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PHASE EFFECTS FOR ELECTRONS IN LIQUID WATER AND WATER VAPOR*

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The objective of these studies is to compare transport, energy loss, and other phenomena for electrons in water in the liquid and vapor phases. Understanding the differences and similarities is an interesting physics problem in its own right. It is also important for applying the relatively large body of experimental data available for the vapor to the liquid, which is of greater relevance in radiobiology. This paper presents a summary of results from a series of collaborative studies carried out by the authors at Oak Ridge National Laboratory (ORNL) and the Gesellschaft für Strahlen- und Umweltforschung (GSF). In these studies, identical calculations were performed using two Monte Carlo computer codes: the ORNL code, OREC, for liquid water and the GSF code, MOCA, for water vapor. More extensive discussion of this work can be found in the following references:

1. J. E. Turner, H. G. Paretzke, R. N. Hamm, H. A. Wright, and R. H. Ritchie, "Comparative Study of Electron Energy Deposition and Yields in Water in the Liquid and Vapor Phases," *Rad. Res.* 92, 47-60 (1982).

2. J. E. Turner, H. G. Paretzke, R. N. Hamm, H. A. Wright, and R. H. Ritchie, "Comparison of Electron Transport Calculations for Water in the Liquid and Vapor Phases," Proc. 8th Symp. Microdosimetry, Jülich, pp. 175-185, Commission of the European Communities, Luxembourg (1982).

3. J. E. Turner, H. G. Paretzke, R. N. Hamm, H. A. Wright, and R. H. Ritchie, "Effects of Phase on Electron Transport in Water," Report ANL-82-88, pp. 91-100, Argonne National Laboratory, Argonne, IL (1982).

4. H. G. Paretzke, J. E. Turner, R. N. Hamm, H. A. Wright, and R. H. Ritchie, "Calculated Yields and Fluctuations for Electron Degradation in Liquid Water and Water Vapor," *J. Chem. Phys.* 84, 3182-3188 (1986).

The principal results are summarized here in a series of figures with self-contained legends. They are grouped into five general areas:

1. Physical differences, Figs. 1 - 4.
2. Average quantities, Figs. 5 - 7.
3. Transport phenomena, Figs. 8 - 9.
4. Fluctuation phenomena, Figs. 10 - 12.
5. Event correlations, Figs. 13 - 14.

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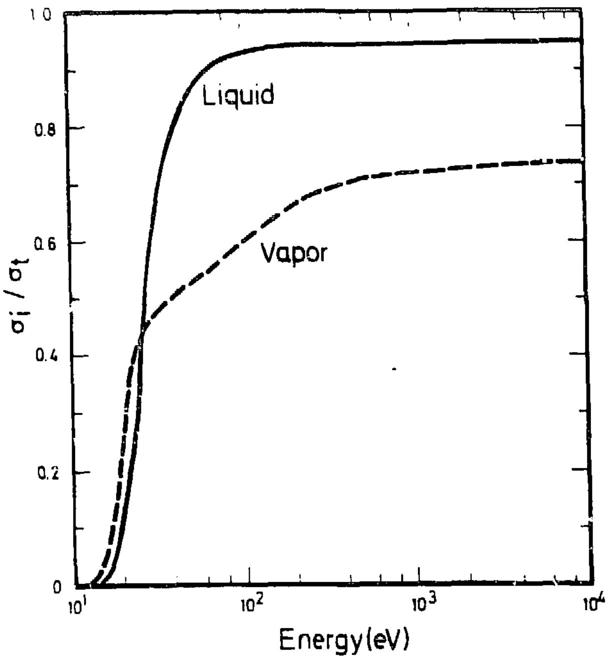

Fig. 1. Ratios of ionization and total inelastic cross sections as functions of electron energy in the two phases (Refs. 1,4). Except at low energies, ionization accounts for a larger share of the inelastic cross section in the liquid, than in the vapor. We calculate W = 25 eV/ip for the average energy to produce an ion pair in the liquid, compared with W = 33 eV/ip measured and calculated for the vapor (Ref. 1).

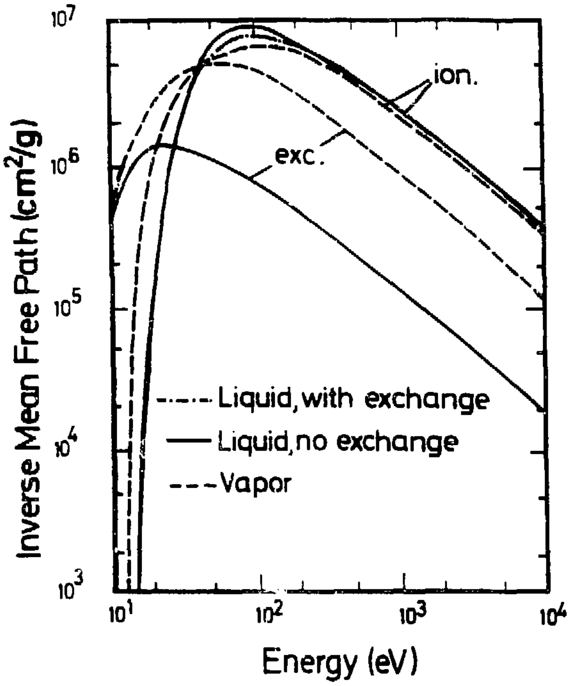

Fig. 2. Inverse mean free paths as functions of electron energy (Ref. 4).

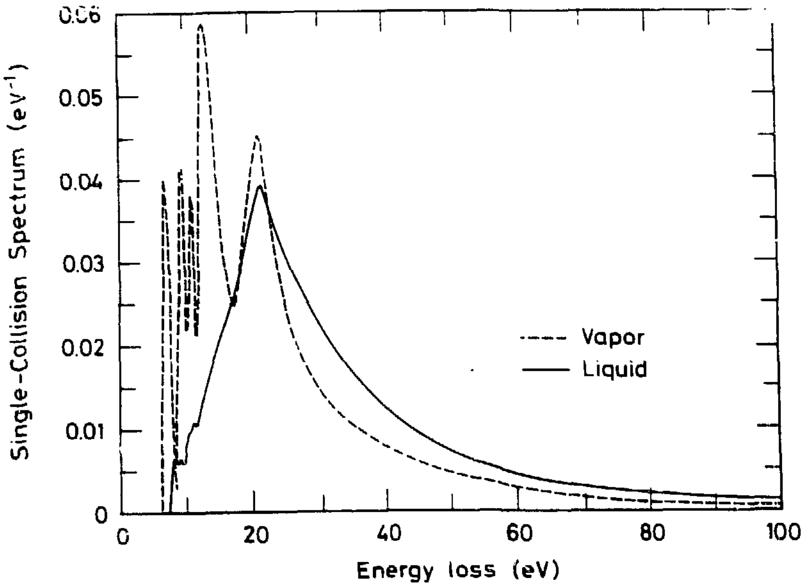

Fig. 3. Normalized single-collision energy-loss spectra for 5-keV electrons. Collision spectra in liquid water are somewhat harder than those in the vapor. This fact, coupled with the lower binding energies of the outer electrons, contribute to the lower W value in the condensed state (Ref. 4).

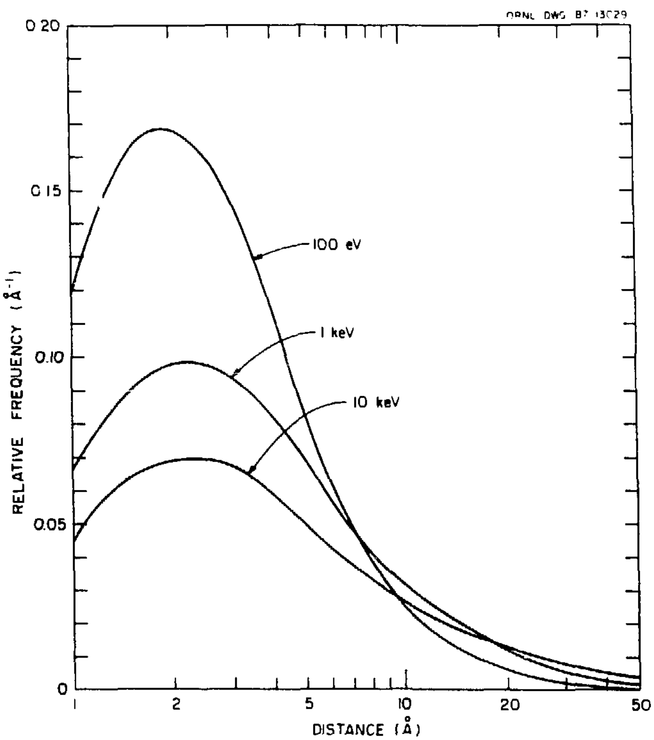

Fig. 4. Nonlocalization of energy losses occurs only in the liquid. The calculated displacement occurs for losses up to 50 eV and is a function of electron energy and energy loss. This figure shows the relative frequency of displacements for collisions by electrons of energy 100 eV, 1 keV, and 10 keV, averaged over all energy losses. See R. N. Hamm, J. E. Turner, R. H. Ritchie, and H. A. Wright, *Rad. Res.* 104, S-20 (1985). (Figure previously unpublished.)

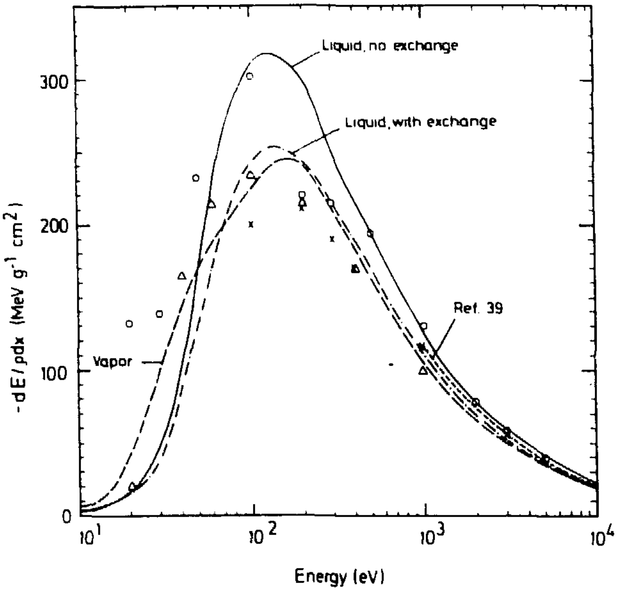

Fig. 5 Mass stopping powers as functions of electron energy (Ref. 4). "Liquid, no exchange" is from Ref. 1; "Liquid, with exchange," Ref. 4; "Vapor," Ref. 1; Open circles, ICRU Report 16 (1964); Crosses, M. Terrisol et al., Proc. Sixth Symp. Microdosimetry (1978); "Ref. 39," ICRU Report 39 (1984).

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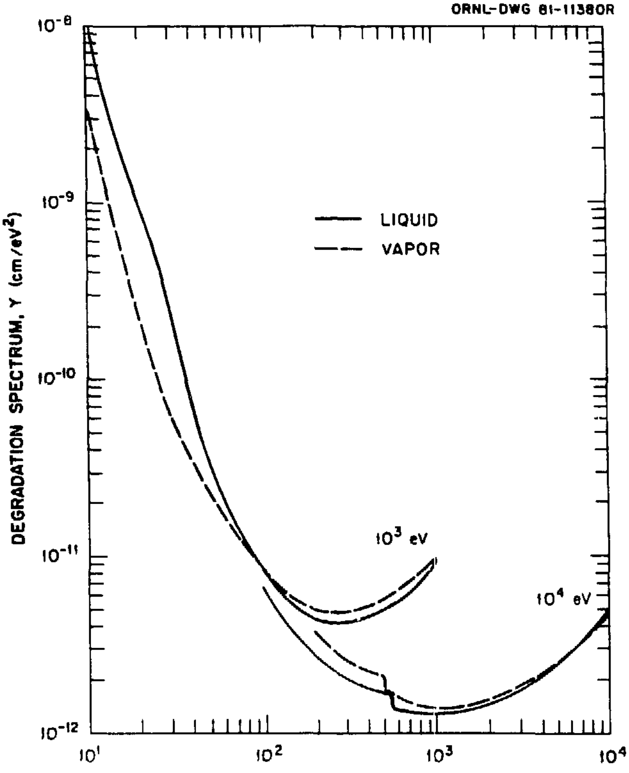

Fig. 6. Slowing-down spectra for 1-keV and 10-keV electrons in the two phases (Ref. 1).

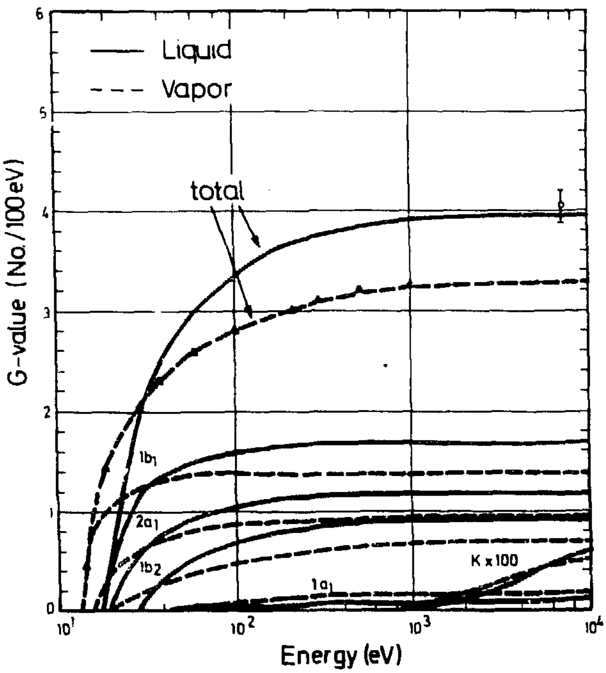

Fig. 7. Calculated total and partial yields for ionizations from various shells in water vapor and liquid water as functions of electron energy (Ref. 4).

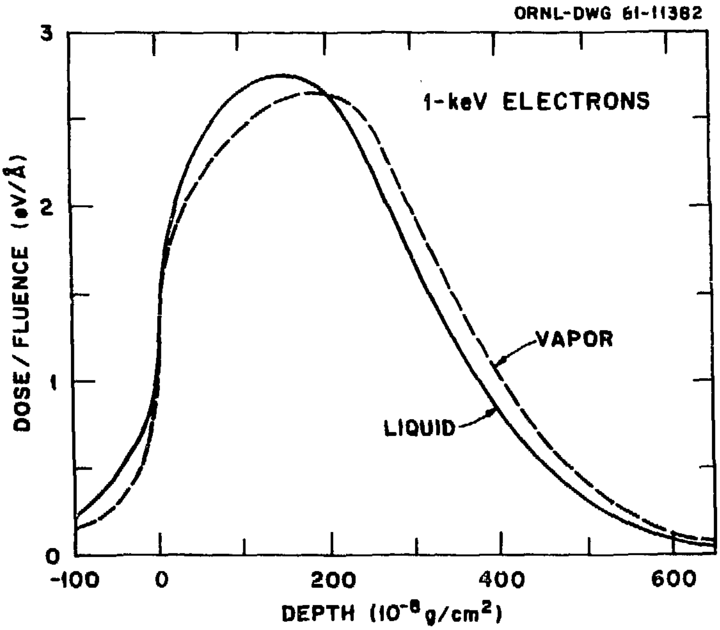

Fig 5 Depth dose curves for a broad, parallel beam of 1-keV electrons, starting at a depth of 0 and traveling initially toward the right. Because of the generally harder collision spectrum, buildup is faster in the liquid. Area under the two curves is the same (energy conservation) (Ref. 1).

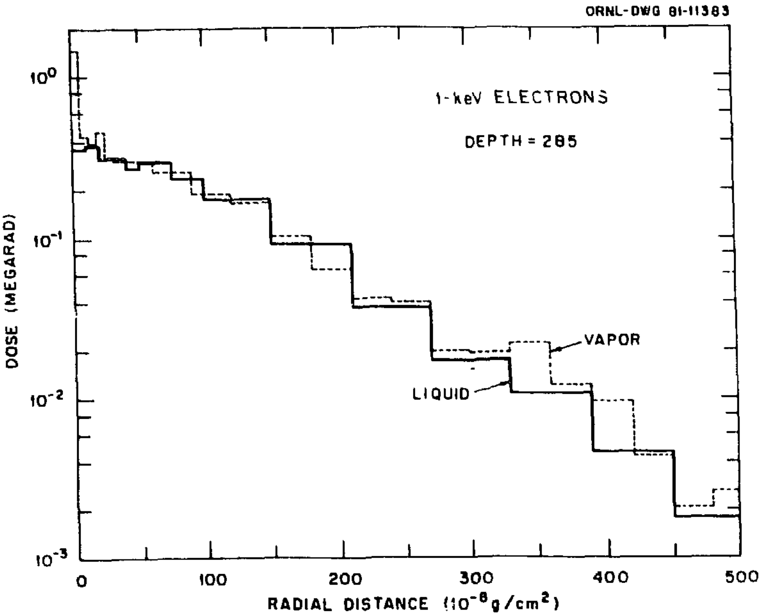

Fig. 9 Radial dose distributions around a pencil beam of 1-keV electrons at a depth of 285 μm. (The same electron histories were used to calculate Figs. 8 and 9.) The nonlocalization of energy losses in the liquid greatly flattens the radial dose close to the track, compared with the vapor (Ref. 1).

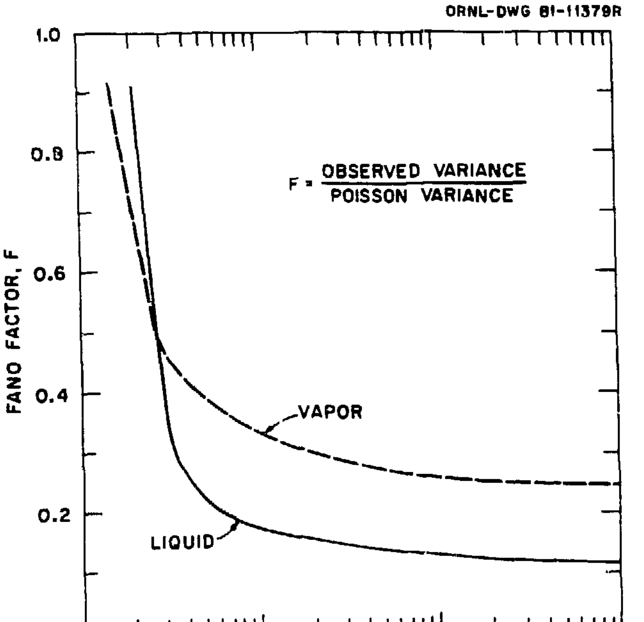

Fig. 10. Fano factors. The lower values at energies above ~30 eV are consistent with the lower W value for the liquid (Ref. 1).

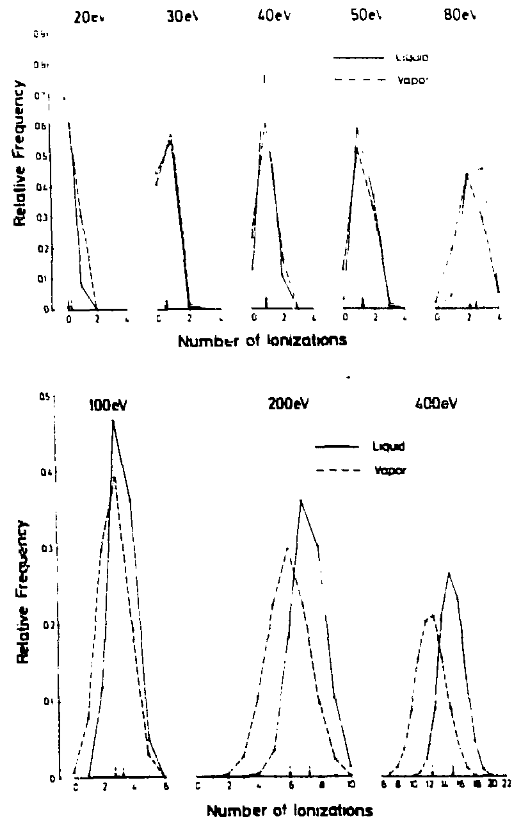

Fig. 11. Distributions of the number of ionizations produced by electrons with initial energies from 20 eV to 400 eV (Ref. 4).

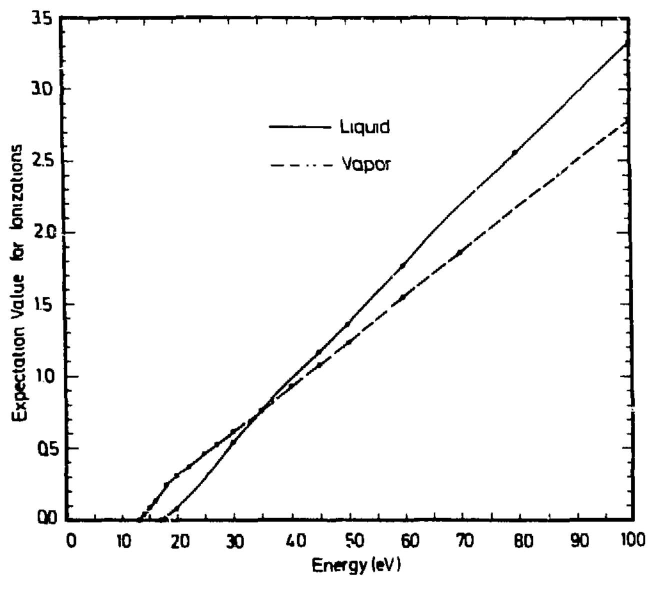

Fig. 12. Mean number of ionizations as a function of electron energy. Above about 35 eV, electron W value is smaller in the liquid (Ref. 4).

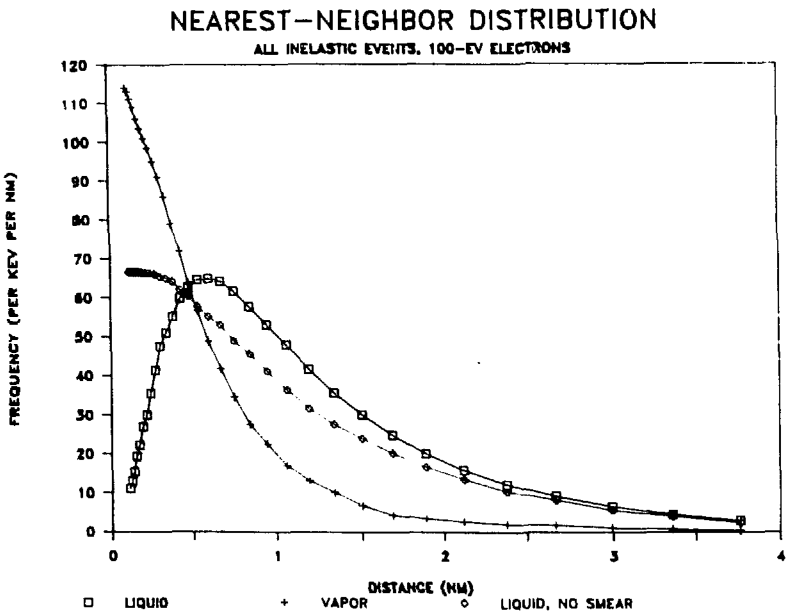

Fig. 13. Preliminary calculations of the nearest-neighbor distributions for all inelastic events in the tracks of 100-eV electrons. The "Liquid-No Smear" curve is obtained by "turning off" the nonlocalization of energy-loss events in the code for the liquid. Work still in progress.

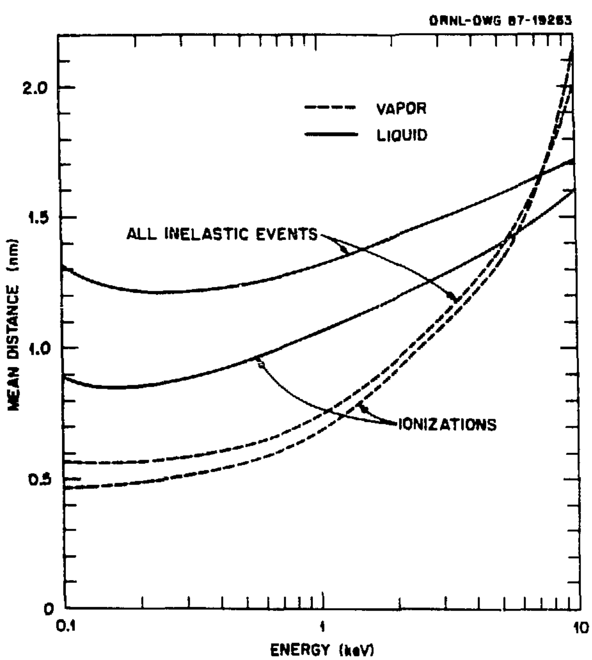

Fig. 14. Preliminary results for mean distance between all inelastic events and between ionizations in tracks of electrons with initial energies up to 10 keV. Work still in progress.