ELASTIC CROSS SECTION CALCULATIONS FOR ELECTRON SCATTERING ON POLYATOMIC MOLECULAR TARGETS: XY_4 (X = C, Si, Ge; Y = H, F, Cl), XF_6 (X = S, W, U), C_2F_6 AND C_6Y_6 (Y = H, F)

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We report calculations of integral cross section (ICS) and differential cross section (DCS) for intermediate- and high-energy electron elastic collisions with polyatomic molecular targets. The calculations have been carried out using an independent atom method with static-polarization model potential.

The objective of the present work was to calculate differential and integral elastic cross sections for electron collisions with polyatomic molecular targets for impact energies ranging from tens electronovolts up to 3000 eV. The calculations have been carried out using an independent atom method (IAM) [1, 2] with static-polarization model potential. In this method differential cross section for elastic electron scattering on molecule is given as:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \sum_{i=1}^{N}\sum_{j=1}^{N} f_i(\theta,k) f_j^*(\theta,k) \frac{\sin(sr_{ij})}{sr_{ij}} \quad , (1)$$

where N is the number of atoms within the molecule, θ is scattering angle and $f_i(\theta,k)$ is the complex scattering amplitude due to the i-th atom of the molecule.

$s = 2k\sin(\theta/2)$ is the magnitude of the momentum transfer during the collision and k is the wave number of incident electron. r_{ij} is the distance between the i-th and j-th atom. Integral elastic cross section (ICS) in this approximation is given by:

$$\sigma(E) = \frac{4\pi}{k}\,\mathrm{Im}\, f(s=0,k) = \\ = \frac{4\pi}{k}\sum_{i=1}^{N}\mathrm{Im}\, f_i(\theta,k) = \sum_{i=1}^{N}\sigma_i(E) \quad , \qquad (2)$$

where $\sigma_i(E)$ is integral cross section of the i-th atom of the molecule, and E is energy of the incident electron. To obtain the elastic electron-atom cross section and atomic scattering amplitudes we solved numerically the radial Schrödinger equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - 2(V_{\mathrm{stat}}(r) + V_{\mathrm{polar}}(r)) - \frac{l(l+1)}{r^2}\right] u_l(r) = 0 \,, \qquad (3)$$

under the boundary conditions

$$u_l(0) = 0,$$
$$u_l(r) \xrightarrow{r\to\infty} A_l j_l(kr) + B_l n_l(kr) \,, \quad (4)$$

where $k^2 = 2E$, $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions, respectively. $V_{\mathrm{stat}}(r)$ is the static potential of

the atom determined following the procedure of Salvat et al. [3].

$$V_{stat}(r) = -\frac{Z}{r}\sum_{i=1}^{3} A_i \exp(-\beta_i r), \quad (5)$$

where Z is the nuclear charge and A_i and β_i are parameters obtained by numerical fitting to the numerical Dirac-Hartree-Fock-Slater screening function [3].

The polarization potential $V_{polar}(r)$ was expressed in the form proposed by Padial et al. [4]

$$V_{polar}(r) = \begin{cases} v(r) & r \le r_c \\ -\alpha/2r^4 & r > r_c \end{cases}, \quad (6)$$

where $v(r)$ is the free-electron-gas correlation energy [5] , α is the static electric dipole polarizability of atom and r_c is the first crossing point of the curves of $v(r)$ and $-\alpha/2r^4$ [6]. The atomic scattering amplitude for the constituent atoms of the molecule was calculated within the partial wave analysis according to

$$f(\theta,k) = \frac{1}{2ik}\sum_{l=0}^{l_{max}}(2l+1)(\exp(2i\delta_l)-1)P_l(\cos(\theta)) + f^{(B)}(\theta,k), \quad (7)$$

where $\delta_l = \arctan(-\frac{B_l}{A_l})$ is phase shift and $P_l(\cos(\theta))$ are Legendre polynomials. $f^{(B)}(\theta,k)$ is the Born scattering amplitude which for potential of the form (6) may be expressed as

$$f^{(B)}(\theta,k) = \pi\alpha k\left(\frac{1}{3} - \frac{1}{2}\sin\frac{\theta}{2} - \sum_{l=1}^{l_{max}}\frac{P_l(\cos(\theta))}{(2l-1)(2l+3)}\right), \quad (8)$$

where l_{max} =100. The differential cross section for electron elastic scattering on the atom was calculated according to the relation

$$\frac{d\sigma}{d\Omega} = |f(\theta,k)|^2. \quad (9)$$

The integral elastic cross section for electron scattering on the constituent atoms of the molecule was calculated as

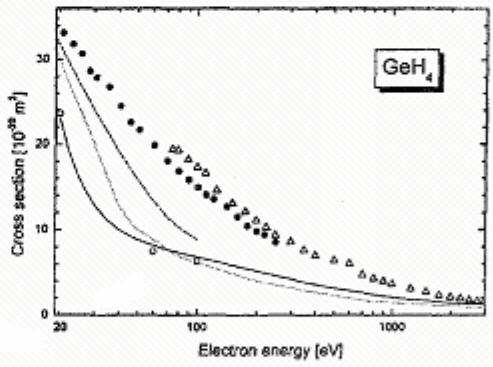

Fig 1. Cross sections for electron scattering from GeH_4 molecule. Calculations: elastic cross section, present results (solid curve); [7] (dotted curve; [8].(chain curve). Experimental: elastic cross section, (○), [9]; absolute total cross section, (•), [10]; (Δ), [11].

$$\sigma(E) = \frac{4\pi}{k^2}\left(\sum_{l=0}^{l_{max}}(2l+1)\sin^2\delta_l + \sum_{l=l_{max}}^{\infty}(2l+1)\sin^2\delta_l^{(B)}\right), \quad (10)$$

where

$$\delta_l^{(B)} \approx tan\delta_l^{(B)} = \frac{\pi\alpha k^2}{(2l-1)(2l+1)(2l+3)}. \quad (11)$$

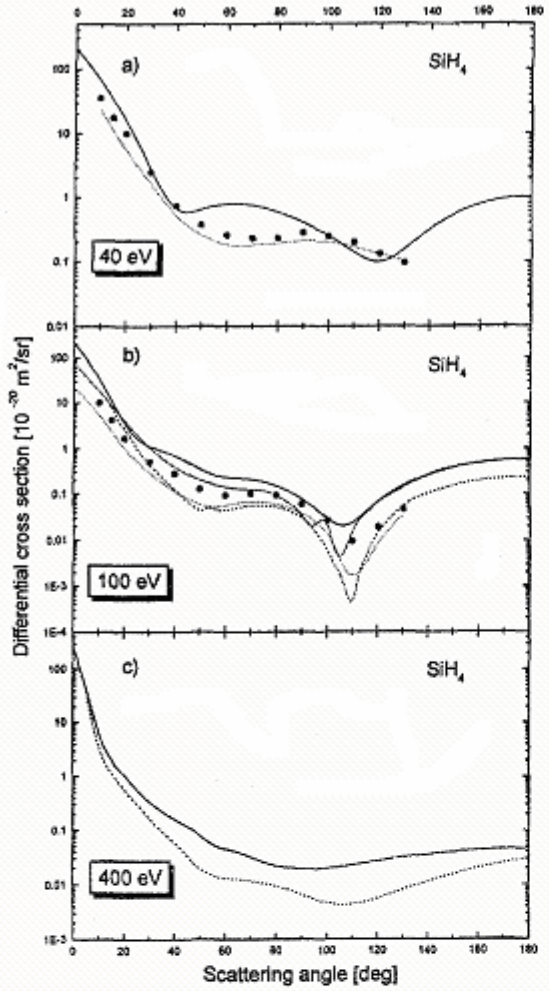

Fig 2. Differential cross section for e^-- SiH_4 collisions:
(a) 40 eV; Experimental results: (circles), [12]. Theoretical results: ·dashed curve – [12]; solid curve – present work.
(b) 100 eV; Experimental results: (circles), [12]. Theoretical results:dotted curve – [12]; dashed curve – [13], chain curve – [14], solid curve – the present work.
(c) 400 eV; Theoretical results: dashed curve – [13]; solid curve – the present work.

Computed ICS and DCS for elastic electron scattering on variety of molecular targets (CH_4, SiH_4, GeH_4, CF_4, SiF_4, GeF_4, CCl_4, $SiCl_4$, $GeCl_4$, SF_6, WF_6, UF_6, C_2F_6, C_6H_6 and C_6F_6), with above methods, for collision energies higher than 40 eV are in good accordance with available experimental data and results of theoretical calculations. In Figs. 1, 2 and 3 we present as an example integral cross section for GeH_4 molecule and differential cross section for SiH_4 and C_2F_6 molecules.

Present ICS for electron collisions with GeH_4 molecule (Fig 1.) is in an excellent agreement with experimental data of Dillon et al. [9]. The values of ICS obtained in present calculation are closer to experimental data than those computed with more sophisticated methods [7,8].

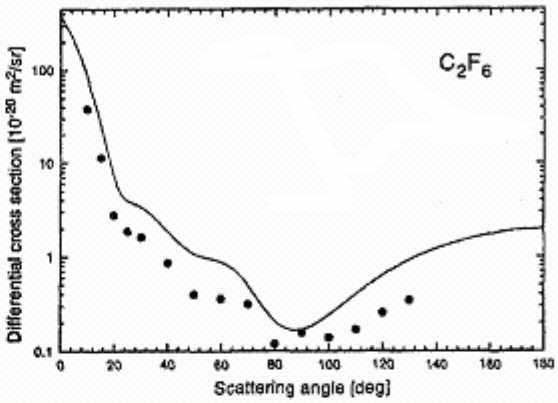

Fig 3. Differential cross section for elastic electron collisions with C_2F_6 molecules at 100 eV::solid curve – the present theoretical results; circles – experimental results [15]

Computed in the present work differential cross section for elastic electron-silane molecule scattering (Fig 2.) for collision energies above 40 eV agree well with experimental and theoretical data of Tanaka et al. [12] and other theoretical results: computed DCS with spherical-complex-optical-potential by Jain [13] and calculations in which relativistic approach was employed [14]. Calculated DCS for e^-- C_2F_6 elastic collisions at 100 eV is in good agreement with experimental data of Takagi et al. [15].

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РОЗРАХУНКИ ПЕРЕРІЗІВ ПРУЖНОГО РОЗСІЮВАННЯ ЕЛЕКТРОНІВ НА БАГАТОАТОМНИХ МОЛЕКУЛАХ: XY_4 (X = C, Si, Ge; Y = H, F, Cl), XF_6 (X = S, W, U), C_2F_6 ТА C_6Y_6 (Y = H, F)

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Представлено розрахунки інтегральних та диференціальних перерізів розсіювання для зіткнень електронів середніх і високих енергій з багатоатомними молекулярними мішенями. Проведено розрахунки з використанням методу незалежних атомів з потенціалом у моделі статичної поляризації.