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LETTER TO THE EDITOR

Critical minima in elastic electron scattering from argon

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Abstract

Relativistic *ab initio* calculations of both low- and high-angle critical minima in the differential cross sections are presented. The theoretical approach is based on the Dirac–Hartree–Fock method. Exchange between incident and target electrons is calculated exactly. Target polarization is described by *ab initio* potential taken from relativistic polarized orbital calculations. The position of our critical minima (39.3 eV, 68°) and (39.5 eV, 141°) agree well with recent measurements performed by Panajatović *et al*.

For many years several measurements of differential cross sections in the elastic electron scattering from noble gases have been reported (e.g. Dehmel *et al* (1976), Haddad and O'Malley (1982), Weyhreter *et al* (1988), Furst *et al* (1989), Gibson *et al* (1996), Mehr (1967), Schackert (1968), Lewis *et al* (1974), Williams and Willis (1975), Vušković and Kurepa (1976), DuBois and Rudd (1976), Srivastava *et al* (1981), Quing *et al* (1982), Cvejanović and Crowe (1994, 1997), Crowe and Cvejanović (1996), Bromberg (1974), Gupta and Rees (1975), Jansen *et al* (1976)). In addition, several calculations have been performed in order to make comparison with experimental data and at the same time to test theoretical methods (e.g. Kemper *et al* (1985), Walker (1971), McEachran and Stauffer (1983), Bartschat *et al* (1988), Mimnagh *et al* (1993), Nahar and Wadehra (1987), Fon *et al* (1983), Saha (1991), Sienkiewicz and Baylis (1987), Haberland *et al* (1986), Plenkiewicz *et al* (1988), Ihra and Friedrich (1992)).

Very recent extensive measurements of Panajatović *et al* (1997) and earlier measurements of Kessler *et al* (1976) provide the excellent possibility of a stringent test for theoretical calculations. They are dealing with critical minima in differential cross sections. The position of a critical minimum is defined by the point on the plane constituted by the scattering angle and projectile energy axis where the differential cross section attains its minimal values. In other words, this point indicates the exact position of the local distinct minimum in a differential cross section. The first methods proposed to search for critical points defined by the above were given by Lucas (1979) and Khare and Raj (1980). Although Bühring (1968) was the first to bring attention to critical energies at which critical minima occur. He already proved their physical significance due to their sensitivity in experimental methods. As stressed by Kessler *et al* (1976) it is virtually impossible to measure the exact depths of differential cross sections. The reason lies in the inherit angular resolution limit of the detectors used.

It is quite obvious that the positions of critical minima are also very sensitive to the theoretical methods chosen. For a proper description they require the exact treatment of exchange potentials and careful choice of a target polarization potential. Another significance of critical minima lies in the fact that their positions indicate the highest values of spin polarization of scattered electrons. The degree of spin polarization is given by $P = (\sigma_\uparrow - \sigma_\downarrow)/(\sigma_\uparrow + \sigma_\downarrow)$, where $\sigma_\uparrow$ and $\sigma_\downarrow$ are the cross sections of scattered electrons with spin momentum pointing 'up' and 'down' with respect to the scattering plane. The biggest difference between the $\sigma_\uparrow$ and $\sigma_\downarrow$ cross section occurs in the angle region, where the differential cross section is minimal. This is explained by the relative weakness of the spin–orbit interaction in comparison to the electrostatic interaction (see Kessler (1985)). The aim of this letter is to test our theoretical approach searching for critical minima in the elastic scattering of electrons from argon. Our very preliminary results have already been published elsewhere (Konopińska *et al* 2001). It should be underlined that our *ab initio* method is fully relativistic. The necessity for a relativistic treatment of electron scattering from argon has already been shown by several authors including Nahar and Wadehra (1991), Yuan and Zhang (1993) and Sienkiewicz and Baylis (1987). Here we also use our method to calculate the spin polarization of the scattered electrons.

We solve the radial Dirac–Hartree–Fock equation (Grant 1970) which can be written in atomic units as

$$\begin{aligned}\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\kappa}{r}\right)P_\kappa(r) &= \{2/\alpha+\alpha[E-V_{\mathrm{fc}}(r)-V_{\mathrm{p}}(r)]\}Q_\kappa(r)+X_Q(r)\\ \left(\frac{\mathrm{d}}{\mathrm{d}r}-\frac{\kappa}{r}\right)Q_\kappa(r) &= -\alpha[E-V_{\mathrm{fc}}(r)-V_{\mathrm{p}}(r)]P_\kappa(r)-X_P(r)\end{aligned}\qquad(1)$$

where P_κ and Q_κ are radial parts of the large and small components of the Dirac wavefunction, the quantum number $\kappa = \pm(j+\frac{1}{2})$ for $l = j \pm \frac{1}{2}$, α is the fine structure constant, E is the energy of the incoming electron, V_{fc} is the relativistic frozen-core potential, V_{p} is the polarization potential and X_Q and X_P are the exchange terms.

The exchange terms and the frozen-core potential V_{fc}—between the scattered electron and target electrons—are calculated from atomic orbitals obtained by the relativistic MCDF program of Desclaux (1975) with some modifications (Sienkiewicz and Baylis 1987). These terms are defined as

$$\begin{aligned}V_{\mathrm{fc}} &= -\frac{Z}{r}+\sum_{j,k}a^k(s,j)Y^k(j,j;r)\\ crX_{P(\mathrm{or}Q)} &= \sum_{j,k}b^k(s,j)Y^k(s,j;r)P_j\ (\mathrm{or}Q_j)\end{aligned}$$

where index 's' refers to the scattered electron, Z is the nuclear charge and the sums are over electrons of the target atom. The radial function Y^k and the angular coefficients a^k and b^k are given by Grant (1970).

The polarization potential V_{p} arises as a second-order correlation correction to the frozen-core approximation. In our approach, it includes the dipole static term and is taken in a numerical form from the *ab initio* calculations of Szmytkowski (1993) performed with the relativistic version of the polarized orbital method.

The phase shifts $\delta_l^\pm$ are obtained by comparison of the numerical solutions of equation (1) with the analytical ones at large r:

$$P_\kappa(r)/r = j_l(kr)\cos\delta_l^\pm - n_l(kr)\sin\delta_l^\pm \qquad (2)$$

where k is the momentum of the incident electron, $j_l(kr)$ and $n_l(kr)$ are the spherical Bessel and Neumann functions, respectively. δ_l^+ is the phase shift calculated for $\kappa = -l-1$ in

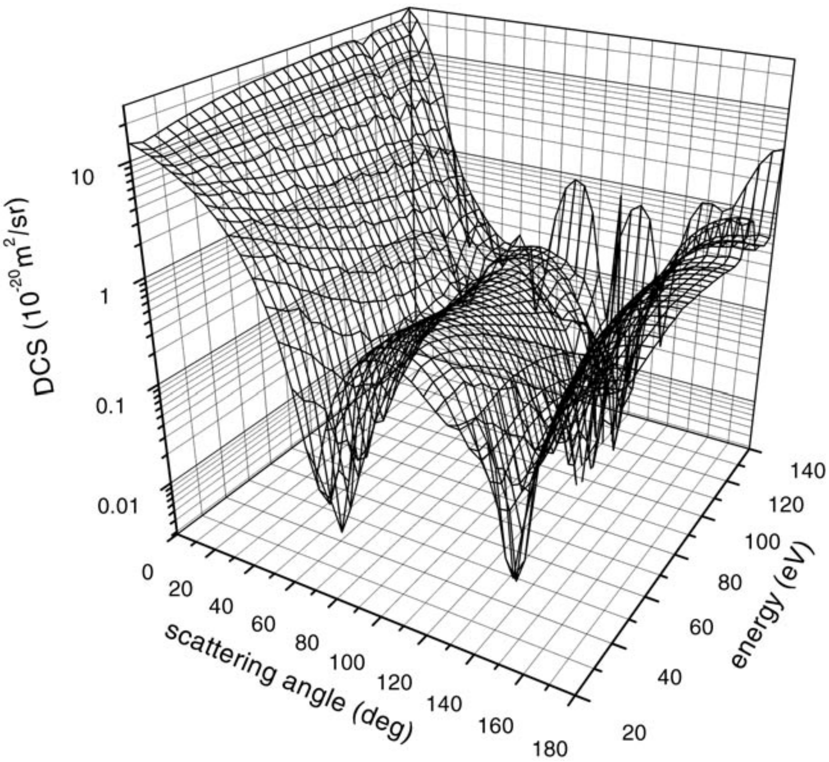

Figure 1. A three-dimensional plot of the differential cross sections: present results.

equation (1) and δ_l^- that for $\kappa = l$. In the case of a relativistic scattering problem we have two scattering amplitudes: the direct one

$$f(\theta) = \frac{1}{2\mathrm{i}k}\sum_l \{(l+1)[\exp(2\mathrm{i}\delta_l^+) - 1] + l[\exp(2\mathrm{i}\delta_l^-) - 1]\}P_l(\cos\theta) \tag{3}$$

and the spin-flip one

$$g(\theta) = \frac{1}{2\mathrm{i}k}\sum_l [\exp(2\mathrm{i}\delta_l^-) - \exp(2\mathrm{i}\delta_l^+)]P_l^1(\cos\theta). \tag{4}$$

Here θ is the scattering angle, while $P_l(\cos\theta)$ and $P_l^1(\cos\theta)$ are the Legendre polynomials and the Legendre associated functions, respectively. The differential cross section for elastic scattering is defined by the relation

$$\sigma_{\mathrm{diff}}(\theta) = |f(\theta)|^2 + |g(\theta)|^2. \tag{5}$$

We have calculated phase shifts for elastic scattering of electrons from argon in the energy range 10–160 eV to cover all the energies used in the measurements of Panajotović *et al* (1997). They are presented in table 1. For any incident energy and any chosen l we have two relativistic phase shifts $\delta_l^{\pm}$ (except for $l = 0$), where '+' corresponds to the spin 'up' and '−' to the spin 'down' solutions of Dirac equation (1). This indicates, respectively, negative and positive values of the quantum number κ.

Our differential cross section results in the considered angular and energy range are presented in a three-dimensional plot (figure 1). The low-angle critical minimum has been

Table 1. Phase shifts for elastic scattering of electron from argon (energies are given in eV). Upper lines correspond to δ_l^+ while lower ones to δ_l^-.

Energy	δ_0^+	$\delta_1^\pm$	$\delta_2^\pm$	$\delta_3^\pm$	$\delta_4^\pm$	$\delta_5^\pm$	$\delta_6^\pm$
10.3	−1.173	−0.545	0.928	0.097	0.038	0.020	0.012
		−0.553	0.929	0.097	0.038	0.020	0.012
15.3	−1.463	−0.762	0.014	0.155	0.059	0.031	0.018
		−0.771	1.463	0.155	0.059	0.031	0.018
20.3	1.451	−0.934	−1.430	0.215	0.080	0.041	0.024
		−0.944	−1.431	0.216	0.080	0.041	0.024
25.3	1.264	−1.076	−1.309	0.277	0.102	0.052	0.030
		−1.086	−1.311	0.278	0.102	0.052	0.030
30.3	1.106	−1.196	−1.170	0.339	0.123	0.062	0.036
		−1.206	−1.172	0.339	0.123	0.062	0.036
36.3	0.943	−1.318	−1.128	0.406	0.150	0.075	0.043
		−1.329	−1.130	0.406	0.150	0.075	0.043
37.3	0.918	−1.337	−1.192	0.421	0.151	0.077	0.045
		−1.348	−1.194	0.422	0.150	0.077	0.045
38.3	0.894	−1.355	−1.183	0.432	0.158	0.080	0.046
		−1.366	−1.185	0.432	0.158	0.080	0.046
39.3	0.870	−1.373	−1.174	0.439	0.164	0.081	0.047
		−1.384	−1.176	0.440	0.164	0.081	0.047
40.3	0.847	−1.391	−1.177	0.453	0.164	0.083	0.049
		−1.401	−1.178	0.453	0.164	0.083	0.049
41.3	0.824	−1.408	−1.159	0.464	0.168	0.085	0.050
		−1.418	−1.161	0.464	0.169	0.085	0.050
42.3	0.802	−1.424	−1.165	0.475	0.176	0.088	0.051
		−1.435	−1.166	0.475	0.176	0.088	0.051
43.3	0.780	−1.440	−1.161	0.482	0.180	0.089	0.052
		−1.451	−1.162	0.482	0.180	0.089	0.052
44.3	0.759	−1.456	−1.153	0.492	0.185	0.091	0.053
		−1.467	−1.154	0.492	0.186	0.091	0.053
50.3	0.640	−1.545	−1.129	0.548	0.206	0.104	0.060
		−1.556	−1.130	0.548	0.206	0.104	0.060
60.3	0.468	1.467	−1.115	0.633	0.251	0.127	0.072
		1.456	−1.116	0.633	0.251	0.127	0.072
75.3	0.254	1.308	−1.092	0.738	0.306	0.155	0.090
		1.297	−1.093	0.738	0.306	0.155	0.090
80.3	0.191	1.262	−1.056	0.766	0.325	0.165	0.096
		1.251	−1.057	0.766	0.325	0.165	0.096
90.3	0.077	1.177	−1.052	0.818	0.359	0.185	0.107
		1.166	−1.053	0.817	0.359	0.185	0.107
100.3	−0.025	1.102	−1.050	0.860	0.392	0.202	0.117
		1.090	−1.051	0.860	0.392	0.202	0.117
110.3	−0.118	1.033	−1.049	0.897	0.420	0.223	0.130
		1.022	−1.050	0.896	0.419	0.223	0.130
120.3	−0.204	0.970	−1.050	0.930	0.457	0.244	0.142
		0.959	−1.051	0.930	0.457	0.244	0.142
130.3	−0.283	0.912	−1.052	0.960	0.485	0.255	0.154
		0.901	−1.053	0.959	0.484	0.255	0.154
140.3	−0.356	0.858	−1.054	0.983	0.502	0.272	0.164
		0.847	−1.055	0.982	0.502	0.272	0.164
150.3	−0.425	0.808	−1.057	1.004	0.527	0.298	0.173
		0.797	−1.059	1.004	0.527	0.298	0.173
160.3	−0.489	0.761	−1.065	1.026	0.546	0.312	0.182
		0.750	−1.066	1.026	0.545	0.312	0.182

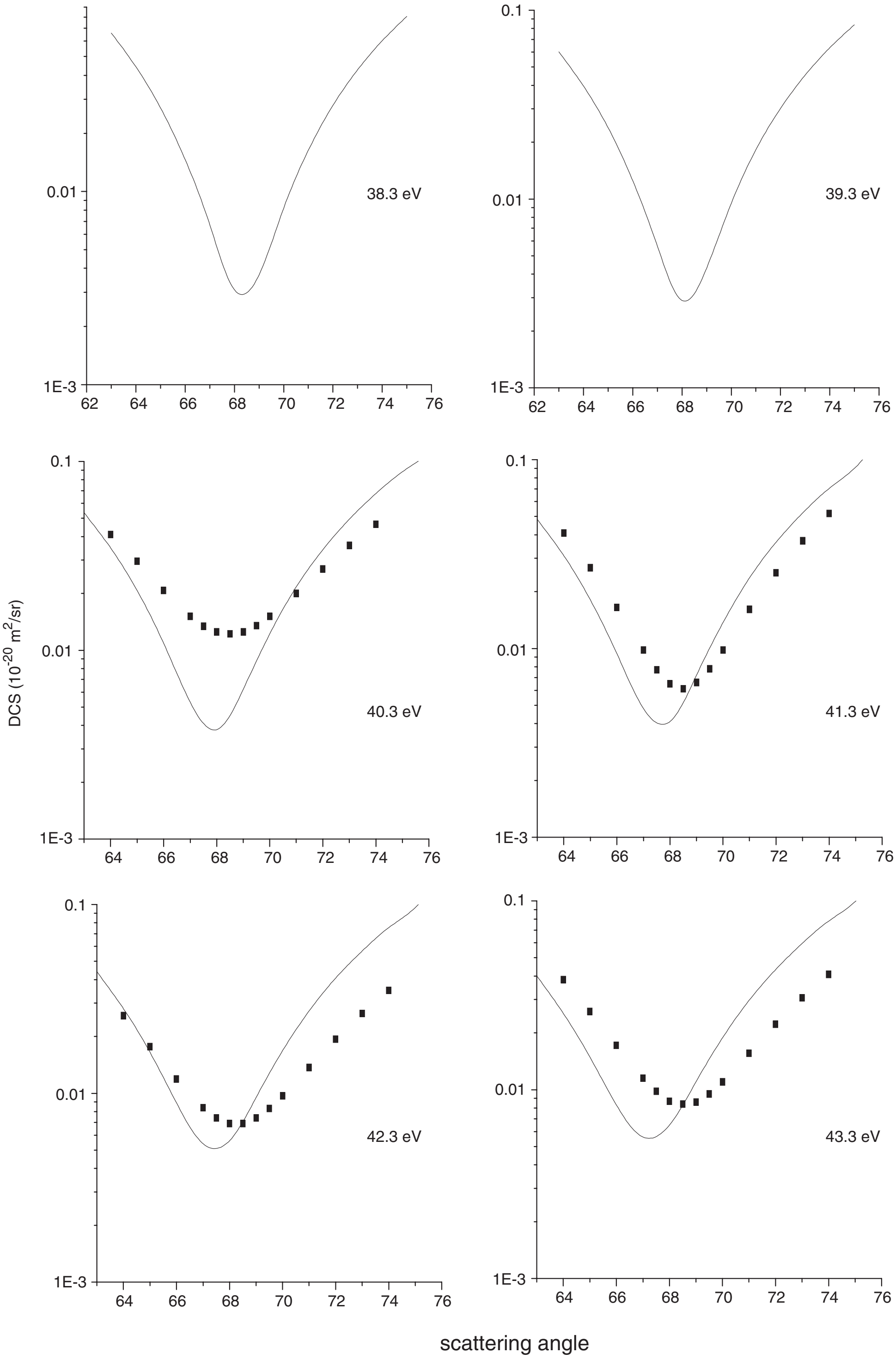

Figure 2. Differential cross sections for electron scattering from argon in the vicinity of low-angle minima: solid curves, present results; squares, the experiment of Panajatović *et al* (1997).

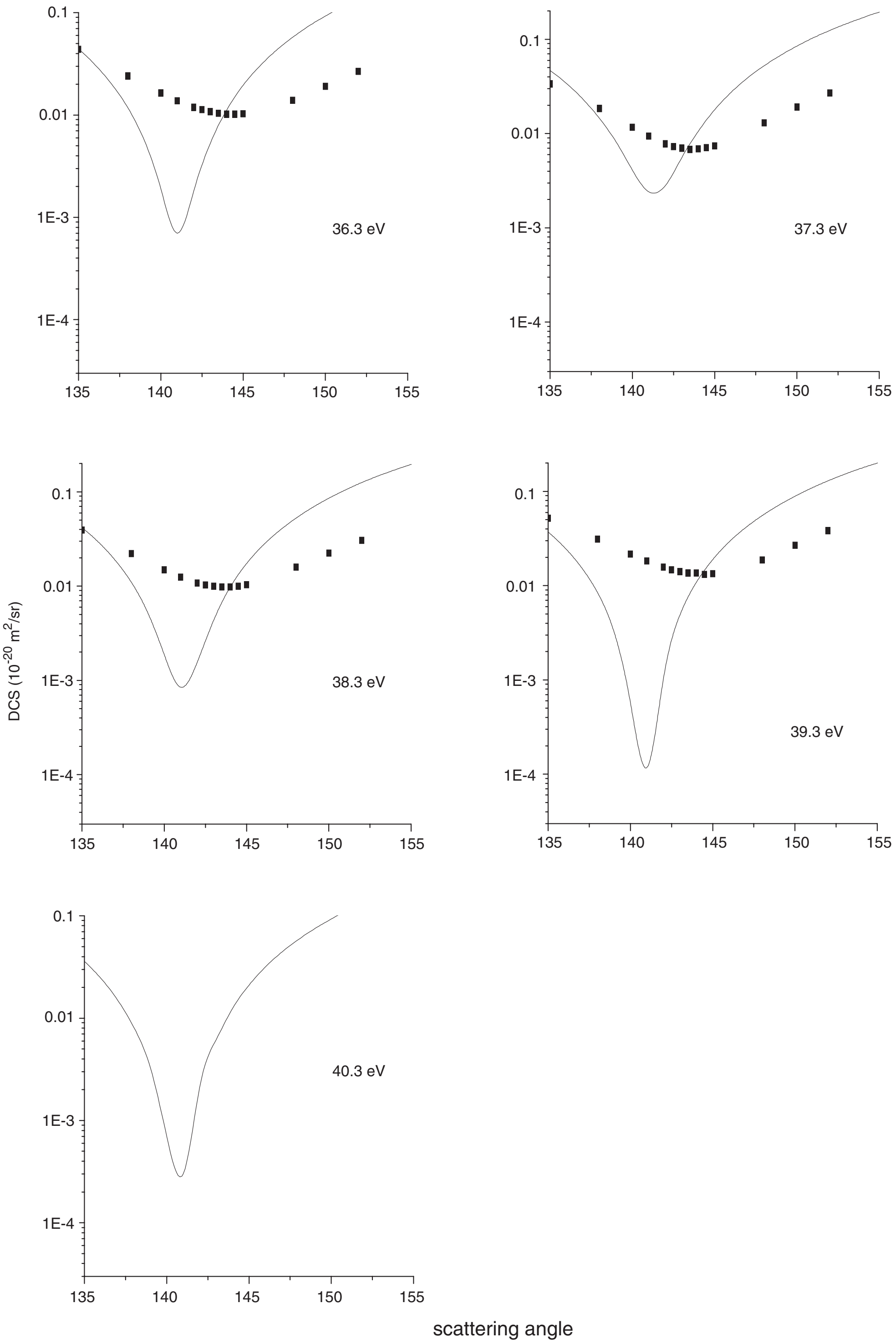

Figure 3. The same as in figure 2 but in the vicinity of high-angle minima.

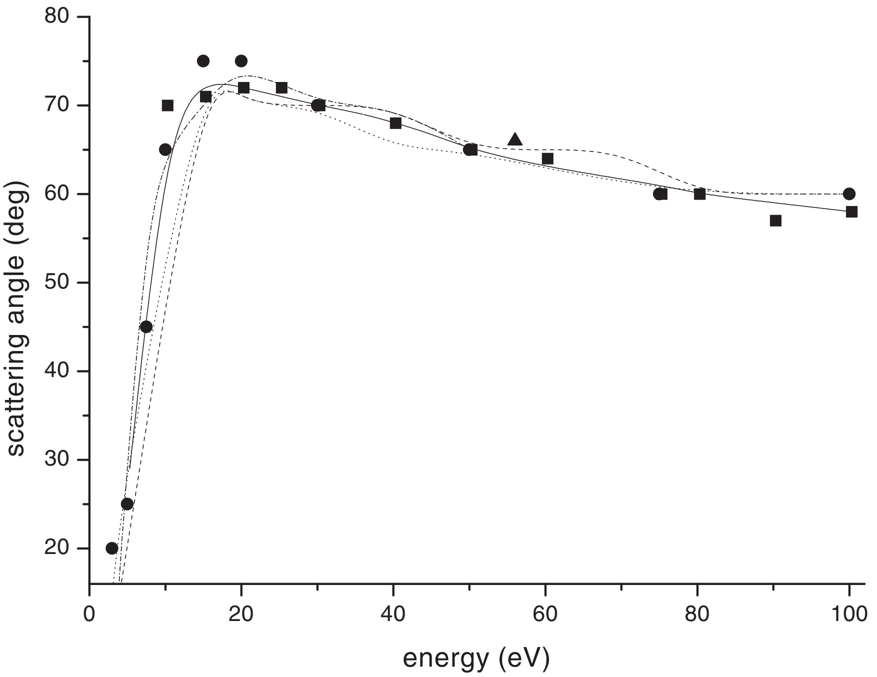

Figure 4. The position of low-angle differential cross section minimum versus incident energy. Experiment: triangles, Kessler *et al* (1976); circles, Srivastava *et al* (1981); squares, Panajatović *et al* (1997). Theory: solid curve, present results; dots, Nahar and Wadehra (1987); dashed curve, Fon *et al* (1983); dot-dashed curve, McEachran and Stauffer (1983).

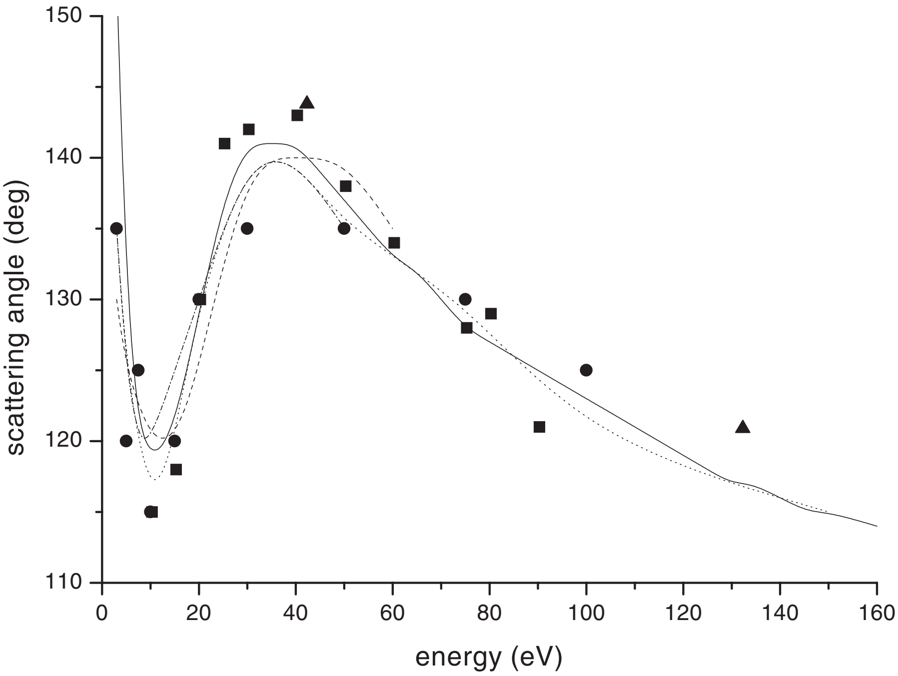

Figure 5. The same as in figure 4 but for high-angle differential cross section minimum.

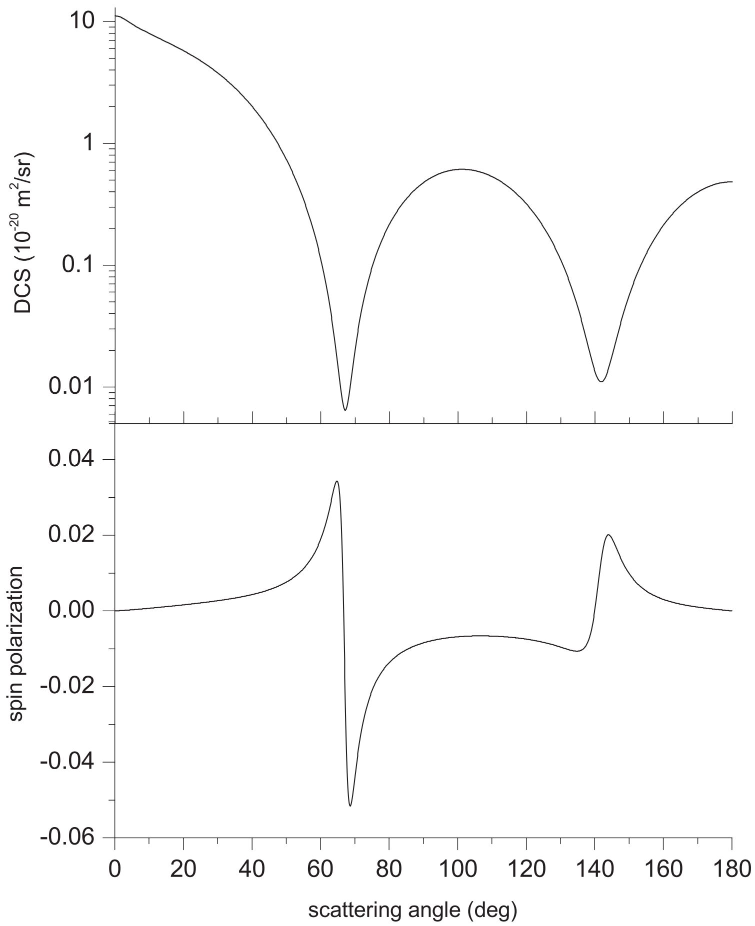

Figure 6. Differential cross sections and spin polarization after scattering of an unpolarized electron beam from argon at 39.4 eV.

found by Panajatović *et al* (1997) to be at 68.5° and 41.30 eV, while ours is at 68.0° and 39.30 eV. The angular positions are almost the same, while our scattering energy is 2 eV lower. In order to give a better insight we present six differential cross sections in the vicinity of critical energy (figure 2). Our theoretical curves follow quite closely experimental points within the considered energy range.

In the case of the high-angle minimum, Panajotović *et al* (1997) have localized it at 143.5° and 37.3 eV, while ours is at 141.0° and 39.5 eV. Comparison of our results with their cross sections is displayed in figure 3. Here, the agreement between our theoretical curves and their experimental points is not as good as in the previous case, although taking into account the logarithmic scale, it is quite reasonable. What is striking, is that our minima of differential cross sections are much narrower and deeper than the experimental ones.

The angular position of the low-angle minimum along incident electron energy is given in figure 4. There is an excellent agreement between our theoretical results and the experimental data of Panajatović *et al* (1997). Results of McEachran and Stauffer (1983), who solved the Schrödinger equation with an adiabatic exchange, cover the energy range up 50 eV and agree well with experiment. The theoretical line of Fon *et al* (1987), who used the *R*-matrix approach, quite closely follows experimental data over the whole energy region, while the model results of Nahar and Wadehra (1987) fit even better with the experimental points, particularly at small scattering energies. Kessler *et al* 's (1976) measurement of the position of the critical minimum position does not agree very well with the experimental point of Panajatović *et al*, neither with our predictions, although his point lies quite closely to both results.

In the case of high-angle minimum (figure 5) the biggest discrepancy between our theoretical results and experimental ones occurs at low energy, i.e. 10–15 eV. Here, only model calculations (Nahar and Wadhera 1987) show good agreement with experiment. At higher energies, all the displayed points and curves show better and more consistent agreement between themselves. The experimental points are well described by our theoretical results and the results of Fon *et al* (1983). It also occurs that two other minima pointed out by Kessler *et al* (1976) as separate critical minima are lying very close to our high-angle minima position curve. Our calculations of minima depths show that the first one is deeper. In figure 6, we present the connection between the positions of the critical minima and the spin polarization features of the scattered electron beam, which is unpolarized before scattering. The chosen energy of 39.4 eV is very close to the energies of the low- and high-angle critical minima, which are 39.3 and 39.5 eV, respectively. The angular positions of the critical minima coincide very well with the positions of the spin-polarization maxima.

In conclusion, our *ab initio* theoretical method is able to describe properly the positions of the critical minima in the case of argon as a target atom. Also, the connection between the positions of the critical minima and spin polarization for an initially unpolarized beam is properly described. Our fully relativistic approach allows for theoretical verification of experimentally obtained critical minima.

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