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Excitation of Ar I $3p^5 4p$, $3p^5 3d$ and $3p^5 5s$ configurations by electrons in the distorted-wave approximation

V E Bubelev and A N Grum-Grzhimailo

Institute of Nuclear Physics, Moscow State University, Moscow 11899, USSR

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Abstract. Excitation cross sections for all fine-structure levels of Ar I $3p^5 4p$, 3d and 5s configurations are calculated for the range of electron energies 16-100 eV in the distorted-wave Born approximation with exchange. Non-empirical intermediate-coupling wavefunctions are used and their quality is checked by calculating the dipole transition probabilities. The results are compared with the experimental data obtained by electrical and optical methods.

1. Introduction

Information about fine-structure Ar I excitation cross sections by electron impact is important in plasma and laser physics and for investigation of the mechanisms of an atomic excitation. At this time the most detailed information, both experimental and theoretical, has been obtained for the $3p^5 4s$ configuration. Experimental studies of excitation cross sections for the neighbouring higher-lying configurations are scanty and far from being complete.

The optical measurements for the 4p levels (Fisher 1933, Herrmann 1936, Volkova and Devyatov 1959, Zapesochnyi and Feltsan 1966, 1967, Ballou *et al* 1973, Bogdanova and Yurgenson 1987, Smirnov 1989) often give discrepant values; it is extremely difficult to take into account the contribution of the secondary process of population of radiating states.

Emission lines from 3d and 5s levels lie in the far infrared or vacuum ultraviolet spectral regions. These regions are uncomfortable for measurements and corresponding data on optical excitation functions are scarce (Mental and Morgan 1976). When using the electrical method it is difficult to measure cross sections for the separate fine-structure levels, due to a poor energy resolution (Chutjian and Cartwright 1981). It is somewhat hard to control inaccuracies which can appear during extrapolation of the differential cross sections.

Calculation difficulties are connected with the necessity of simultaneous application of qualitative wavefunctions and adequately taking into account both direct and exchange scattering amplitudes in the broad energy range. A few plane-wave Born approximation (PWBA) calculations have been carried out. Ganas and Green (1971) and Peterson and Allen (1972) obtained the cross sections for optically allowed transitions to the levels $3d(J=1)$ and $5s(J=1)$. Semi-empirical radial wavefunctions were used for the description of the target. Calculations with the Hartree-Fock type wavefunctions and taking into account a configuration interaction have been performed by Albat *et al* (1975) for an excitation of the two $4p(J=0)$ states and of the ^1D

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component of the $4p(J=2)$ states. The exchange amplitude has been ignored. Plane-wave results for the 4p states in the Ochkur approximation for an exchange amplitude and with the use of Hartree–Fock–Slater wavefunctions have been discussed by Ballou *et al* (1973). A large disagreement between theory and experiment was observed both in the levels excited predominantly by the direct scattering, and in the levels excited only by the exchange scattering (in the model used). All of the above-mentioned theoretical investigations apply to intermediate-coupling wavefunctions with semi-empirical coefficients of expansion on the basis of pure *LS* states taken from the spectroscopic data on the energy levels. Semiquantitative evaluations of the excitation cross sections for Ar I have also been performed for the purposes of plasma physics (Peterson and Allen 1972, Eggarter 1975, Bretagne *et al* 1986). Presently, we do not know of any calculations for the separate $3d(J\neq 1)$ and $5s(J\neq 1)$ levels. The recent experiments of Chutjian and Cartwright (1981) are free from the cascade contribution in the level cross sections which we investigated, but the results have not yet been theoretically interpreted.

In this paper we perform systematical calculations of the excitation cross sections for all the fine-structure levels of the $3p^5 4p$, 3d and 5s configurations in the distorted-wave Born approximation with exchange (DWBA). Some of the differential and correlation characteristics of excitation of the $3d(J=1)$ states in the DWBA without exchange have been published earlier (Balashov *et al* 1988). In this work the Ar I target is described by the non-empirical intermediate-coupling wavefunctions. Some preliminary results on the excitation cross sections for the $3p^5 4p$ configuration were published earlier (Bubelev and Grum-Grzhimailo 1990). In section 2 we calculate the wavefunctions of Ar I and check their quality; in section 3 we describe our formalism, consider a choice of the distortion potential and give some details of the calculations. In section 4 we demonstrate and discuss the results for the cross sections.

2. Wavefunctions of the target

2.1. Construction of wavefunctions

We use intermediate-coupling wavefunctions of the form

$$|\gamma J, i\rangle = \sum_{LS} A_{LS}^{J,i} |\gamma LS\rangle \tag{1}$$

where i is the number of the level with the prescribed total angular momentum J and configuration $\gamma(\gamma = 3p^5 nl)$. Wavefunctions (1) are found in three stages. First the *LS* basis states are calculated in the single configuration term-dependent Hartree–Fock approximation with the $3p^5$ frozen core. Then an atomic Hamiltonian with spin–orbit interaction $\Sigma_i \zeta(r_i)(\boldsymbol{l}_i \cdot \boldsymbol{s}_i)$ is diagonalized and the coefficients $A_{LS}^{J,i}$ are found. Spin–orbit interaction is dominated by the $3p^5$ core ($\zeta_{3p} \gg \zeta_{nl}$, $\zeta_{3p} = 894\ \mathrm{cm}^{-1}$). In table 1 the contribution of the *LS*-basis states to the fine-structure level wavefunctions of Ar I are listed for the purpose of subsequent discussion (Racah notation is used throughout). Experimental thresholds and *LS* compositions from the semi-empirical procedure are also indicated.

In the last stage the angular coefficients in the Hartree–Fock equation for an outer electron are recalculated taking into consideration the values of $A_{LS}^{J,i}$, which have been found already, and a new radial function is calculated for the prescribed level (Fliflet *et al* 1975). Such an approach allows us to factorize angular and radial parts when calculating matrix elements and concurrently retain the term dependence of the orbitals

Table 1. Ar I $3p^5nl[K]_J$ experimental thresholds E_{th}(eV) and eigenvector purities.

Level	E_{th}	*LS* composition	
		This work[a]	Other
$4s'[\frac{1}{2}]_0$	11.72	100% ^{3}P	
$4s[\frac{3}{2}]_1$	11.62	22.8% ^{1}P+77.2% ^{3}P	20.3% ^{1}P+79.7% ^{3}P[b]
$4s'[\frac{1}{2}]_1$	11.83	77.2% ^{1}P+22.8% ^{3}P	79.7% ^{1}P+20.3% ^{3}P
$4s[\frac{3}{2}]_2$	11.55	100% ^{3}P	
$4p[\frac{1}{2}]_0$	13.27	45.6% ^{1}S+54.4% ^{3}P	16.7% ^{1}S+83.3% ^{3}P[c]
$4p'[\frac{1}{2}]_0$	13.48	54.4% ^{1}S+45.6% ^{3}P	83.3% ^{1}S+16.7% ^{3}P
$4p[\frac{1}{2}]_1$	12.91	96.1% ^{3}S+1.2% ^{1}P+2.7% ^{3}P	
$4p[\frac{3}{2}]_1$	13.15	31.6% ^{1}P+16.3% ^{3}P+52.0% ^{3}D	
$4p'[\frac{3}{2}]_1$	13.28	35.9% ^{1}P+16.1% ^{3}P+47.9% ^{3}D	
$4p'[\frac{1}{2}]_1$	13.33	3.9% ^{3}S+31.2% ^{1}P+64.9% ^{3}P	
$4p[\frac{5}{2}]_2$	13.09	1.5% ^{3}P+36.8% ^{1}D+61.6% ^{3}D	
$4p[\frac{3}{2}]_2$	13.17	56.2% ^{3}P+33.1% ^{1}D+10.6% ^{3}D	
$4p'[\frac{3}{2}]_2$	13.30	42.2% ^{3}P+30.0% ^{1}D+27.7% ^{3}D	
$4p[\frac{5}{2}]_3$	13.08	100% ^{3}D	
$3d[\frac{1}{2}]_0$	13.84	100% ^{3}P	
$3d[\frac{1}{2}]_1$	13.86	1.4% ^{1}P+96.5% ^{3}P+2.2% ^{3}D	98% ^{3}P[d]
$3d[\frac{3}{2}]_1$	14.15	59.1% ^{1}P+40.9% ^{3}D	46% ^{1}P+53% ^{3}D
$3d'[\frac{3}{2}]_1$	14.30	39.5% ^{1}P+3.5% ^{3}P+56.9% ^{3}D	53% ^{1}P+2% ^{3}P+45% ^{3}D
$3d[\frac{3}{2}]_2$	13.90	88.4% ^{3}P+4.6% ^{1}D+7.0% ^{3}D	93% ^{3}P+3% ^{1}D+4% ^{3}D
$3d[\frac{5}{2}]_2$	14.06	27.3% ^{1}D+18.2% ^{3}D+54.6% ^{3}F	19% ^{1}D+13% ^{3}D+68% ^{3}F
$3d'[\frac{5}{2}]_2$	14.21	32.8% ^{1}D+21.7% ^{3}D+45.4% ^{3}F	41% ^{1}D+27% ^{3}D+32% ^{3}F
$3d'[\frac{3}{2}]_2$	14.23	11.6% ^{3}P+35.3% ^{1}D+53.1% ^{3}D	7% ^{3}P+37% ^{1}D+56% ^{3}D
$3d[\frac{7}{2}]_3$	14.01	2.9% ^{3}D+27.3% ^{1}F+69.9% ^{3}F	3% ^{3}D+19% ^{1}F+78% ^{3}F
$3d[\frac{5}{2}]_3$	14.10	53.2% ^{3}D+40.5% ^{1}F+6.3% ^{3}F	46% ^{3}D+49% ^{1}F+5% ^{3}F
$3d'[\frac{5}{2}]_3$	14.24	43.9% ^{3}D+32.2% ^{1}F+23.9% ^{3}F	51% ^{3}D+32% ^{1}F+17% ^{3}F
$3d[\frac{7}{2}]_4$	13.98	100% ^{3}F	
$5s'[\frac{1}{2}]_0$	14.24	100% ^{3}P	
$5s[\frac{3}{2}]_1$	14.09	54.8% ^{1}P+45.2% ^{3}P	
$5s'[\frac{1}{2}]_1$	14.25	45.2% ^{1}P+54.8% ^{3}P	
$5s[\frac{3}{2}]_2$	14.07	100% ^{3}P	

[a] Quantities less than 0.1% not given.
[b] Padial *et al* (1981).
[c] Albat *et al* (1975).
[d] Martin (1984).

(each fine-structure level $\gamma J, i$ has its own radial wavefunction $P_{nl}^{J,i}(r)$). The latter can be found important in the first instance for the $3p^5$3d configuration, where the 3d orbital is strongly term dependent (Hansen 1972).

2.2. A check of the quality of wavefunctions

We have carried out calculations of all the dipole transition probabilities between 4s, 5s, 4p, 3d levels and the ground state for checking the suitability of the wavefunctions in the calculations of matrix elements. The probabilities (r variant) are listed in tables 2–4 together with the experimental data and other theoretical values. Our results for infrared transitions 5s–4p and 3d–4p may be of self-dependent interest since experimental data are not accurate and incomplete, and there also exists a deficit of calculations.

Table 2. Ar I 4s–4p and 4p–5s transition probabilities ($10^6\ s^{-1}$). Experimental values from Wiese *et al* (1989) for 4s–4p and from Wiese *et al* (1969) for 4p–5s. Calculations from Lilly (1976).

4p–4s	This work	Wiese *et al*	Lilly	4p–5s	This work	Wiese *et al*	Lilly
$4p'[\frac{1}{2}]_0$–$4s'[\frac{1}{2}]_1$	50.3	44.5 ± 3.6	44.1	–$5s'[\frac{1}{2}]_1$	1.66	2.1[b]	0.97
$4p'[\frac{1}{2}]_1$–	22.9	15.3 ± 0.8	17.2		3.95	3.4[b]	3.29
$4p'[\frac{3}{2}]_2$–	29.7	22.3 ± 1.1	22.5		10.7	10.0[b]	9.79
$4p'[\frac{3}{2}]_1$–	16.2	13.9 ± 1.1	13.0		2.57	2.2[b]	2.39
$4p[\frac{1}{2}]_0$–	4.38	<0.001	0.00		0.03	0.38[c]	0.40
$4p[\frac{3}{2}]_2$–	6.55	5.03 ± 0.5	5.2		1.85	1.56[a]	1.40
$4p[\frac{3}{2}]_1$–	0.89	1.1 ± 0.08	0.9		0.15	0.28[c]	0.20
$4p[\frac{5}{2}]_2$–	1.46	1.5 ± 0.12	1.2		0.05	0.21[c]	0.11
$4p[\frac{1}{2}]_1$–	0.28	0.2 ± 0.06	0.17		1.01	1.98[a]	1.52
$4p'[\frac{1}{2}]_1$–$4s'[\frac{1}{2}]_0$	14.4	11.7 ± 0.6	12.5	–$5s'[\frac{1}{2}]_0$	6.91	5.1[b]	5.29
$4p'[\frac{3}{2}]_1$–	25.2	18.6 ± 1.5	20.4		14.0	11.0[b]	10.9
$4p[\frac{3}{2}]_1$–	3.18	2.43 ± 0.2	2.6		3.32	2.49[a]	2.58
$4p[\frac{1}{2}]_1$–	1.07	1.0 ± 0.15	0.86		2.28	1.58[a]	2.82
$4p'[\frac{1}{2}]_0$–$4s[\frac{3}{2}]_1$	2.18	0.24 ± 0.02	0.09	–$5s[\frac{3}{2}]_1$	0.01	0.18[b]	0.10
$4p'[\frac{1}{2}]_1$–	1.89	1.83 ± 0.1	1.9		0.023	0.034[b]	0.03
$4p'[\frac{3}{2}]_2$–	10.3	8.47 ± 0.7	9.2		0.10	0.033[b]	0.05
$4p'[\frac{3}{2}]_1$–	0.27	0.02 ± 0.002	0.1		0.36	0.45[c]	0.34
$4p[\frac{1}{2}]_0$–	53.1	40.2 ± 3.2	43.9		2.13	1.5[b]	1.13
$4p[\frac{3}{2}]_2$–	5.69	4.90 ± 0.7	4.9		2.85	2.7[b]	2.59
$4p[\frac{3}{2}]_1$–	31.9	25.0 ± 1.3	25.7		5.44	4.6[b]	4.63
$4p[\frac{5}{2}]_2$–	26.8	21.5 ± 1.1	20.8		10.1	10.0[b]	8.9
$4p[\frac{1}{2}]_1$–	5.78	5.43 ± 0.4	4.65		1.47	2.74[a]	1.93
$4p'[\frac{1}{2}]_1$–$4s[\frac{3}{2}]_2$	1.57	6.39 ± 0.3	7.40	–$5s[\frac{3}{2}]_2$	0.34	0.35[b]	0.24
$4p'[\frac{3}{2}]_2$–	5.75	3.80 ± 0.3	4.5		0.39	0.14[b]	0.29
$4p'[\frac{3}{2}]_1$–	0.26	0.63 ± 0.05	1.0		0.057	0.059[c]	0.05
$4p[\frac{3}{2}]_2$–	33.5	24.5 ± 2.0	27.0		4.70	3.3[b]	3.48
$4p[\frac{3}{2}]_1$–	2.82	5.18 ± 0.26	5.60		0.61	0.46[c]	0.48
$4p[\frac{5}{2}]_2$–	11.0	9.28 ± 0.74	9.80		2.04	1.2[b]	1.87
$4p[\frac{5}{2}]_3$–	42.5	33.1 ± 2.6	34.9		11.5	12.0[b]	10.3
$4p[\frac{1}{2}]_1$–	18.0	18.9 ± 1.5	17.4		3.90	4.9[b]	4.99

[a] Uncertainties within 25%.
[b] Uncertainties within 50%.
[c] Uncertainties larger than 50%.

In the majority of cases our calculations overestimate (about 20–30%) the experimental probabilities for the well studied 4s–4p transition array and are inferior as a whole to the effective operator method with adjustable parameters (Lilly 1976). An intent analysis of table 2 shows that systematic large discrepancies appear for our results from the values of Lilly (1976) for the weak transitions from $4p(J=0)$ levels. The wavefunctions of these levels are most likely inadequate in our calculations, and this is also seen from table 1. It is significant that our results for the 4p–3d transition array (i.e. the transitions from the levels with strongly term-dependent 3d wavefunction) are in satisfactory agreement with the calculations of Lilly (1976) and with the available experimental data (Wiese *et al* 1969). Disagreement of the two calculations exists for some weak transitions for which experimental data are absent. This overall harmonious picture deteriorates by a strong divergence in the $J=3$–$J=3$ transitions. We cannot explain the reasons of such divergence at present.

Table 3. Ar I 4p–3d transition probabilities (10^6 s^{-1}). Experimental values from Wiese *et al* (1969). Calculations from Lilly (1976).

4p–3d	This work	Wiese *et al*	Lilly	4p–3d	This work	Wiese *et al*	Lilly
$4p[\frac{1}{2}]_1$–$3d'[\frac{3}{2}]_1$	0.06	—	0.00	$4p[\frac{1}{2}]_1$–$3d[\frac{5}{2}]_1$	0.00	—	0.00
$4p[\frac{3}{2}]_2$–	0.20	—	0.07	$4p[\frac{5}{2}]_3$–	0.42	0.14[b]	0.35
$4p[\frac{3}{2}]_1$–	1.08	—	0.16	$4p[\frac{5}{2}]_2$–	6.85	6.4[b]	5.8
$4p[\frac{3}{2}]_2$–	0.71	0.48[a]	0.64	$4p[\frac{3}{2}]_1$–	12.7	8.2[b]	11.3
$4p[\frac{1}{2}]_0$–	0.29	0.47[b]	0.93	$4p[\frac{3}{2}]_2$–	0.37	—	0.27
$4p'[\frac{3}{2}]_1$–	3.13	5.1[b]	3.34	$4p'[\frac{3}{2}]_1$–	0.00	—	0.15
$4p'[\frac{3}{2}]_2$–	0.40	—	0.34	$4p'[\frac{3}{2}]_2$–	0.00	—	0.01
$4p'[\frac{5}{2}]_2$–	7.32	8.0[b]	5.97	$4p'[\frac{1}{2}]_1$–	0.00	—	0.00
$4p'[\frac{1}{2}]_0$–	8.69	5.8[b]	6.25	$4p[\frac{5}{2}]_3$–$3d[\frac{7}{2}]_3$	0.00	—	2.74
$4p[\frac{5}{2}]_3$–$3d'[\frac{5}{2}]_3$	0.02	—	1.21	$4p[\frac{5}{2}]_2$–	16.7	12[b]	14.5
$4p[\frac{3}{2}]_2$–	0.04	—	0.01	$4p[\frac{3}{2}]_2$–	0.05	0.1[b]	0.17
$4p[\frac{3}{2}]_2$–	0.21	—	0.05	$4p'[\frac{3}{2}]_2$–	0.00	—	0.06
$4p'[\frac{3}{2}]_2$–	20.5	17[b]	17.7	$4p[\frac{5}{2}]_3$–$3d[\frac{7}{2}]_4$	17.7	—	16.6
$4p[\frac{1}{2}]_1$–$3d'[\frac{3}{2}]_2$	0.36	—	0.05	$4p[\frac{1}{2}]_1$–$3d[\frac{3}{2}]_2$	0.79	5.5[b]	10.7
$4p[\frac{5}{2}]_3$–	0.32	—	0.39	$4p[\frac{5}{2}]_3$–	0.50	—	0.45
$4p[\frac{5}{2}]_2$–	0.31	—	0.37	$4p[\frac{5}{2}]_2$–	0.04	0.14[b]	0.04
$4p[\frac{3}{2}]_1$–	0.55	0.41[a]	0.52	$4p[\frac{3}{2}]_1$–	0.32	0.29[b]	0.29
$4p[\frac{3}{2}]_2$–	4.33	4.23[a]	4.43	$4p[\frac{3}{2}]_2$–	2.97	2.8[b]	2.5
$4p'[\frac{3}{2}]_1$–	0.07	—	0.02	$4p'[\frac{3}{2}]_1$–	0.10	—	0.10
$4p'[\frac{3}{2}]_2$–	1.34	—	1.00	$4p'[\frac{3}{2}]_2$–	0.57	0.44[b]	0.57
$4p'[\frac{1}{2}]_1$–	15.0	7.0[b]	12.4	$4p'[\frac{1}{2}]_1$–	0.07	0.12[b]	0.15
$4p[\frac{1}{2}]_1$–$3d'[\frac{5}{2}]_2$	0.25	—	0.00	$4p[\frac{1}{2}]_1$–$3d[\frac{1}{2}]_1$	11.4	8.3[b]	12.4
$4p[\frac{5}{2}]_3$–	0.08	—	0.13	$4p[\frac{5}{2}]_2$–	0.35	0.044[b]	0.37
$4p[\frac{5}{2}]_2$–	0.71	0.93[a]	1.32	$4p[\frac{3}{2}]_1$–	0.08	—	0.08
$4p[\frac{3}{2}]_1$–$3d'[\frac{5}{2}]_2$	0.25	—	0.00	$4p[\frac{3}{2}]_2$–$3d[\frac{1}{2}]_1$	1.23	—	1.1
$4p[\frac{3}{2}]_2$–	0.04	—	0.01	$4p[\frac{1}{2}]_0$–	0.36	—	0.39
$4p'[\frac{3}{2}]_1$–	17.9	15[b]	15.4	$4p'[\frac{3}{2}]_1$–	0.08	0.036[b]	0.09
$4p'[\frac{3}{2}]_2$–	2.08	2.50[b]	1.80	$4p'[\frac{3}{2}]_2$–	0.13	0.16[b]	0.12
$4p'[\frac{1}{2}]_1$–	0.00	—	0.02	$4p'[\frac{1}{2}]_1$–	0.18	0.19[b]	0.13
$4p[\frac{1}{2}]_1$–$3d[\frac{3}{2}]_1$	0.00	—	0.00	$4p'[\frac{1}{2}]_0$–	0.02	—	0.01
$4p[\frac{5}{2}]_2$–	1.38	1.07[a]	1.33	$4p[\frac{1}{2}]_1$–$3d[\frac{1}{2}]_0$	11.8	9.1[b]	13.2
$4p[\frac{3}{2}]_1$–	10.1	12[b]	9.26	$4p[\frac{3}{2}]_1$–	1.09	—	1.04
$4p[\frac{3}{2}]_2$–	0.05	—	0.12	$4p'[\frac{3}{2}]_1$–	0.09	0.14[b]	0.08
$4p[\frac{1}{2}]_0$–	9.67	4.8[b]	6.66	$4p'[\frac{1}{2}]_1$–	0.45	0.45[b]	0.41
$4p'[\frac{3}{2}]_1$–	1.06	—	0.53	$4p[\frac{5}{2}]_3$–$3d[\frac{5}{2}]_3$	0.03	3.5[b]	3.68
$4p'[\frac{3}{2}]_2$–	0.03	—	0.01	$4p[\frac{5}{2}]_2$–	1.21	2.2[b]	1.73
$4p'[\frac{1}{2}]_1$–	0.00	—	0.11	$4p[\frac{3}{2}]_2$–	16.2	—	13.8
$4p'[\frac{1}{2}]_0$–	0.19	—	0.38	$4p'[\frac{3}{2}]_2$–	0.00	0.011[b]	0.01

[a] Uncertainties within 25%.
[b] Uncertainties within 50%.

Our calculations of transitions to the ground state (table 4) give good results for all the lines except for the two weakest from the states $3d[\frac{1}{2}]_1$ and $5s'[\frac{1}{2}]_1$. In the case of the $3d[\frac{1}{2}]_1$ level it is important to take into account configuration mixing, as it is seen in comparison with the calculations of Lee and Lu (1973) and Lee (1974) by the multichannel quantum defect method and of Gruzdev and Loginov (1975) in the Hartree–Fock approximation with configuration mixing. For the state $5s'[\frac{1}{2}]_1$ our results are in accordance with the calculations of Lee and Lu (1973), Lee (1974) and Gruzdev and Loginov (1975) but disagree with experiment and with the empirically allowed

Table 4. Absorption oscillator strength (in unit 10^{-3}) of Ar I for transitions from the ground state.

Level	This work	Observed		Calculated			
$4s[\frac{3}{2}]_1$	69	59 ± 3[a]	63 ± 5[b]	59[c]	61[d]	80[e]	71[f]
$4s'[\frac{1}{2}]_1$	224	228 ± 21	240 ± 20	300	231	210	286
$5s[\frac{3}{2}]_1$	33	27 ± 2	25 ± 2	34	29	45	34.4[g]
$5s'[\frac{1}{2}]_1$	27	13 ± 3	10.6 ± 0.8	25	24	39	11.1
$3d[\frac{1}{2}]_1$	12	—	0.89 ± 0.07	1.1	4.6	1.6	—
$3d[\frac{3}{2}]_1$	112	93 ± 6	79 ± 6	53	88	45	—
$3d'[\frac{3}{2}]_1$	88	107 ± 15	86 ± 7	110	350	128	—

[a] Lawrence (1968).
[b] Westerveld *et al* (1979).
[c] Lee (1974).
[d] Gruzdev and Loginov (1975).
[e] Lee and Lu (1973).
[f] Aymar *et al* (1970).
[g] Aymar (1972).

for configuration mixing calculations of Aymar (1972). This transition is very sensitive to the effects of configuration mixing (Gruzdev and Loginov 1975) and it has to be taken into account.

The present analysis shows that the accuracy of our wavefunctions for the calculation of the dipole transition probabilities is in conformity, as a whole, with the accuracy expected for the calculations of the electron impact cross sections. In some cases, for example for the states $4p(J=0)$, $3d[\frac{1}{2}]_1$, $5s'[\frac{1}{2}]_1$ it is hard to expect reliable results. These conclusions must be taken with caution, when referring to the excitation from the ground state which will be considered, because in the latter case the scattering amplitudes are dominated by the inner region of atom within the radius of the $3p^6$ subshell.

3. Theory and calculation details

The convenience of our variant of the intermediate-coupling model is that the radial and angular parts of the wavefunctions (1) are factorized and it leads to the corresponding factorization of the direct and exchange multiple cross sections. We can almost literally use the finished formulae of the DWBA for the integral cross sections in the pure coupling schemes (see, for example, Sobel'man *et al* 1981). Corrections are only required in the angular factors. We write down the final expressions for the cross sections of $3p^6\ {}^1S_0$-$3p^6nl$: J, i excitations (in πa_0^2):

$$\sigma(E)=\sigma^{\mathrm{d}}(E)+\sigma^{\mathrm{int}}(E)+\sigma^{\mathrm{ex}}(E) \tag{2}$$

$$\sigma^{\mathrm{d}}(E)=\frac{1}{E}\sum_k Q_k^{\mathrm{d}} \sum_{\lambda\lambda'} [R_k^{\mathrm{d}}(\lambda,\lambda',l)]^2 \tag{3}$$

$$\sigma^{\mathrm{int}}(E)=-\frac{1}{E}\sum_k Q_k^{\mathrm{d}} \sum_{\lambda\lambda'}\left[R_k^{\mathrm{d}}(\lambda,\lambda',l)\left(\sum_\varkappa (-1)^\varkappa \begin{Bmatrix} k & 1 & l \\ \varkappa & \lambda & \lambda' \end{Bmatrix} R_\varkappa^{\mathrm{e}}(\lambda,\lambda',l)\right)\right] \tag{4}$$

$$\sigma^{\mathrm{ex}}(E)=\frac{1}{E}\sum_k Q_k^{\mathrm{e}}\sum_{\lambda\lambda'}\left[\sum_{\varkappa}(-1)^{\varkappa}\begin{Bmatrix} k & 1 & l \\ \varkappa & \lambda & \lambda' \end{Bmatrix} R_{\varkappa}^{\mathrm{e}}(\lambda,\lambda',l)\right]^2 \tag{5}$$

$$R_k^{\mathrm{d}}(\lambda,\lambda',l)=\sqrt{(2\lambda+1)(2\lambda'+1)}\begin{pmatrix}1 & l & k\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & \lambda' & k\\ 0 & 0 & 0\end{pmatrix}$$
$$\times\int_0^\infty \mathrm{d}r\int_0^\infty \mathrm{d}r'\,P_{nl}^{J,i}(r)P_{3\mathrm{p}}(r)\frac{r_<^{\varkappa}}{r_>^{\varkappa+1}}P_{E\lambda}(r')P_{E'\lambda}(r') \tag{6}$$

$$R_{\varkappa}^{\mathrm{e}}(\lambda,\lambda',l)=\sqrt{(2\lambda+1)(2\lambda'+1)}\begin{pmatrix}1 & \lambda' & \varkappa\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\lambda & l & \varkappa\\ 0 & 0 & 0\end{pmatrix}$$
$$\times\int_0^\infty \mathrm{d}r\int_0^\infty \mathrm{d}r'\,P_{nl}^{J,i}(r)P_{3\mathrm{p}}(r')\frac{r_<^{\varkappa}}{r_>^{\varkappa+1}}P_{E\lambda}(r)P_{E'\lambda'}(r') \tag{7}$$

$$Q_k^{\mathrm{d}}=96\frac{(2J+1)(2l+1)}{(2k+1)^2}\delta_{S0}\delta_{Lk}\delta_{LJ}(A_{LS}^{J,i})^2 \tag{8}$$

$$Q_k^{\mathrm{e}}=24\frac{(2J+1)(2l+1)}{(2k+1)^2}\delta_{Lk}[\delta_{S0}(A_{LS}^{J,i})^2+\delta_{S1}(A_{LS}^{J,i})^2]. \tag{9}$$

Here σ^{d}, σ^{ex} and σ^{int} are direct, exchange and interference cross sections; E, E' are the energies of incident and scattered electrons in Ryd; $\left(\begin{smallmatrix}a & b & c\\ \alpha & \beta & \gamma\end{smallmatrix}\right)$ and $\left\{\begin{smallmatrix}a & b & c\\ e & f & g\end{smallmatrix}\right\}$ are 3-j and 6-j symbols; $P_{E\lambda}(r)$ is a partial wave, distorted by an atomic potential and normalized to the asymptotic $(1/\pi^{1/2}E^{1/4})\sin(E^{1/2}r-\pi\lambda/2+\delta_\lambda)$; δ_λ is a scattering phase.

It is known (Bartschat and Madison 1987) that results are best for the 3p^6–3p^{5}4s($J=1$) excitation when the static potential of the final atomic state is used for distortion in the entrance and exit channels. For the levels 3p^{5}4p($J=2$) we have carried out calculations with the ground-state potential and the excited-state potential for both channels and also with the ground-state potential for incident electron and with the excited state potential for scattered electron. It was revealed that the first variant gives unsatisfactory results in the region of the cross section maximum and the two other variants lead to rather similar and more acceptable results (figure 1). The rest of the calculations were performed with the excited-state potential both for incident and scattered electrons (this potential changes from one fine-structure level to another). Polarization and exchange potentials are ignored. It simplifies the calculations but can be a source of inaccuracy of the method at low energies. Allowing for the local exchange potential of the form of Furness and McCarthy (1973) has not improved the total cross sections appreciably for the 3p^{5}4p states.

An orthogonalization of the incident El and scattered E'p partial waves to nl and 3p orbitals accordingly was carried out when calculating the exchange integrals (7). Up to 25 partial waves were taken into account in the formulae (3)–(5) depending on the incident energy. The rest of the partial waves were summed up in (3) in the plane-wave approximation. All the possible values of k and $\varkappa$ in the exchange cross sections were taken into account. The upper limit of r' was brought up to 200 au in the slowly convergent integrals (6). Experimental excitation thresholds were used throughout.

A computer program was created to calculate target wavefunctions, dipole transition probabilities and excitation cross sections in the DWBA (and PWBA). A special routine can compute the differential cross sections and density matrix of the total angular momentum, which determines the correlation and polarization parameters of an excitation. In this paper we limit ourselves to the total cross sections.

4. Results and discussion

Our results for all 26 levels (arranged in order of increasing threshold) are listed in table 5, and in figures 1–8 the theory is compared with experiment. We also have performed calculations for the levels $3p^5 4s$. Our results for the state $4s'[\frac{1}{2}]_1$ are about 6% lower at a maximum of the cross section; and for the weaker transition to the state $4s[\frac{3}{2}]_1$ the results are about 20% higher than the FOMBT values of Padial *et al* (1981). This discrepancy may be accounted for the difference in the model for the distorted waves and slightly different contributions of ^1P and ^3P components to the $3p^5 4s(J=1)$ states (table 1) in our calculations and in the calculations of Padial *et al* (1981).

4.1. *Configuration $3p^5 4p$*

The main features of the electron impact excitation for this configuration are similar to those for the configuration $2p^5 3p$ of neon (Bubelev and Grum-Grzhimailo 1990). The levels $3p^5 4p(J=0,2)$ are excited in our model both by direct and by exchange scattering, as follows from (2)–(9). The levels $3p^5 4p(J=1,3)$ are excited only by exchange scattering. We shall discuss an excitation of groups of levels with different J separately.

Table 5. Cross sections for excitation of the $3p^5 4p$, 3d and 5s levels of Ar I (10^{-19} cm^2). Excitation thresholds E_{th} are also listed.

	Level	E_{th} (eV)	Energy (eV)							
			16	18	20	25	30	40	50	100
1	$4p[\frac{1}{2}]_1$	12.91	13.9	22.9	38.1	52.2	42.0	13.5	5.00	0.51
2	$4p[\frac{5}{2}]_3$	13.08	19.0	26.0	32.8	33.4	23.3	7.56	3.11	0.27
3	$4p[\frac{5}{2}]_2$	13.10	14.5	19.9	25.3	27.7	24.3	17.7	15.9	8.59
4	$4p[\frac{3}{2}]_1$	13.15	6.03	8.50	11.1	11.6	8.06	2.46	0.95	0.08
5	$4p[\frac{3}{2}]_2$	13.17	10.3	14.6	19.5	22.1	19.5	14.2	12.8	7.05
6	$4p[\frac{1}{2}]_0$	13.27	116.0	123.0	129.0	132.0	122.0	95.0	78.0	40.6
7	$4p'[\frac{3}{2}]_1$	13.28	5.60	8.10	10.7	11.3	7.90	2.40	0.93	0.07
8	$4p'[\frac{3}{2}]_2$	13.30	10.5	15.1	20.2	22.7	19.7	13.7	12.4	6.58
9	$4p'[\frac{1}{2}]_1$	13.33	10.1	10.4	9.76	6.74	3.51	0.94	0.38	0.10
10	$4p'[\frac{1}{2}]_0$	13.48	125.0	135.0	143.0	146.0	136.0	107.0	88.0	46.0
11	$3d[\frac{1}{2}]_0$	13.84	12.1	20.5	24.2	23.1	16.7	6.50	2.70	0.27
12	$3d[\frac{1}{2}]_1$	13.86	50.0	71.8	81.0	77.1	59.4	31.2	20.5	11.5
13	$3d[\frac{3}{2}]_2$	13.90	26.1	86.3	99.3	91.6	65.2	25.4	10.7	1.10
14	$3d[\frac{7}{2}]_4$	13.98	36.2	53.6	58.2	48.2	31.7	11.5	4.76	0.45
15	$3d[\frac{7}{2}]_3$	14.01	22.2	29.8	31.6	26.5	19.0	10.1	6.42	2.80
16	$3d[\frac{5}{2}]_2$	14.06	9.80	16.6	19.7	15.8	10.1	3.76	1.50	0.12
17	$5s[\frac{3}{2}]_2$	14.07	17.7	21.7	22.2	17.1	10.8	3.73	1.52	0.11
18	$5s[\frac{3}{2}]_1$	14.09	17.7	23.5	27.4	31.1	31.3	30.9	30.5	25.6
19	$3d[\frac{5}{2}]_3$	14.10	9.20	12.3	13.4	11.9	9.66	6.83	5.04	2.76
20	$3d[\frac{3}{2}]_1$	14.15	64.7	64.8	69.4	83.0	89.0	89.0	88.3	77.8
21	$3d'[\frac{5}{2}]_2$	14.21	7.80	14.2	17.3	13.9	9.00	3.33	1.31	0.11
22	$3d'[\frac{3}{2}]_2$	14.23	6.00	11.5	14.4	11.8	7.68	2.83	1.08	0.08
23	$3d'[\frac{5}{2}]_3$	14.24	11.1	15.6	17.2	14.8	11.4	6.94	4.80	2.40
24	$5s'[\frac{1}{2}]_0$	14.24	2.96	3.68	3.77	2.90	1.81	0.63	0.26	0.02
25	$5s'[\frac{1}{2}]_1$	14.25	15.4	20.7	24.0	26.8	26.4	25.4	25.0	21.0
26	$3d'[\frac{3}{2}]_1$	14.30	56.8	58.0	59.0	68.8	72.7	71.5	70.5	61.6

4.1.1. 3p^{5}4p(J=2). The calculations for these levels give satisfactory agreement with the measurements of Chutjian and Cartwright (1981) in a broad energy range, though a tendency to overestimate these data at the maximum is observed (figure 1). At the energy 100 eV the theory is in accord with the PWBA computations of Ballou *et al* (1973). A quadrupole direct excitation of the ^{1}D component contributes mainly to the cross section and gives a typical broad excitation function for the levels with $J=2$. The proximity of the cross section for these levels in magnitude follows from the proximity of the mixing coefficients of the ^{1}D component (table 1). Exchange scattering contributes only a little. The direct cross section at a maximum in the DWBA is larger than in the PWBA, which is not an unusual situation (Sobel'man *et al* 1981). Optical data are several times greater than both the electrical data of Chutjian and Cartwright (1981) and our calculations.

4.1.2. 3p^{5}4p(J=0). The DWBA cross sections are almost an order greater than the experimental data of Chutjian and Cartwright (1981) for both levels. When using the mixing ^{1}S and ^{3}P coefficients from Albat *et al* (1975) (table 1) our results at high energies come to agreement with the PWBA calculations of Ballou *et al* (1973). One cannot make a reliable conclusion about the validity of the DWBA in the case of excitation of the 3p^{5}4p($J=0$) states as we are not sure of the good quality of the

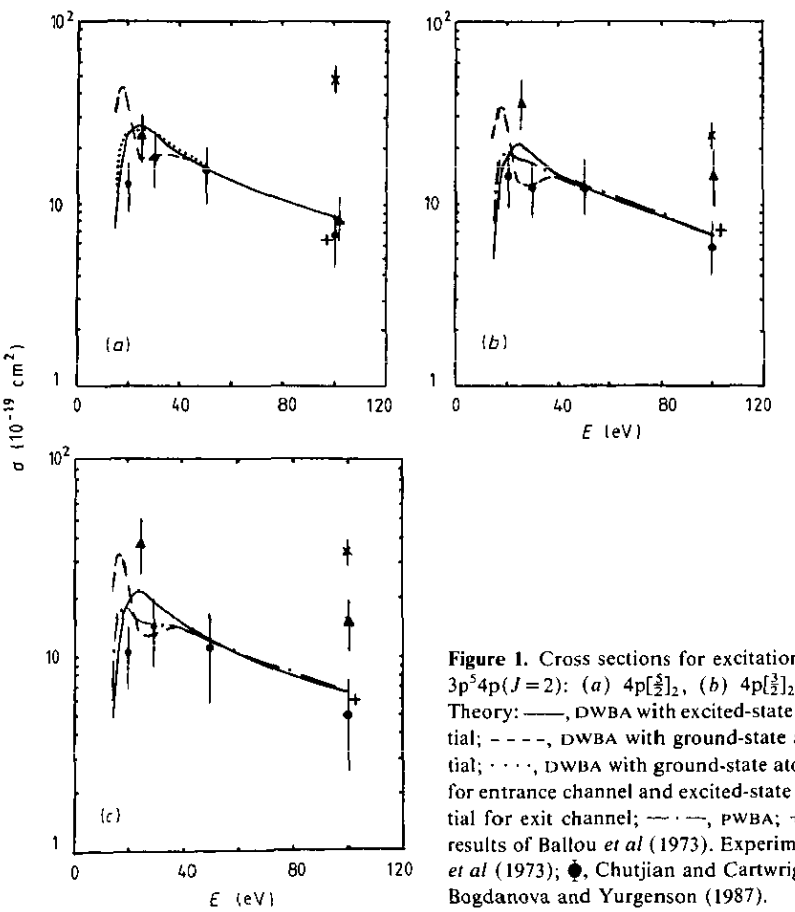

Figure 1. Cross sections for excitation of the levels 3p^{5}4p($J=2$): (*a*) 4p[$\frac{5}{2}$]$_2$, (*b*) 4p[$\frac{3}{2}$]$_2$, (*c*) 4p'[$\frac{3}{2}$]$_2$. Theory: ——, DWBA with excited-state atomic potential; – – – –, DWBA with ground-state atomic potential; · · · ·, DWBA with ground-state atomic potential for entrance channel and excited-state atomic potential for exit channel; — · —, PWBA; +, plane-wave results of Ballou *et al* (1973). Experiment: ⧗, Ballou *et al* (1973); ●, Chutjian and Cartwright (1981); ▲, Bogdanova and Yurgenson (1987).

wavefunctions of these states (see section 2). A comparison of the PWBA results of Ballou *et al* (1973) and Albat *et al* (1975) at high energies (figure 2(*b*)) demonstrates that taking into account configuration mixing can reduce the cross sections by at least a factor of two. Furthermore, the calculations of Albat *et al* (1975) in the eikonal close-coupling method for excitation by protons show that taking into account coupling with the channel $3p^5 4s\ ^1P$ can in addition strongly decrease the cross sections at a maximum. (The results of Albat *et al* (1975) in figure 2(*b*) were extracted from the proton cross sections by scaling the energy of an incident particle). A large magnitude of the radiative transition probabilities between the states $3p^6\ ^1S$–$3p^5 4s(J=1)$–$3p^5 4p(J=0)$ (tables 1 and 4) is also an argument in favour of strong influence of the virtual dipole transitions via the states $3p^5 4s(J=1)$ on the excitation cross sections of the levels with $J=0$. Note that an exchange amplitude which was ignored in Albat *et al* (1975) reduces the cross section by 20% at a maximum. It seems that the description of an excitation of the states $3p^5 4p(J=0)$ in argon is an even more arduous problem than for the states $2p^5 3p(J=0)$ in neon (Machado *et al* 1984, Bubelev and Grum-Grzhimailo 1990).

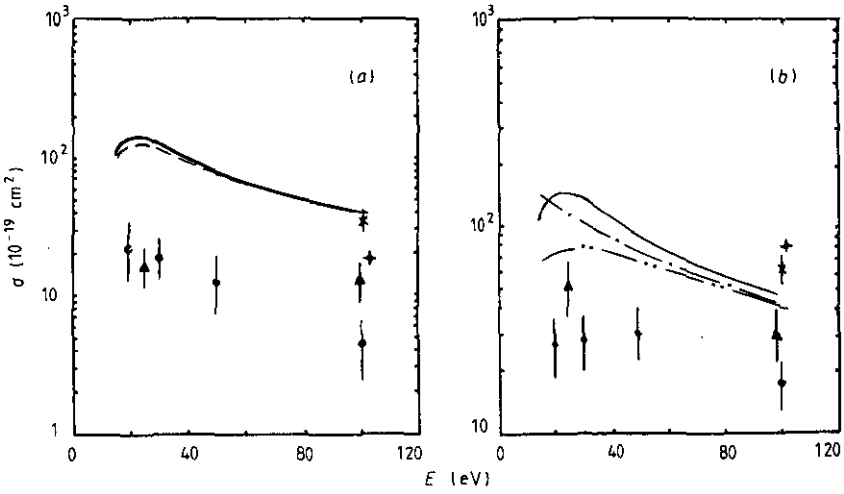

Figure 2. Cross sections for excitation of the levels $3p^5 4p(J=0)$: (*a*) $4p[\frac{1}{2}]_0$, (*b*) $4p'[\frac{1}{2}]_0$. Theory: - - - -, DWBA for the individual level $4p[\frac{1}{2}]_0$; ——, DWBA for the sum of cross sections for the levels $4p[\frac{1}{2}]_0$ and $4p'[\frac{3}{2}]_1$; ——, DWBA; — · —, PWBA from Albat *et al* (1975); — · · —, close-coupling calculations from Albat *et al* (1975) (see text). Other designations are as in figure 1. Experimental results of Chutjian and Cartwright in (*a*) are for the sum of cross sections for the levels $4p[\frac{1}{2}]_0$ and $4p'[\frac{3}{2}]_1$.

4.1.3. $3p^5 4p(J=1)$. Exchange cross sections for these four levels are demonstrated in figure 3. They drop rapidly as a function of the electron energy, and are in accord with the data of Chutjian and Cartwright (1981) and Bogdanova and Yurgenson (1987) in the region of a maximum. At the energies 50 eV, and particularly 100 eV, our results for the states $4p[\frac{3}{2}]_1$ and $4p[\frac{1}{2}]_1$ are an order of magnitude lower than those measured by Chutjian and Cartwright (1981). At the same time our calculations for the level $4p[\frac{1}{2}]_1$ are in satisfactory agreement with these data up to 100 eV. We agree with Ballou *et al* (1973) that the virtual transitions via intermediate states mainly contribute to the excitation cross sections of the levels with $J=1$ at high energies. The most possible

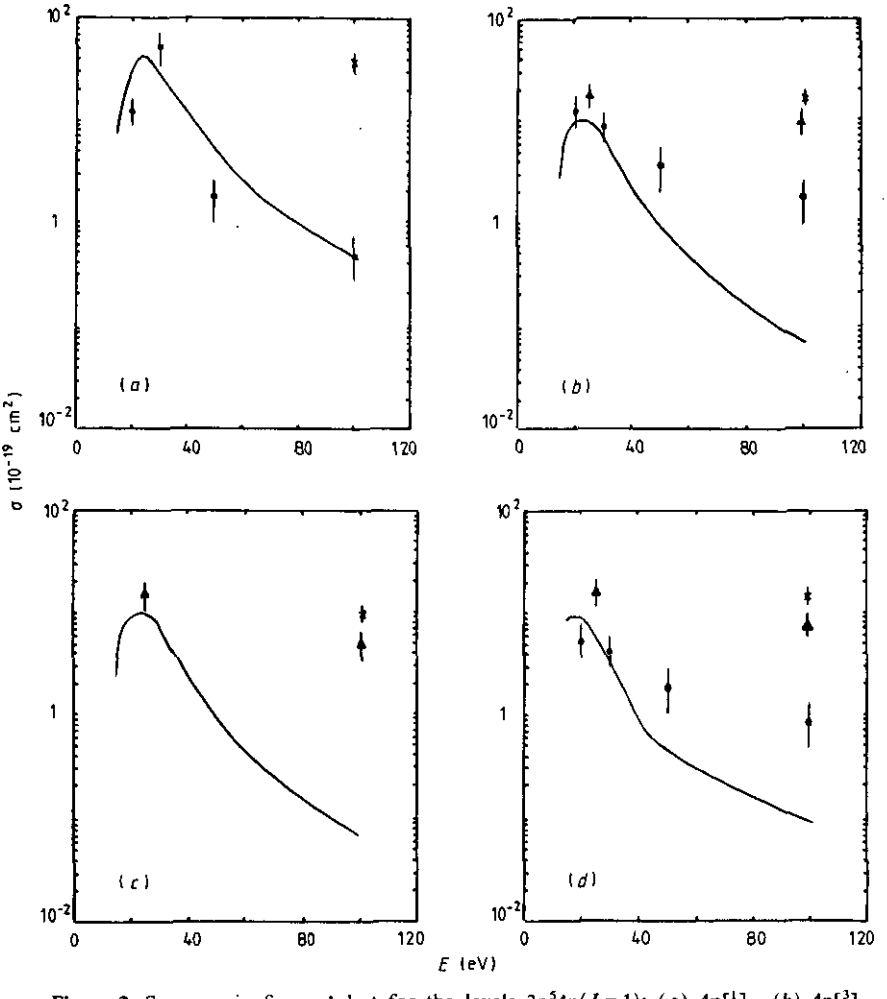

Figure 3. Same as in figure 1 but for the levels $3p^5 4p(J=1)$: (*a*) $4p[\frac{1}{2}]_1$, (*b*) $4p[\frac{3}{2}]_1$, (*c*) $4p'[\frac{3}{2}]_1$, (*d*) $4p'[\frac{1}{2}]_1$.

process will be in this case an excitation of the ^1P component through the direct amplitude of the second order. Naturally, the corresponding contribution to the cross section of the $4p[\frac{1}{2}]_1$ state plays a minor role even at 100 eV, as this state contains a negligible portion of ^1P (table 1).

4.1.4. $3p^5 4p(J=3)$. Our calculations for an excitation of the $4p[\frac{5}{2}]_3$ level are in good overall agreement with the measurements of Chutjian and Cartwright (1981) (figure 4), but some tendency is observed to underestimate the cross section at 100 eV. At 100 eV the results are close to the calculations of Ballou *et al* in the Ochkur approximation.

4.2. Configuration $3p^5 3d$

In our model the levels $3p^5 3d(J=1,3)$ are excited through both direct and exchange scattering, and the levels $3p^5 3d(J=0,2,4)$ are excited through exchange scattering only.

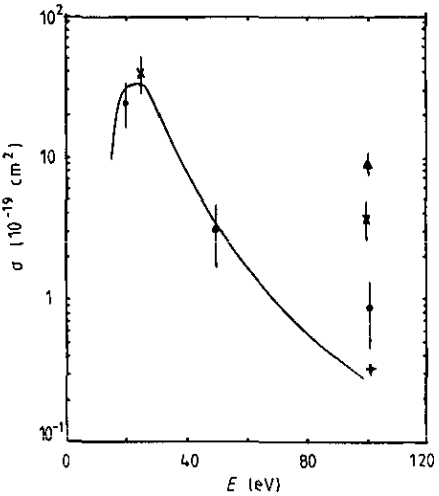

Figure 4. Same as in figure 1 but for the level $3p^5 4p[\frac{5}{2}]_3$.

4.2.1. $3p^5 3d(J=1)$. Cross sections for the states $3d[\frac{3}{2}]_1$ and $3d'[\frac{3}{2}]_1$ have a broad maximum and drop slowly as a function of energy (figures 5(*a*) and (*b*)). This is typical behaviour of an excitation function for the dipole-allowed transitions. As our calculations reproduce the corresponding oscillator strengths quite satisfactorily (table 4), the fact that our results essentially exceed the experimental data can in the first instance be an effect of neglecting some essential features of a scattering process. We can assume an influence of the channels $3p^5 4p(J=0)$, which are coupled by strong dipole transitions with the two levels under discussion (table 3) and have a large excitation cross section over a broad energy range (figure 2). The third level $3d[\frac{1}{2}]_1$ contains only a very small portion of the singlet component (table 1) and the behaviour of the cross section in the region of maximum is determined by an exchange amplitude of the transition to the ^{3}P component. The corresponding cross section drops rapidly as a function of energy (figure 5(*c*)). This cross section has been measured only in sum with the cross section of the level $3d[\frac{1}{2}]_0$. From the data on the oscillator strengths (table 4) one can expect that our calculations for the state $3d[\frac{1}{2}]_1$ will overestimate the cross sections by an order of one at the high energies, and effects of configuration mixing have to play a substantial role. This is also confirmed in figure 5(*c*).Our results are much better at smaller energies where exchange excitation of the ^{3}P component predominates.

4.2.2. $3p^5 3d(J=3)$. The cross sections at large energies are determined by the direct octupole amplitude (figure 6(*a*)) which drops much faster than the dipole one as a function of energy (figure 5(*a*) and (*b*)). Our calculation for the level $3d[\frac{7}{2}]_3$ is in satisfactory agreement with the experimental data of Chutjian and Cartwright (1981) exceeding somewhat the data at a maximum. Experimental and theoretical information about the cross section for the other two levels with $J=3$ is absent from the literature. Our calculation can be compared only with the data in sum with the cross sections for the neighbouring states of the $3p^5 5s$ configuration (figures 6(*b*), 7(*d*)).

4.2.3. $3p^5 3d(J=0)$. Cross sections for the level $3d[\frac{1}{2}]_0$, which is excited by exchange scattering, is demonstrated in figure 5(*c*). The shape of the cross section in the region

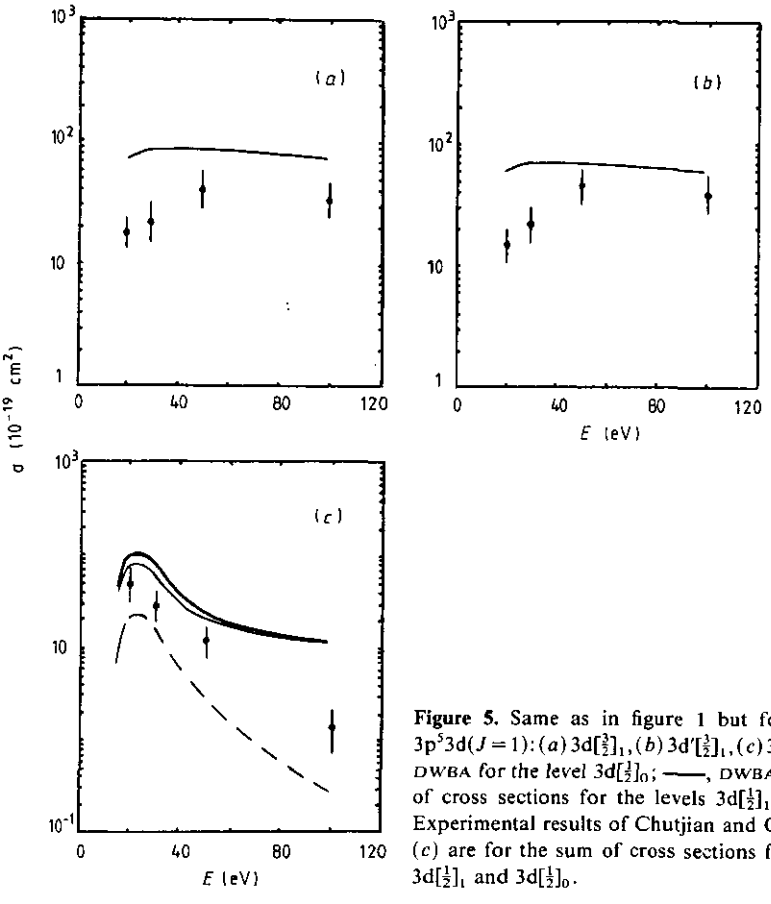

Figure 5. Same as in figure 1 but for the levels $3p^5 3d(J=1)$: (*a*) $3d[\frac{3}{2}]_1$, (*b*) $3d'[\frac{3}{2}]_1$, (*c*) $3d[\frac{1}{2}]_1$. - - - -, DWBA for the level $3d[\frac{1}{2}]_0$; ——, DWBA for the sum of cross sections for the levels $3d[\frac{1}{2}]_1$ and $3d[\frac{1}{2}]_0$. Experimental results of Chutjian and Cartwright in (*c*) are for the sum of cross sections for the levels $3d[\frac{1}{2}]_1$ and $3d[\frac{1}{2}]_0$.

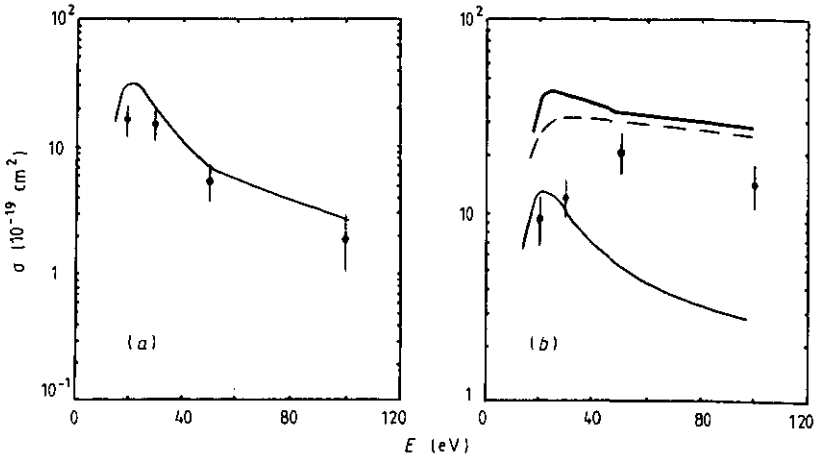

Figure 6. Same as in figure 1 but for the levels $3p^5 3d(J=3)$: (*a*) $3d[\frac{7}{2}]_3$, (*b*) $3d[\frac{5}{2}]_3$. - - - -, DWBA for the level $5s[\frac{3}{2}]_1$; ——, DWBA for the sum of cross sections for the levels $3d[\frac{5}{2}]_3$ and $5s[\frac{3}{2}]_1$. Experimental results of Chutjian and Cartwright in (*b*) are for the sum of cross sections for the levels $3d[\frac{5}{2}]_3$ and $5s[\frac{3}{2}]_1$.

of maximum is similar to that for the level $3d[\frac{1}{2}]_1$ owing to the fact that both states are excited through the ^3P component by exchange scattering.

4.2.4. $3p^5 3d(J=2)$. A situation with these levels (figure 7) looks very much like the situation with the levels $3p^5 4p(J=1)$ (figure 3). Calculations for the state $3d[\frac{3}{2}]_2$ agree satisfactorily at high energies with the measurements of Chutjian and Cartwright (1981) whereas for the state $3d[\frac{5}{2}]_2$ the calculated cross section at 100 eV is an order of magnitude smaller than the experimental value. Such a difference in the ratio between theoretical and experimental results for these two levels can be accounted for by the

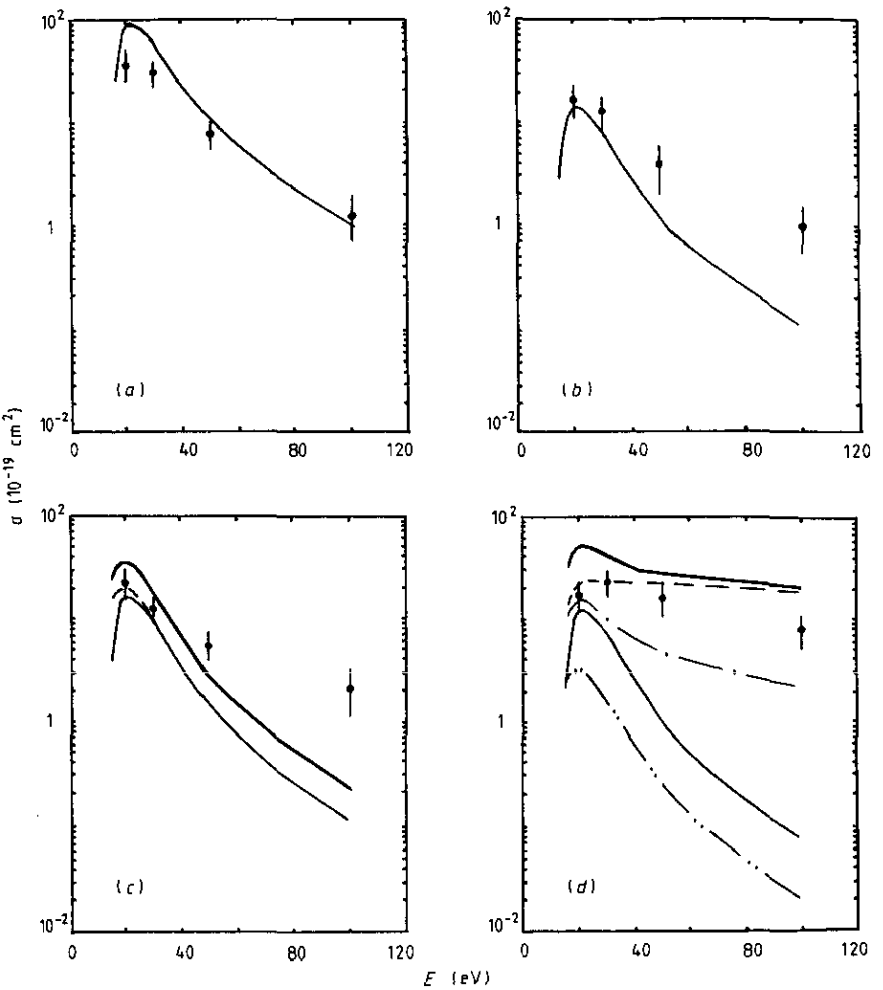

Figure 7. Same as in figure 1 but for the levels $3p^5 3d(J=2)$: (*a*) $3d[\frac{3}{2}]_2$; (*b*) $3d'[\frac{5}{2}]_2$, (*c*) $3d[\frac{5}{2}]_2$, (*d*) $3d'[\frac{3}{2}]_2$. In (*c*): - - - -, DWBA for the level $5s[\frac{3}{2}]_2$; ——, DWBA for the sum of cross sections for the levels $3d[\frac{5}{2}]_2$ and $5s[\frac{3}{2}]_2$. Experimental results of Chutjian and Cartwright are for the sum of cross sections for the levels $3d[\frac{5}{2}]_2$ and $5s[\frac{3}{2}]_2$. In (*d*): - - - -, DWBA for the level $5s'[\frac{1}{2}]_1$; — · —, DWBA for the level $3d'[\frac{5}{2}]_3$; — · · —, DWBA for the level $5s'[\frac{1}{2}]_0$; ——, DWBA for the sum of cross sections for the levels $5s'[\frac{1}{2}]_1$, $5s'[\frac{1}{2}]_0$, $3d'[\frac{5}{2}]_3$, $3d'[\frac{3}{2}]_2$. Experimental results of Chutjian and Cartwright are for the sum of cross sections for the levels $5s'[\frac{1}{2}]_1$, $5s'[\frac{1}{2}]_0$, $3d'[\frac{5}{2}]_3$, $3d'[\frac{3}{2}]_2$.

essential distinction in the contribution of the ^{1}D component to the wavefunction (table 1). At those energies where the exchange amplitude is small, the cross section for the level $3d'[\frac{5}{2}]_2$ with large ^{1}D component can be governed by the direct second-order amplitude, which has to take into account virtual transitions via intermediate states. This amplitude must also be essential for the other two levels with $J = 2$. Corresponding excitation cross sections are displayed in figure 7(c) and (d), however, these levels have not been resolved from the neighbouring states of the 3p^{5}5s configuration in the experiments of Chutjian and Cartwright (1981).

4.2.5. 3p^{5}3d($J = 4$). Our calculations agree satisfactorily with the data of Chutjian and Cartwright (1981) for the level $3d[\frac{7}{2}]_4$ over the whole energy range under consideration (figure 8).

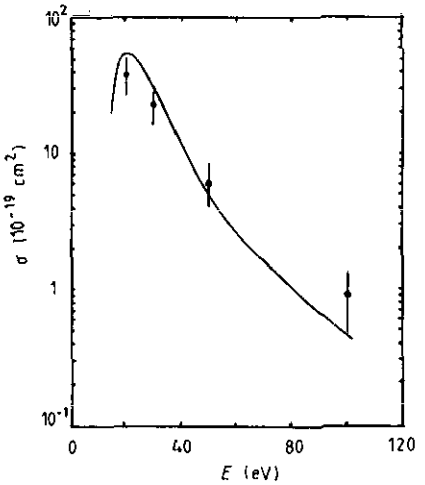

Figure 8. Same as in figure 1 but for the level $3p^5 3d[\frac{7}{2}]_4$.

4.3. Configuration 3p^{5}5s

The results of our calculations are shown in figures 6(b), 7(c) and 7(d). The evaluated excitation cross section for the $5s'[\frac{1}{2}]_1$ level is expected to be greater than the experimental data by a factor of two at large energies, in accordance with table 4. This is indirectly confirmed in figure 7(d). It is interesting to note that calculations give practically identically shaped cross sections for the levels 3p^{5}5s($J = 0, 2$) and for the neighbouring levels 3p^{5}3d($J = 2$), also excited through exchange amplitude (figure 7(c) and (d)).

5. Conclusions

Systematic calculations of the electron impact excitation cross sections for all fine-structure levels of Ar I 3p^{5}4p, 3d and 5s configurations have been carried out in the distorted-wave Born approximation with exchange in the range of energy 16–100 eV. For some of the levels the values of cross sections were obtained for the first time. In

the range from maximum of cross sections and to 100 eV a satisfactory agreement with experimental data is achieved for the levels, which are excited predominantly through direct or exchange amplitude of the highest multipolarity ($3p^5 4p(J=2,3)$; $3p^5 3d(J=3,4)$). Information on the contribution of the *LS*-basis states to the fine-structure level wavefunctions and control of the quality of the wavefunctions with the use of the data on radiative transition probabilities were extremely useful for analysis of both the agreement of theory with experiment and the shape of cross sections as a function of energy. The reason for disagreement of our calculations with the experiments of Chutjian and Cartwright (1981) seem to be transparent for some levels. Analysis shows that for the levels $4p(J=0)$ a configuration mixing and coupling with channel $4s(J=1)$ have to be taken into account; for the level $3d[\frac{1}{2}]_1$ and, probably, for the $5s'[\frac{1}{2}]_1$ a configuration mixing; for the levels $4p[\frac{3}{2}]_1$, $4p[\frac{5}{2}]_1$, $4p[\frac{1}{2}]_1$, $3d[\frac{5}{2}]_2$ and, probably, $3d[\frac{5}{2}]_2$, $3d[\frac{3}{2}]_2$, the direct second-order amplitude. Though the simple variant of the DWBA gives quite reasonable results for many of the levels considered, its applicability is restricted in the above-mentioned cases, where the second-order amplitude has to be taken into account.

The use of the Hartree–Fock wavefunctions for the $3p^5 nl$ states of argon, even term dependent and intermediate coupling, is, in general, an excessive simplification. This is confirmed by our results for the dipole transition probabilities. Nevertheless, we hold that the present calculations and the discussion can serve as a reliable reference point for future investigations in more accurate models.

Measurements by the electrical method with a resolution of about 0.01 eV are desirable for the detailed comparison of calculations with experiment for the levels of $3p^5 5s$ and some levels of the $3p^5 3d$ configurations. Also desirable are calculations of the differential excitation cross sections for the levels considered in this paper.

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References

Albat R, Gruen N and Wirsam B 1975 *J. Phys. B: At. Mol. Phys.* **8** L82
Aymar M 1972 *Physica* **57** 178
Aymar M, Feneuille S and Klapisch M 1970 *Nucl. Instrum. Methods* **90** 137
Balashov V V, Grum-Grzhimailo A N and Khrapov A A 1988 *Vestnik MGU ser.* 3, *Fiz. Astron.* **29** N2 78
Ballou J K, Lin C C and Fajen F E 1973 *Phys. Rev.* A **8** 1797
Bartschat K and Madison D H 1987 *J. Phys. B: At. Mol. Phys.* **20** 5839
Bogdanova I P and Yurgenson S V 1987 *Opt. Spektrosk.* **62** 471
Bretagne J, Callede G, Legentil M and Puech V 1986 *J. Phys. D: Appl. Phys.* **19** 761
Bubelev V E and Grum-Grzhimailo A N 1990 *Opt. Spektrosk.* **69** 295
Chutjian A and Cartwright D C 1981 *Phys. Rev.* A **23** 2178
Eggarter E 1975 *J. Chem. Phys.* **62** 833
Fischer O 1933 *Z. Phys.* **86** 646

Fliflet A W, Kelly H P and Hansen J E 1975 *J. Phys. B: At. Mol. Phys.* **8** L268
Furness J B and McCarthy I E 1973 *J. Phys. B: At. Mol. Phys.* **6** 2280
Ganas P S and Green A E S 1971 *Phys. Rev.* A **4** 182
Gruzdev P V and Loginov A V 1975 *Opt. Spektrosk.* **38** 411
Hansen J E 1972 *J. Phys. B: At. Mol. Phys.* **5** 1083
Herrmann O 1936 *Ann. Phys., Lpz.* **25** 143
Lawrence G M 1968 *Phys. Rev.* **175** 40
Lee C M 1974 *Phys. Rev.* A **10** 584
Lee C M and Lu K T 1973 *Phys. Rev.* A **8** 1241
Lilly R A 1976 *J. Opt. Soc. Am.* **66** 245
Machado L E, Leal E P and Csanak G 1984 *Phys. Rev.* A **29** 1811
Martin N L S 1984 *J. Phys. B: At. Mol. Phys.* **17** 163
Mental J E and Morgan H D 1976 *Phys. Rev.* A **14** 957
Padial N T, Meneses G D, da Paixao F J and Csanak G 1981 *Phys. Rev.* A **23** 2194
Peterson L R and Allen J E 1972 *Chem. Phys.* **56** 6068
Smirnov Yu M 1989 *Effective Cross Sections for Excitation of Atoms and Ions by Electron Impact* (Moscow: Izdat. Standartov) (in Russian)
Sobel'man I I Vainshtein L A and Yukov E A 1981 *Excitations of Atoms and Broadening of Spectral Lines* (Berlin: Springer)
Volkova L M and Devyatov A M 1959 *Opt. Spektrosk.* **7** 819
Westerveld W B, Mulder Th F A and van Eck J 1979 *J. Quant. Spectrosc. Radiat. Transfer* **21** 533
Wiese W L, Brault J W, Danzmann K, Helbig V and Kock M 1989 *Phys. Rev.* A **39** 2461
Wiese W L, Smith M W and Miles B M 1969 *Atomic Transition Probabilities* vol 2 (NSRDS-NBS22) (Washington, DC: National Bureau of Standards)
Zapesochnyi I P and Feltsan P V 1966 *Opt. Spektrosk.* **20** 521
—— 1967 *Ukr. Fiz. Zh.* **12** 633