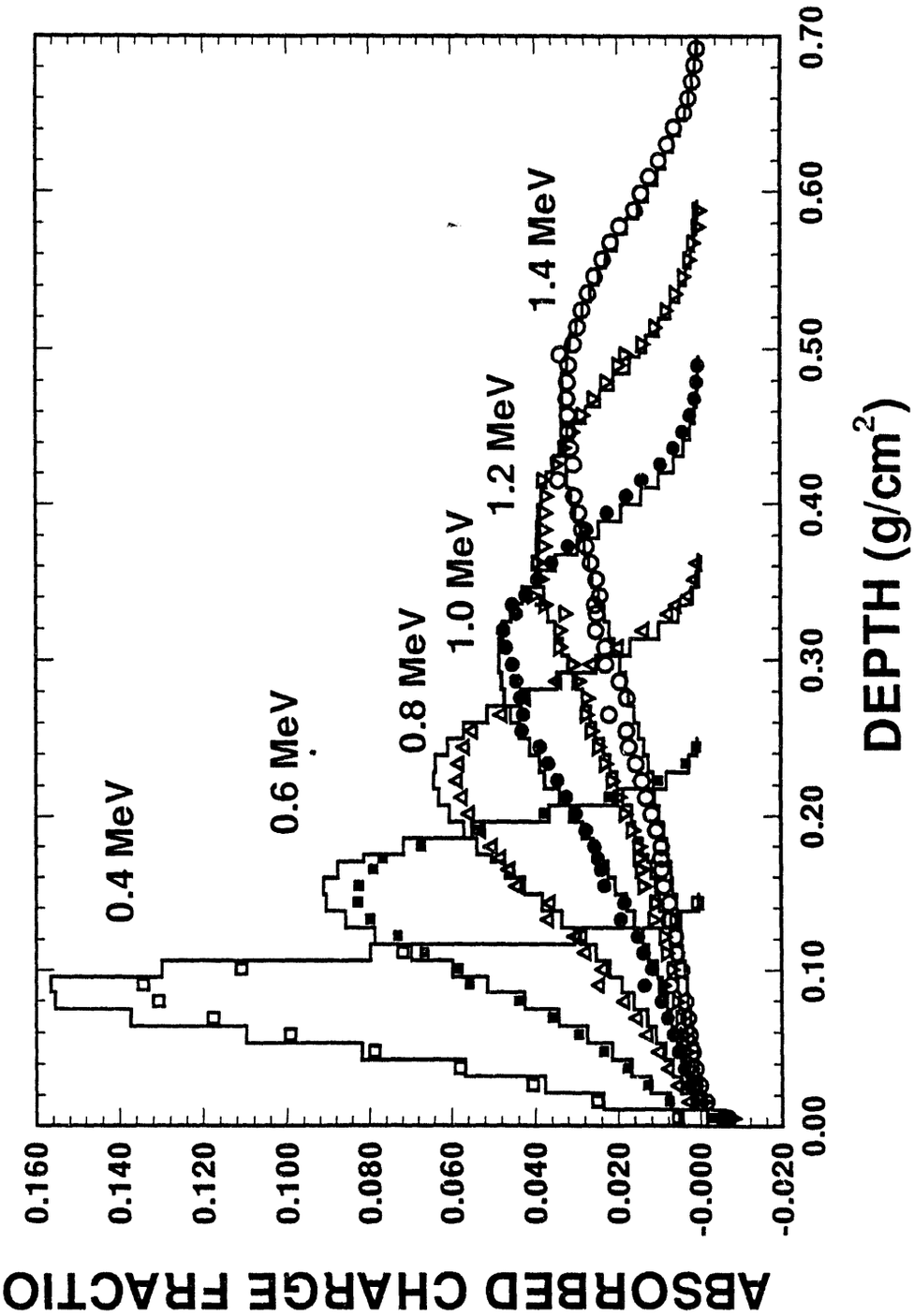

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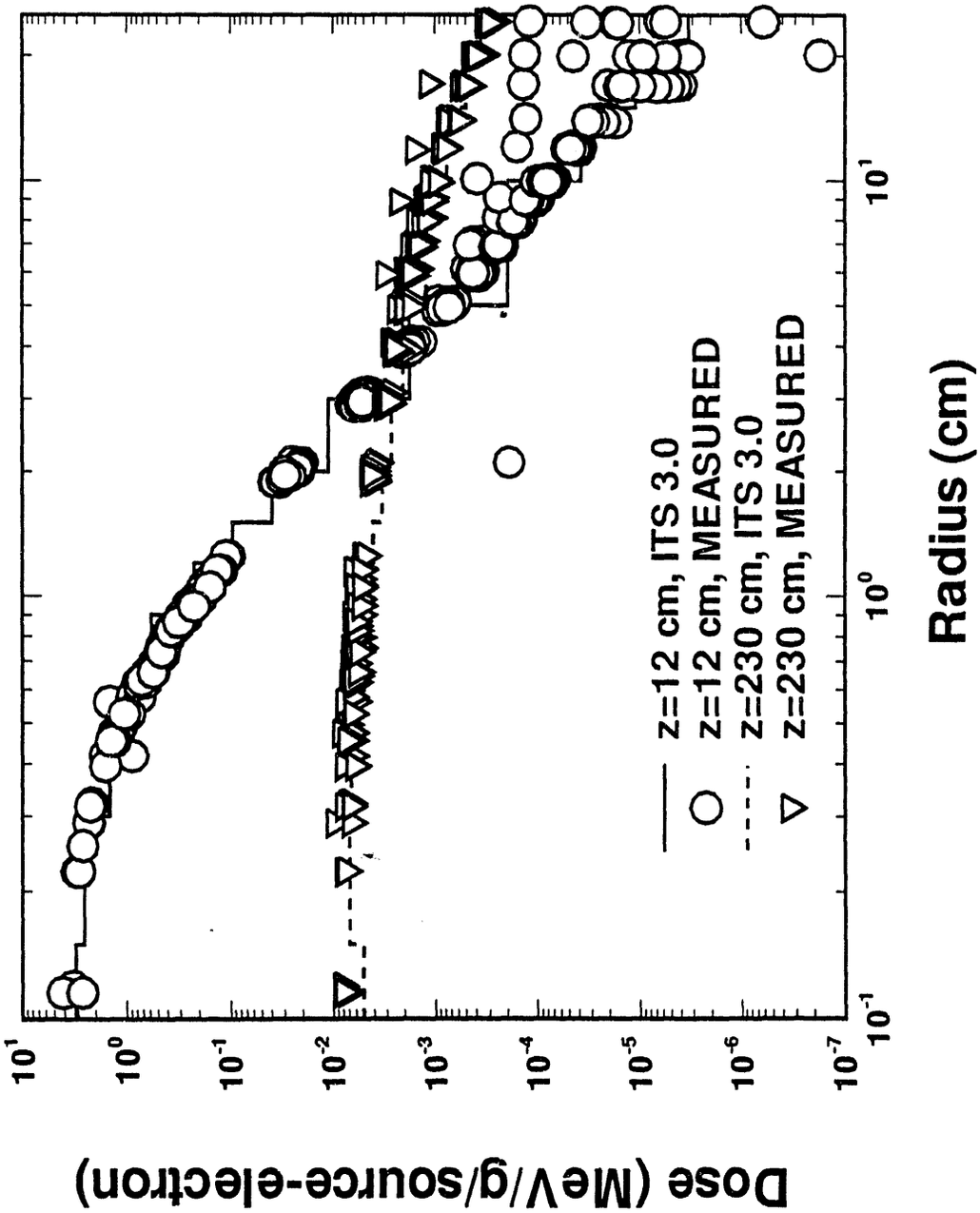

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