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APPLICATIONS OF ATOMIC AND MOLECULAR DATA TO RADIATION PHYSICS

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The general purpose of our work is to provide atomic and molecular collision cross sections useful for radiological physics, dosimetry, and other applications. It is true that the complete understanding of radiation actions on matter, especially on biological cells, requires a vast range of knowledge far beyond the scope of our study, such as molecular biology. Nevertheless, the knowledge of elementary collision processes involving photons and electrons interacting with atoms or molecules is the most fundamental and is indispensable; any scientifically sound discussion about mechanisms of radiation actions must include some elements of the physics and data of atomic and molecular collisions.[1,2]

For applications to radiation physics, the cross section data must fulfill what I call the trinity of requirements: the data must be (1) correct, (2) absolute, and (3) comprehensive. The meaning of the terms "correct" and "absolute" is evident. By the term "comprehensive", I mean that the data pertain to a wide range of variables involved, e.g., the incident energy, the energy transfer to a target, and the scattering angle. Much too often, the data we see in the literature are discordant (causing suspicion as to correct-

ness), relative (as opposed to absolute), and fragmentary (rather than comprehensive). (This is so because much of the work on atomic and molecular collisions is motivated by interest in basic physics; to prove or disprove a point in physics, it is often sufficient and is indeed efficient to generate data that are relative or limited to a small range of variables.) The thrust of my group's work is to provide comprehensive data, to provide criteria for data assessment, and to develop systematics. Indeed, at the present meeting, Kim[3] discusses many ways for judging the reliability of secondary-electron spectra. Dillon[4] shows how to fit oscillator-strength spectra and related data to the most appropriate analytic expression, for interpolation and extrapolation, and in turn for their effecient use in modeling and other applications. Dehmer[5] reports on prevailing systematics found in the photoionization data specifically on molecules (as opposed to atoms).

Specific problems of my current research include some demonstration of the value of atomic and molecular data in radiological physics and dosimetry. Here I choose to discuss some selected topics. First, the systematics[6] of the atomic oscillator-strength spectra and related quantities have been thoroughly studied for all neutral atoms with $Z \leq 38$. Figures 1 and 2 exemplify results. Second, M. J. Berger, J. E. Turner, and I have been working for a few years with others on an extensive survey of stopping-power data needed in radiological and dosimetric applications - a task for the International Commission on Radiation Units and Measurements. In the course of this study, we found it more and more important to determine the mean excitation energy I in the famous Bethe stopping-power formula by use of the oscillator-strength spectra;

a preliminary account[7] of the work has been published.

As soon as one starts discussing the stopping-power data, one encounters the following question, natural for anyone that has studied condensed-phase physics: Aren't oscillator-strength spectra different for condensed phases from the spectra for isolated atoms or molecules composed of the same atomic elements? Certainly for metals and other materials, there are great differences in the oscillator-strength spectrum upon going from isolated atoms or molecules to condensed phases. Certainly we know much about the oscillator-strength spectra of atoms and molecules in the entire range of excitation energy. In contrast, comprehensive knowledge on condensed-phase materials is hard in general to come by. (As an exception, L. R. Painter and co-workers are conducting extensive work on solids and liquids of many molecules of radiological interest.) As an initial effort toward fully assessing the reliability of data on solids, we have surveyed all data related to the optical properties of metallic aluminum, and have come up with a recommended set of the optical response function.[8] Figure 3 represents an overview of the data.[9] The same data have been used also in the most rigorous evaluation of the Fermi density effect on the stopping power.[9]

Finally, another area of current work[10,11] concerns the generalized oscillator strength for the inner-shell ionization of atoms - a topic motivated by need in electron microscopy for the structure determination of biological molecules and of solid-state materials.

REFERENCES

1. M. Inokuti: Atomic processes pertinent to radiation physics. Electronic and Atomic Collisions, edited by N. Oda and K. Takayanagi (North-Holland Publishing Company, Amsterdam, 1980) pp. 31-45.

2. M. Inokuti: Radiation physics as a basis of radiation chemistry and biology. To be published as Chapter 11 of a monograph Applications of Atomic Collision Physics. Vol. IV. Condensed Matter, edited by H.S.W. Massey, B. Bederson, and E. W. McDaniel (Academic Press, New York).

3. Y.-K. Kim: Energy and Angular Distributions of Secondary Electrons by Charged-Particle Collisions, the present meeting.

4. M. A. Dillon: Analytical Properties of Oscillator-Strength Distributions, the present meeting.

5. J. L. Dehmer: Molecular Photoionization Dynamics, the present meeting.

6. M. Inokuti, J. L. Dehmer, T. Baer, and J. D. Hanson: Oscillator-strength sums, stopping powers, and total inelastic-scattering cross sections of all atoms through strontium. Phys. Rev. A 23, 95-109 (1981).

7. M. Inokuti and J. E. Turner: Mean excitation energies for stopping power as derived from oscillator-strength distributions. In Proceedings of the Sixth Symposium on Microdosimetry, Brussels, 1978, edited by J. Booz and H. G. Ebert (Harwood Academic Publishers, London (1978) pp. 675-687.

8. E. Shiles, T. Sasaki, M. Inokuti, and D. Y. Smith: Self-consistency and sum-rule tests in the Kramers-Kronig analysis of optical data: Applications to aluminum. Phys. Rev. B 22, 1612-1628 (1980).

9. M. Inokuti and D. Y. Smith: Fermi density effect on the stopping power of metallic aluminum. Phys. Rev. B 25, 61-66 (1982).

10. S. T. Manson and M. Inokuti: Near-threshold structure in the atomic K-shell spectra for ionization by photons or fast charged particles. J. Phys. B 13, L323-L326 (1980).

11. M. Inokuti and S. T. Manson: Cross sections for inelastic scattering of electrons by atoms - Selected topics related to electron microscopy. To appear in the Proceedings of the Conference on Electron Beam Interactions with Solids for Microscopy, Microanalysis, and Microlithography, Asilomar, California, April 1982. (Electron Scanning Microscopy, Inc., 1982).

Fig. 1 The total inelastic-scattering cross section σ_{tot} (measured in $\mathring{A}^2$) for 50-keV electrons, plotted against atomic number Z.

The solid line shows the result of calculations that incorporates relativistic kinematics for the incident electron. For comparison, the dotted line shows the results of calculations that disregard relativistic kinematics.

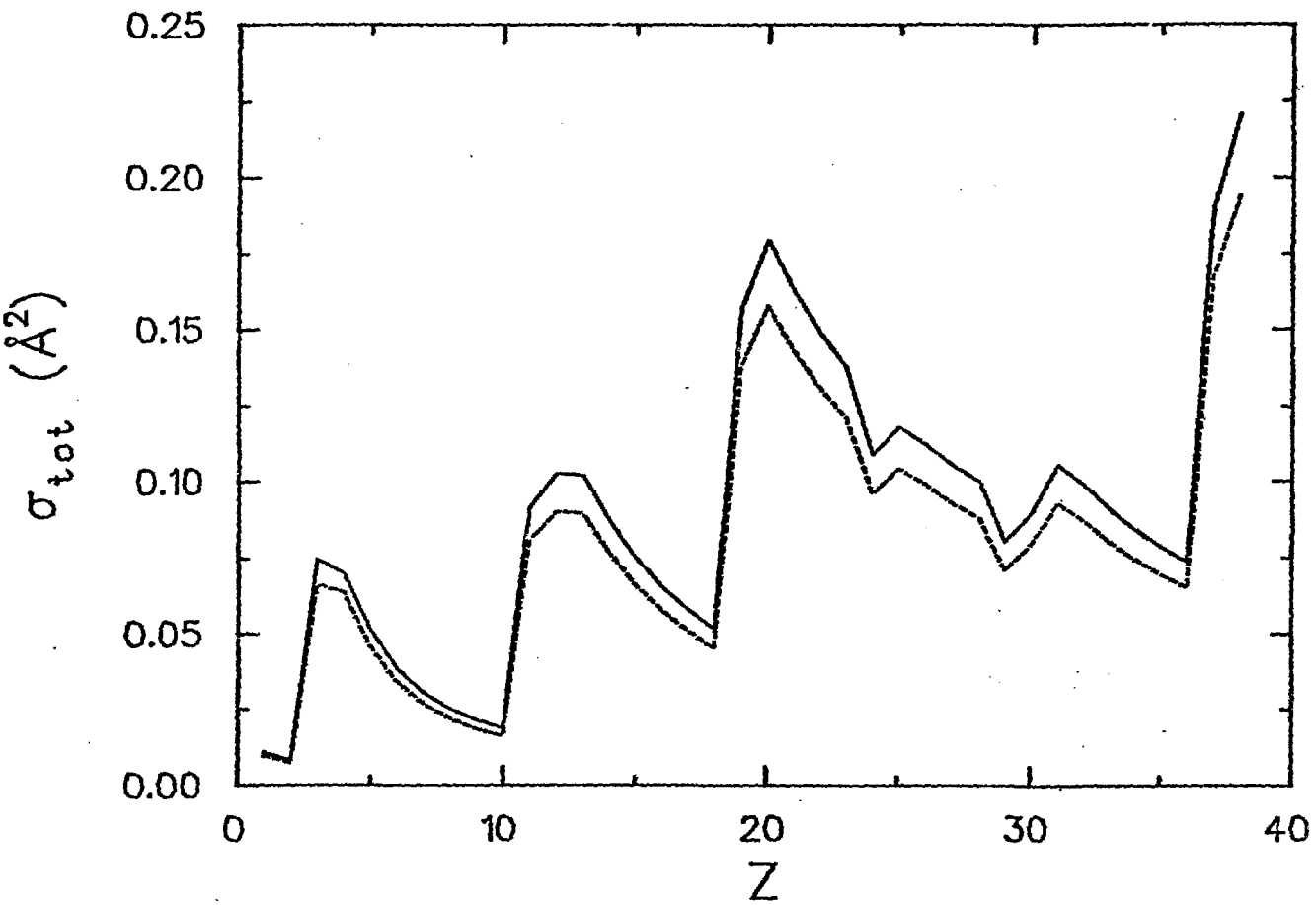

Fig. 2 The mean energy transfer E_{Av} per inelastic collision (measured in eV) for 50-keV electrons, plotted against atomic number Z.

The general features of the curve are the same for all charged particles incident with sufficiently high speed. The dotted line shows the limiting E_{Av} for any extremely relativistic particle.

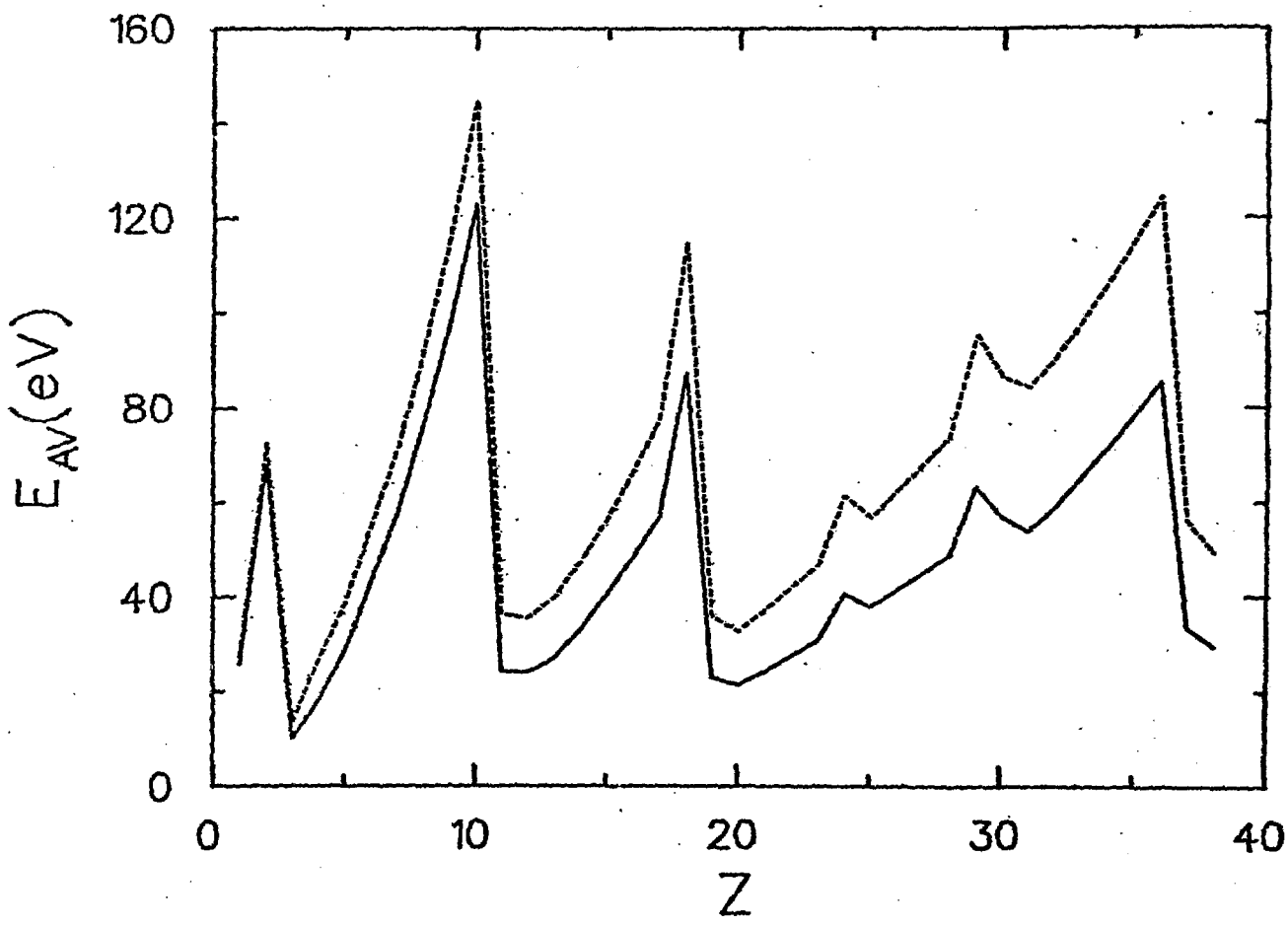

Fig. 3 Dielectric-response function of metallic aluminum.

The real part $\varepsilon_1(E)$ is negative with large absolute values at low E, vanishes at E_{pc} = 15.0 eV (i.e., the plasma energy for conduction electrons), and is positive and approaches unity at higher E. The imaginary part, $\varepsilon_2(E)$, is largest at low E and decreases with E except at thresholds for newer modes of excitation (first at the beginning of interband excitation of valence electrons, next at the L-shell threshold, and finally at the K-shell threshold, on going to higher and higher E). The quantity $\mathrm{Im}[-1/\varepsilon(E)]$ which governs the energy transfer from fast charged particles, shows a prominent maximum near E_{pc}, and is small at both lower and higher E.