ASTRONOMY & ASTROPHYSICS
SUPPLEMENT SERIES

Astron. Astrophys. Suppl. Ser. **138**, 323–326 (1999)

Electron impact excitation of Si I

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Received February 17; accepted April 15, 1999

Abstract. An analytic atomic independent-particle-model is used to generate wave functions for the valence and excited states of the neutral silicon atom. These wave functions are used to calculate generalized oscillator strengths, and from these quantities the cross sections are obtained in the Born approximation. Various excitations from the ground state, $3p^2(^3P_0)$, are considered, and results are presented for electron impact energies up to 5 keV.

Key words: atomic data — atomic processes

1. Introduction

In this article we present the results of calculations of generalized oscillator strengths and integrated cross sections for the electron impact excitation of Si I from the ground state $3p^2(^3P_0)$ to various s,p,d excited states. Si I is an astrophysically important atom. It is seen in absorption spectra from the interstellar medium and stellar photospheres (Anders & Grevesse 1989). In order to interpret such data it is important to have accurate electron excitation cross sections and other atomic data for the observed transitions. Very little experimental information is available on atomic cross sections, consequently theory must be relied on to provide the majority of required data.

In the present theoretical approach the 14-electron system of the Si I atom is represented by an independent-particle-model, in which each electron moves independently in an effective potential having the form

$$V(r) = -(2/r)\{\ 13\ [\ H\ (e^{r/d}\ -\ 1)\ +\ 1]^{-1}\ +\ 1\} \qquad (1)$$

where r is the electron-nucleus distance in the units of the Bohr radius a_0, and d, H are adjustable parameters. This potential is inserted into the radial Schrödinger equation which is solved numerically to obtain the wave functions and energy eigenvalues. The parameters d, H are determined by fitting the eigenvalues to the experimental single-particle energy levels. The values $d = 0.6703$, $H = 1.4952$ were obtained from the best fit.

2. Generalized oscillator strengths

The formulas for computing the generalized oscillator strengths (GOS) are based on the first Born approximation and the LS-Coupling scheme, and may be found in earlier work by the present author (Ganas 1998). The following notation appears in the subsequent discussion. The quantity $x = K^2a_0^2$, where K is the momentum tranfer. Also $x_t = W/R$ where W is the excitation energy in eV and R is the Rydberg energy. The quantity $\xi = x/x_t$.

Plots of the GOS are shown in Fig. 1. As ξ increases, the GOS for the transitions 3p − ns decrease in oscillatory fashion, while the GOS for 3p − nd decrease monotonically. The GOS for 3p − np also decrease monotonically, but pass through a maximum first.

The calculation of cross sections can be facilitated by parametrizing the GOS with simple analytic forms:

$$f(\xi) = A\ (e^{-\alpha\xi}\ +\ \beta\xi e^{-\gamma\xi})^2 \qquad \text{for 3p} - \text{ns, 3p} - \text{nd} \quad (2)$$

$$f(\xi) = \xi A\ (e^{-\alpha\xi}\ +\ \beta\xi e^{-\gamma\xi})^2 \qquad \text{for 3p} - \text{np.} \quad (3)$$

The quantities A, α, β, γ in Eqs. (2) and (3) are adjustable parameters which are varied so as to obtain the best fit to the numerically generated GOS. The quantity A in Eq. (2) is the oscillator strength, which is the limit of the GOS as $\xi \to 0$. When using Eq. (2), A is set equal to the value of the oscillator strength, and three-parameter fits are obtained. Four-parameter fits are obtained when using Eq. (3). The values of the four parameters which yield the best fits are given in Table 1. Sample fits are shown in Fig. 1. Equations (2) and (3) actually only reproduce the GOS when it is significantly large.

3. Cross sections

The formulas used to obtain the cross sections may be found in earlier work (Ganas 1998). The computed cross sections are presented in Fig. 2. No experimental cross sections are available, so a direct comparison with experiment is not possible. However, an estimate of their accuracy can be obtained from the accuracy of the

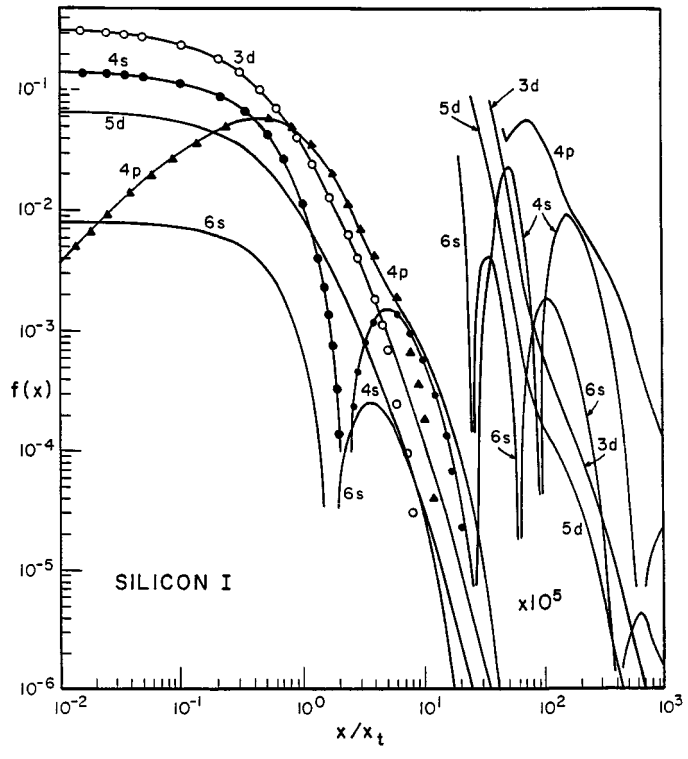

Fig. 1. GOS for 3p − ns, 3p − np, 3p − nd transitions in Si I as functions of reduced square of momentum transfer. The curves are the result of the present work. The solid dots, open circles, and triangles are representative fits using Eqs. (2) and (3). Values of the GOS below 10^{-5} have been multiplied by 10^5

Table 1. Values of the dimensionless parameters A, α, β, γ in Eqs. (2) and (3)

3p to	A	α	β	γ
4s	0.1448	1.0789	−0.0673	0.2328
5s	0.0223	0.6123	−0.3292	0.4205
6s	0.0080	0.7854	−0.2698	0.3864
3d	0.3279	1.7004	0.2788	0.6793
4d	0.1400	1.3839	0.1839	0.5470
5d	0.0697	1.2591	0.1465	0.4879
4p	0.3657	0.4706	−0.6195	0.8108
5p	0.0962	0.4002	−0.5659	0.6804

oscillator strengths for the allowed transitions. The Born cross sections are very sensitive to the values of the oscillator strengths (Inokuti 1971). In Table 2 we present a comparison between the oscillator strengths obtained from the present calculations and those obtained from experiment and other calculations. For the 3p − 4s transition, our calculated value is in good agreement with various experimental data, but is lower than the majority of theoretical data. For 3p − 5s, the present value is in good agreement with experimental and theoretical data, but for the 3p − 6s there is a factor of 2 difference between our value and experiment. However the oscillator

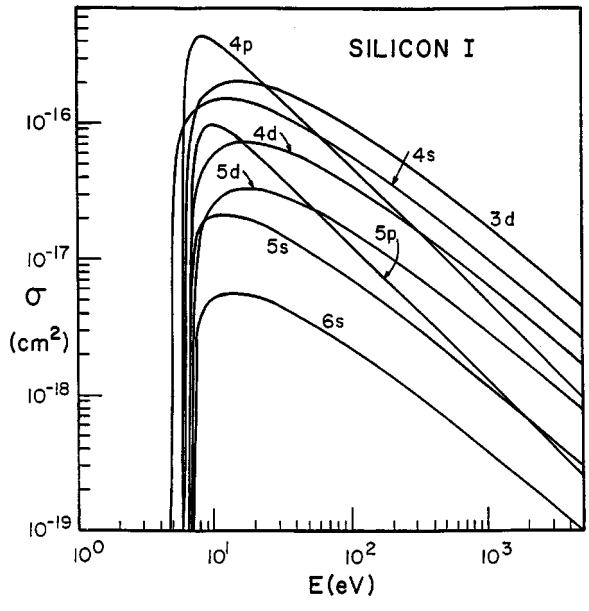

Fig. 2. Integrated cross sections for 3p − ns, 3p − np, and 3p − nd excitations in Si I versus electron impact energy

strength for 3p − 6s is much smaller than it is for 3p − 5s or 3p − 4s.

For the 3p − 3d(^{3}D$_1$) transition, our calculated value is in good agreement with the experimental data of Smith et al. (1987), and with various theoretical data. For the 3p − 3d(^{3}P$_1$) transition, our value is higher than the experimental and theoretical data, by a factor of 2 in some cases. However, the oscillator strength for 3p − 3d(^{3}P$_1$) is much smaller than for 3p − 3d(^{3}D$_1$). For 3p − 4d, there is generally reasonable agreement between our results and those of experiment and other calculations. For the higher transitions 3p − 5d, 3p − 6d and 3p − 7d, there is no experimental information available.

If we limit our consideration to the three transitions with the largest oscillator strengths: 3p − 3d(^{3}D$_1$), 3p − 4s(^{3}P$_1$), and 3p − 4d(^{3}D$_1$), and if we compare these oscillator strengths with those of Smith et al. (1987), which are the most extensive experimental data available on Si I, we find that our results have an accuracy in the range 7% to 23%. We therefore estimate our high energy cross sections to have an accuracy somewhere in this range. Our low energy cross sections are likely to be inaccurate due to the breakdown of the Born approximation near the threshold of inelastic scattering.

4. Conclusion

The purpose of the present calculations has been to generate cross sections for the electron impact excitation of Si I in the Born approximation. These atomic cross sections are potentially useful as required data for modelers of astrophysical plasmas, and should also serve as a guide

for more advanced calculations on the complex open-shell system represented by Si I.

Results are given over a large energy range, but due to the limitations of the Born approximation, only those results above 60 eV may be considered to have good accuracy. Used with this caution, the present results may be helpful to users of atomic data.

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Table 2. Oscillator strengths for Si I for the transitions $3p^2(^3P_0) \rightarrow 3pns(^3P_1)$ and $3p^2(^3P_0) \rightarrow 3pnd(^3P_1, ^3D_1)$

3p to	This Calculation	Experiment	Other Calculations
$4s(^3P_1)$	0.1448	$0.158^a, 0.16^b, 0.16 \pm 0.02^c$ $0.162 \pm 0.024^d, 0.170 \pm 0.041^d$ $0.174 \pm 0.015^e, 0.2104 \pm 0.01^f$	$0.1622^g, 0.207^h$ $0.214^i, 0.215^j, 0.226^k$ $0.2358^l, 0.236^{m,n}$
$5s(^3P_1)$	0.0223	0.023 ± 0.008^d 0.024 ± 0.018^d	$0.0229^g, 0.029^m$ $0.0291^n, 0.033^{i,k}$
$6s(^3P_1)$	0.0080	0.0046 ± 0.0038^d 0.0047 ± 0.0012^d	0.012^k
$7s(^3P_1)$	0.00383		
$3d(^3P_1)$	0.0820	$0.0308^a, 0.040 \pm 0.010^d$ 0.041 ± 0.011^d 0.0491 ± 0.002^f	$0.0389^g, 0.042^i, 0.053^m$ $0.0539^{l,n}, 0.2291^g$ $0.269^m, 0.296^i, 0.271^n$ 0.321^k
$3d(^3D_1)$	0.2459	$0.151^a, 0.229 \pm 0.034^d$ 0.229 ± 0.059^d	$0.2291^g, 0.269^m, 0.296^i$ $0.271^n, 0.321^k$
$4d(^3P_1)$	0.0350	0.022 ± 0.004^d 0.031 ± 0.019^d	$0.0081^g, 0.012^m$ $0.0121^n, 0.020^i$
$4d(^3D_1)$	0.1050	0.085 ± 0.058^d 0.087 ± 0.032^d	$0.0037^k, 0.0871^g$ $0.146^i, 0.155^m, 0.156^n$
$5d(^3P_1)$	0.0174		$0.0219^g, 0.0346^n$
$5d(^3D_1)$	0.0522		$0.0682^g, 0.0851^n$
$6d(^3P_1)$	0.0099		$0.0293^n, 0.0472^g$
$6d(^3D_1)$	0.0296		$0.0168^g, 0.0503^n$
$7d(^3P_1)$	0.0061		$0.0183^n, 0.0261^g$
$7d(^3D_1)$	0.0184		$0.0072^g, 0.0381^n$

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