A GEOMETRICAL OPTICS MODEL FOR ELECTRON SCATTERING BY MOLECULES

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In calculating the electron elastic cross section of hydrocarbon isomers [1], we were surprised to verify that, for energies between 10eV and 40eV, the cross sections differed by a factor that could be calculated with a simple model burrowed from Geometrical Optics. The result was surprising because the range of energies implies electron wavelengths with the same order of the inter atomic distance. Therefore one would expect interference between the many atoms, which lies in the domain of the Wave Optics, while there is no such a thing in Geometrical Optics.

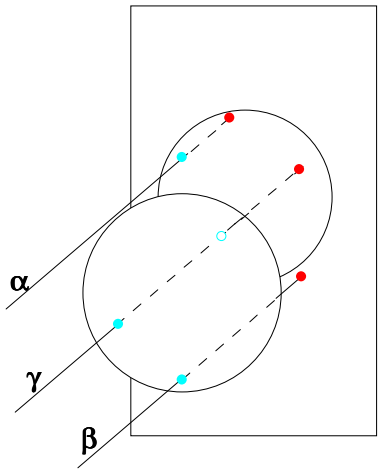

Fig. 1. Three light rays hitting 2 atoms. Ray α hits only the atom behind. Ray β hits only the atom in the front. Ray γ hits both atoms but its shadow in the screen is counted only once.

In Fig. 1 we explain the Geometrical Optics model. In this model the atoms are represented by spheres whose radii depend only on the atomic species and on the incident electron energy. The molecule is considered as a rigid assembly of these atomic spheres. We shine light with many orientations upon the molecule and then collect the molecular shadow in a screen behind the molecule (red dots in the figure). In the case of the hydrocarbon isomers [1] we verified that the area of the shadow, named "shadow cross section", is proportional to the electron-molecule cross section.

After the success of the model for the hydrocarbons the next natural step was to extend it to other atoms and molecules. In Fig. 2 we present some first results, which are still not optimized. In this figure we plot the ratio of the cross section obtained with the Schwinger multichannel method (SMC) and the shadow cross section for a collection of molecules.

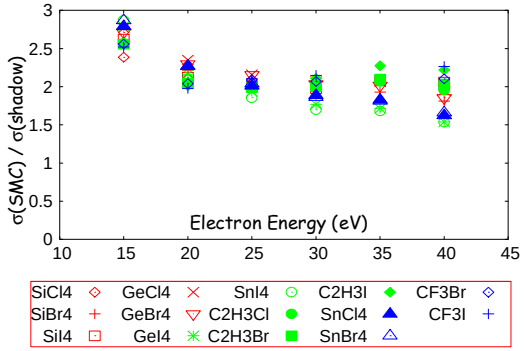

Fig. 2. SMC cross section $\sigma(SMC)$ divided by the shadow cross section. Observe that the ratio is approximately equal to 2 for many molecules and electron energies.

A question remains to be answered: how do the atomic sphere radii defining the shadows compare with those of standard tables (atomic and covalent radii) [2]? Or equivalently, how well the standard radii can be used to define the shadow spheres? The answer is that the comparison is poor, and the stardard radii are not a good choice to use as shadow sphere raddi. The shadow radii are not even monotonic with covalent or atomic radii. For instance, Sn and I have smaller shadow radii than Si and Cl respectively.

References

[1] A R Lopes, M H F Bettega, M A P Lima and L G Ferreira, J. Phys. B: At. Mol. Opt. Phys. **37**, 997-1012 (2004).

[2] http://www.webelements.com