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# KLL Auger decay of atomic silicon

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#### Abstract

The KLL Auger electron spectrum of free silicon atoms has been recorded using electron impact ionization. Besides normal KLL Auger lines, the spectrum shows a rich satellite structure. The KLL Auger transitions following a shake off or a shake up of the outermost electron during the K ionization are found to create the strongest satellite spectra. The satellite intensities relative to the total normal KLL Auger intensity were determined semiempirically. The spectral structures have been identified using Hartree-Fock calculations obtained with Cowan's code.

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#### 1. Introduction

Silicon as the second most abundant element in the earth's crust and the seventh most abundant element in the universe has been widely studied not only on account of its abundance, but also for the sake of its extensive use especially in electronic industry. Though silicon has been a subject of many electron-spectroscopic studies, there exist only a few on atomic silicon. The main experimental difficulty lies in the high temperature of over  $1500^{\circ}C$  needed to create a vapor pressure adequate for measurements. Silicon plasma created with laser ablation has been studied (e.g. [1, 2, 3, 4]), but only Partanen *et al.* [5] and Jänkälä *et al.* [6] have studied free initially neutral silicon atoms by measuring the 2s and 2p photoelectron spectra and the subsequent Auger electron spectra.

The low ionization cross section of the K-shell of silicon atoms creates further experimental problems. The K-shell of silicon has been studied from solid and molecular silicon compounds using for example photoabsorption (e.g. [7, 8, 9, 10]) and electron spectroscopy (e.g. [9, 10, 11, 12, 13]). Researches on the K-shell of pure silicon thin films have also been reported (e.g. [14, 15, 16]). For example Nath *et al.* [14] have studied thin silicon films on graphite using synchrotron radiation photoemission spectroscopy and they obtained the 1s binding energy of 1840.0eV for a bulk-like 5 Å silicon film. According to our calculations the 1s ionization energy of atomic silicon is 1850.4eV. This energy is outside the useful range of such soft X-ray synchrotron radiation sources as MAX II in Lund, Sweden. Excitation by electron impact for measuring Auger electron spectra is thus a good alternative method.

We are running a project to study systematically KLL Auger spectra of free atoms. At room temperature only rare gases appear as monoatomic but by using evaporation ovens many solid materials can be evaporated as atomic vapours. This provides a possibility to study various atomic samples. Previously we have examined the KLL Auger spectrum of atomic aluminium [17] and remeasured and analyzed the KLL Auger spectra of atomic sodium and magnesium [18]. In reference [18] we have also made a comparison between the KLL Auger spectra of atomic samples from neon to aluminium (Z = 10 - 13). In this study we present the KLL Auger spectrum of free silicon atoms. The spectral structures are identified by using Hartree-Fock calculations obtained with Cowan's code [19].

#### 2. Experiments

Measurements were performed in our home laboratory at the University of Oulu. Auger electron energies were analyzed dispersively using a modified Gammadata Scienta SES-200 hemispherical electron energy analyzer updated with a SES-R4000 power supply unit. Electrons were detected with a position sensitive multi-channel plate detector and a high-resolution CCD camera. Silicon vapour was ionized using 5keV electron impact. A curved spectrometer entrance slit of 0.8mm was used with a pass energy of 500eVproducing a total experimental broadening of 1.0eV. The strongest line group was also measured with an entrance slit of 0.5mm giving an experimental broadening of 0.7eV. The ionizing electron beam was at  $90^{\circ}$  angle to the nozzle through which the silicon vapour reached the interaction region. The Auger electrons were observed at  $90^{\circ}$  angle to both of these.

To achieve a sufficient pressure of silicon vapour of about  $10^{-3}mbar$  in the crucible, a rather high temperature of approximately  $1620^{\circ}C$  is required [20]. Therefore the sample was vaporized using induction heating which has proven to be very practical at high temperatures. It has been used extensively in our previous studies and a detailed description of our induction heating system is given in reference [21]. Silicon is chemically very reactive as liquid and vapour, thus possible crucible materials are boron nitride (BN) and graphite [20]. Induction heating demands a crucible made of electrically conductive material. In our measurements different kind of crucibles were tested. The most reliable system was found to be an insulating BN crucible placed inside a conductive graphite or molybdenum crucible.

The kinetic energy calibration for the Auger electron spectrum was done with the Kr  $L_3M_{4,5}M_{4,5}$   ${}^{1}G_4$  Auger line. The Kr  $L_3M_{4,5}M_{4,5}$  spectrum was first recalibrated using the Ne  $KL_{2,3}L_{2,3}$   ${}^{1}D_2$  Auger line with a kinetic energy of 804.458eV [22]. The absolute energies for the Kr LMM lines have been reported only in references [23], and [24]. Werme et al. [23] reported the energy of the line group including transitions Kr  $L_3M_{4,5}M_{4,5}$   ${}^{3}P$ ,  ${}^{1}D_2$  and  ${}^{1}G_4$  to be 1460.4  $\pm$  1.1eV. Levin et al. [24] reported the energy of 1460.0eV  $\pm$  0.2eV for the transition Kr  $L_3M_{4,5}M_{4,5}$   ${}^{1}G_4$ . By calculating a weighted mean value of the components Kr  $L_3M_{4,5}M_{4,5}$   ${}^{3}P$ ,  ${}^{1}D_2$  and  ${}^{1}G_4$  from the data of Levin et al. a value of 1460.3eV is obtained. In our measurements, the energy of the Kr  $L_3M_{4,5}M_{4,5}$   ${}^{1}G_4$  Auger line was determined to be 1460.49eV  $\pm$  0.15eV, which deviates somewhat from the value given by Levin et al. The energy calibrated KLL Auger spectrum of atomic silicon is shown in figure 1 a). The kinetic energies and intensity ratios determined for the lines of this experimental spectrum are given in table 1.

#### 3. Theoretical results and comparison with experiment

The kinetic energies and transition rates of the KLL Auger transitions of silicon were calculated with Cowan's code [19]. Initial and final state wave functions were calculated in the intermediate coupling scheme using the Hartree-Fock method with relativistic corrections (HFR). The Auger final states with electron configurations  $1s^22s^02p^6val$ and  $1s^22s^22p^4val$  (valence structure identical) having the same total angular momentum quantum number and the same parity were allowed to mix by applying the configuration interaction (CI) method. Spin-orbit interaction was calculated using the Blume-Watson theory and Slater integrals were not scaled. The differences between the average energies of the initial and final state electron configurations were used as the kinetic energies of continuum electrons.

Kinetic energies and Auger transition rates were calculated for five different initial 1s hole state electron configurations:  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{2}$ ,  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{1}4p^{1}$ ,  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{1}$ ,  $1s^{1}2s^{2}2p^{6}3s^{1}3p^{2}$  and  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{3}$ . The Auger final state electron configurations for the calculated transitions were  $1s^{2}2s^{0}2p^{6}val$ ,  $1s^{2}2s^{1}2p^{5}val$  and  $1s^{2}2s^{2}2p^{4}val$ , where the valence structure is identical to that of the initial state electron configuration of the transition.

The simulated spectrum of silicon constructed using the calculations is shown in figure 1 b). To achieve a correspondence between the linewidths of the experimental and simulated spectrum, the experimental broadening of 1.0eV was used as the Gaussian width in the simulation. A semiempirical value of 0.51eV for the natural width of the Si  $KL_2L_3$  given by Krause *et al.* [25] was used as the Lorentzian contribution. The uppermost spectrum in figure 1 b) is the sum of the calculated normal KLL Auger spectrum and the satellite spectra. Transitions from different initial state electron configurations are shown separately below and the initial state electron configuration is given in the beginning of the spectrum. The LS terms above the normal KLL Auger lines are determined by coupling the final state holes on the L shell. The intensity ratios between the KLL Auger spectrum.

At the temperature of  $1620^{\circ}C$ , the Boltzmann distribution gives the state population probabilities of the ground state electron configuration  $[Ne]3s^23p^2$  to be 0.12 for  ${}^{3}P_{0}$ , 0.35 for  ${}^{3}P_{1}$ , 0.52 for  ${}^{3}P_{2}$ , 0.005 for  ${}^{1}D_{2}$  and  $1 \cdot 10^{-6}$  for  ${}^{1}S_{0}$ . These ground state terms are the parent terms for the  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{2}$  Auger initial states. Because the  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{2}$ initial states are almost pure in LS-coupling scheme and outer valence usually preserves its initial coupling during electron impact ionization, practically only those Auger initial states with parent terms  ${}^{3}P_{0,1,2}$  are occupied. This has been taken into account by weighting the population probabilities of the KLL Auger initial states originating from the parent states  ${}^{3}P_{0,1,2}$  by the ground state population probabilities given above. The population probabilities of the KLL Auger initial states were also weighted with a statistical weight 2J + 1 according to the total angular momentum quantum number J of the state. The Auger transitions from the initial states with the parent terms  ${}^{1}D_{2}$  and  ${}^{1}S_{0}$ have been left out due to the very low population probability of these states in the ground state, even though some minor contribution may come via the mixing of these states with the states having a  ${}^{3}P$  parent term. This was seen in the case of the 2p photoionization of atomic silicon [6], but state mixing was clearly stronger for the 2p ionized states than what is obtained now for the 1s ionized states.

According to optical data [26] the energy separations between the  $[Ne]3s^23p^2$  ground state  ${}^{3}P_{0}$  and other  $[Ne]3s^23p^2$  states are 0.010eV for  ${}^{3}P_{1}$ , 0.028eV for  ${}^{3}P_{2}$ , 0.781eVfor  ${}^{1}D_{2}$  and 1.909eV for  ${}^{1}S_{0}$ . Cowan's code gives values of 0.008eV, 0.025eV, 1.098eV, and 2.720eV respectively. The values for the  ${}^{3}P$  terms are in good agreement with the optical data, but the rest of them deviate notably. The overestimation of the splitting is related to the fact, that the calculations were carried out not including the configuration interaction between the electron configurations with different valence structures as was done in reference [6]. Also no scaling of Slater integrals was adopted to compensate the omission of electron correlation. Cowan's code gives similar kind of overestimation of the splitting for  $Si^{6+}$   $1s^22s^22p^4$   $^3P$ ,  $^1D$  and  $^1S$  states. According to our calculations these states spread across an energy range of 14.717eV, while the optical data gives a splitting of 12.317eV [26]. By including configuration interaction between the  $Si^{6+}$   $1s^22s^22p^4$  states a more reasonable splitting of 11.876eV was obtained. In the Auger final state electron configuration  $1s^22s^22p^43s^23p^2$ , the coupling between  $2p^4$  and  $3p^2$  causes further splitting and the states are spread over an energy range of 18.672eV. In the normal KLL Auger spectrum, this coupling is manifested approximately so that the  $2p^4$  states as the parent states give the energy separation between the  $KL_{2,3}L_{2,3}$  peaks and the coupling with  $3p^2$  creates additional structure which widens the peaks. The strong effect of the parent state can also be witnessed in the mixing of the  $1s^22s^22p^43s^23p^2$  states so that considerable mixing happens only between the states with the parent terms  $^3P$  and  $^1D$ , but not with the states having the parent term  $^1S$  even though the state with the parent.

As can be seen in figures 1 a) and b), the main  $KL_{2,3}L_{2,3}$  peak, labelled as 10, has a double peak stucture in the simulated spectrum, whereas the experimental spectrum shows only one peak. Thus the calculations exaggerate the splitting of the states, which was already noted for the ground state. The splitting between the tops of peak 10 in the simulated spectrum is approximately 2eV and this results to a total FWHM of peak 10 of about 3.6eV while an experimental FWHM of about 2.6eV was determined from spectrum in figure 1 a). Such a big overestimation of the splitting cannot originate from the initial states, because the included initial states spread over an energy range of 0.698eV according to single-configuration calculation. Thereby we conclude that the overestimation of the splitting originates from the  $1s^22s^22p^43s^23p^2$  final states. The lower kinetic energy part of peak 10 consists mainly of transitions to the mixed final states with leading states  $(^1D)^3P$  and  $^3D$ . The higher kinetic energy part of line 10 consists of transitions to nearly pure LS-coupled final states  $(^1D)^1G$  and  $^3F$ . This kind of overestimation of the splitting between mixed states and pure states was also seen in the main  $KL_{2,3}L_{2,3}$  ( $^1D$ ) line of the calculated KLL Auger spectrum of aluminium [17].

The simulated spectrum in figure 1 b) agrees fairly well with the experimental one (figure 1 a)) in respect of the satellite Auger spectra. It can be stated quite reliably that the experimental spectrum includes the satellite KLL Auger spectra with initial state configurations  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{1}$ ,  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{1}4p^{1}$  and  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{3}$ . Corresponding satellite spectra were also detected for the KLL Auger spectrum of atomic aluminium [17] which with an atomic number of 13 is beside silicon in the periodic table. In figure 1 b) the calculated satellite spectrum with an initial state configuration  $1s^{1}2s^{2}2p^{6}3s^{1}3p^{2}$  seems to coincide with the experimental spectral features in figure 1 a), but due to the low intensity of the lines this recognition is to some extent uncertain. Calculations were also computed for the satellite KLL Auger transitions with initial state configurations  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{1}5p^{1}$  and  $1s^{1}2s^{2}2p^{6}3s^{1}3p^{2}4s^{1}$ . However, the calculated transitions did not match to any distinguished experimental spectral features.

The experimental and calculated normal and satellite KLL Auger transition intensities of atomic silicon are given in table 2. The total satellite intensities relative to the total normal KLL Auger intensity were determined semiempirically. The 3p shake off and  $3p \rightarrow 4p$  shake up satellite spectra with intensity ratios of 19% and 12% are the strongest. These results are in line with the 3p shake off and  $3p \rightarrow 4p$  shake up intensities of 17% and 15% obtained for atomic aluminium [17, 18].

Line 7 in the experimental spectrum 1 a) is not entirely explained by the calculated satellite Auger spectra shown below. The previously studied KLL Auger spectra of atomic sodium and magnesium [18] included satellite transitions where a shake up from the 3s to 4s orbital during the KLL Auger process takes place. Suchlike transitions might also happen in silicon with shake up from the 3p to 4p orbital producing the strongest spectral structures approximately in the region of line 7, but no calculations were carried out for this satellite.

The Lorentzian linewidth of the silicon main line  $KL_{2,3}L_{2,3}$  (<sup>1</sup>D) was determined from the experimental spectrum measured with the spectrometer entrance slit of 0.5mm to be  $2.1 \pm 0.1 eV$ . The line was fitted as one line, even though it can be seen from the simulated spectrum in figure 1 b) that line  $KL_{2,3}L_{2,3}$  (<sup>1</sup>D) labelled as line 10 actually comprises of many lines which are not resolved. Krause *et al.* [25] have determined for these individual lines a semiempirical natural width of 0.51 eV. The Lorentzian linewidths of lines  $KL_1L_1$  (<sup>1</sup>S) and  $KL_1L_{2,3}$  (<sup>1</sup>P) were determined from the experimental spectrum measured with the spectrometer entrance slit of 0.8mm to be  $4.3 \pm 0.2 eV$  and  $2.2 \pm 0.2 eV$ . These lines were also fitted as one line. The  $L_1$  hole state of silicon can decay further via fast Coster-Kronig transition and this widens the  $KL_1L_1$  and  $KL_1L_{2,3}$  lines with respect to the  $KL_{2,3}L_{2,3}$  lines. This affects especially the linewidth of the  $KL_1L_1$  (<sup>1</sup>S) line which has both holes on the  $L_1$  shell.

#### 4. Conclusions

The KLL Auger spectrum of atomic silicon was measured using electron impact for the ionization of the 1s orbital. The experimental spectrum was interpreted using calculations obtained with Cowan's code. The calculations were carried out in the intermediate coupling scheme using the Hartree-Fock method with relativistic corrections. The main *KLL* Auger lines were identified and *KL*<sub>1</sub>*L*<sub>1</sub>, *KL*<sub>1</sub>*L*<sub>2,3</sub>, and *KL*<sub>2,3</sub>*L*<sub>2,3</sub> group intensities were determined to be 8%, 28% and 64%, respectively. The KLL Auger satellite spectra with initial state configurations  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{1}$ ,  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{1}4p^{1}$ , and  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{3}$  were identified from the experimental spectrum. The intensity ratios of the strongest satellite spectra with the initial state configurations  $1s^{1}2s^{2}2p^{6}3s^{2}3p^{1}4p^{1}$  relative to the total normal KLL Auger intensity were determined semiempirically to be 19% and 12%, respectively. For some of these satellite lines the intensity in the experimental spectrum was too low for the lines to be resolved. The intensities of these lines were determined with the help of the calculations and thus the total satellite intensities are semiempirical.

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Figure 1: a) Experimental KLL Auger spectrum of atomic silicon. b) Simulated KLL Auger spectrum of atomic silicon.

Table 1: Experimental kinetic energies and intensities (relative to line 10) of the KLL and satellite Auger spectra of atomic silicon. The designation of the peaks is the same as in figure 1. The intensity errors are the maximum deviations from the mean intensity obtained from three fittings. The kinetic energy error bars include the uncertainty of fitting obtained from these three fittings and also the error of the energy calibration line. The LS terms given in brackets are determined by coupling the final state holes on the L shell.

Peak	$E_k  [eV]$	Int. [%]	Iniatial state	Final state	
1	1493.8(2)	16.5(3)	$1s3p^2$	$2s^0 3p^2 \ (^1S)$	
2	1524.9(4)	8.0(6)	1s3p	$2s2p^{5}3p~(^{1}P)$	
3	1530.6(2)	4.2(2)	1s3p4p	$2s2p^{5}3p4p~(^{1}P)$	
4	1537.9(2)	39.6(5)	$1s3p^2$	$2s2p^53p^2 \ (^1P)$	
5	1544.8(5)	<pre></pre>	$1s3s3p^2$	$2s2p^53s3p^2~(^3P)$	
			1s3p4p	$2s2p^{5}3p4p~(^{3}P)$	
		0.7(11)	1s3p	$2s2p^{5}3p~(^{3}P)$	
		(	$1s3p^3$	$2s2p^53p^3 \ (^1P)$	
6	1555.6(3)	15.5(11)	$1s3p^2$	$2s2p^53p^2 \ (^3P)$	
7	1575.5(4)	0.2(1)	$1s3s3p^2$	$2p^43s3p^2$ ( <sup>1</sup> S)	
		9.3(1)	1s3p	$2p^4 3p \ (^1S)$	
		(	1s3p	$2p^4 3p \ (^1D)$	
8	1582.9(2)	24.5(3)	$1s3s3p^2$	$2p^4 3s 3p^2 \ (^1D)$	
		l	1s3p4p	$2p^4 3p 4p \ (^1S)$	
9	1589.0(3)	(100, 100)	1s3p4p	$2p^4 3p 4p \ (^1D)$	
		20.2(23)	$1s3p^2$	$2p^4 3p^2 \ (^1S)$	
10	1595.9(2)	100.0(96)	$1s3p^2$	$2p^4 3p^2 \ (^1D)$	
11	1600.6(2)	16.8(87)	$1s3p^2$	$2p^4 3p^2 \ (^3P)$	
12	1608.1(2)	1.6(2)	$1s3p^3$	$2p^4 3p^3$ (1D)	

Table 2: Experimental and calculated Si normal KLL Auger and satellite transition intensities as percentages of the total intensity of the decay channel. The ratio given below the initial state of a satellite transition is between the satellite intensity and the total normal KLL Auger intensity. These values are semiempirical. For the satellite transitions, the given experimental intensity values are indicative because most of the lines were part of a wider peak including several lines which could not be resolved. The error bars of the KLL Auger intensities are given in brackets.

Final state		$2s^0val$	$2s^12p^5val$	¢	$2p^4val$
		$^{1}S$	$^{1}P$ $^{3}P$	$^{1}S$	$^{1}D$ $^{3}P$
Initial state					
$1s3p^2$	Exp.	8(2)	20(3) $8(2)$	6(2)	50(6) $8(7)$
(Normal KLL)	Calc.	6	20 7	7	54 7
Group int.	Exp.	8(2)	28(4)		64(5)
	Calc.	6	26		68
1s3p4p	Exp.	$6^a$	$17   7^a$	$7^a$	$59  4^a$
12%	Calc.	6	20 7	7	57 4
Group int.	$\operatorname{Exp.}^{b}$	6	24		69
÷	Calc.	6	26		67
1s3p	Exp.	$6^a$	21 $6^a$	$7^a$	$56  4^a$
19%	Calc.	6	20 7	7	57 4
Group int.	$\operatorname{Exp.}^{b}$	6	27		67
1	Calc.	6	26		68
$1s3s3p^2$	Exp.	$1^a$	$0^{a}$ 54	$15^a$	$29^{c}$ $2^{c}$
5%	Calc.	1	0 48	13	36 2
Group int.	$Exp.^{b}$	1	54		45
Ĩ	Calc.	1	48		51
$1s3p^3$	Exp.	-		_	56 -
2%	Calc.	6	20 7	7	56 5
Group int.	Calc.	6	26		68

<sup>a</sup>These values are semiempirical. The intensities of these lines were too low for the lines to be resolved in the experiment and the given values are determined with the help of the strongest observed line and the intensity ratio obtained from the calculations between this particular line and the strongest observed line.

<sup>b</sup>Group intensities are obtained with the help of the experiment and the calculations. <sup>c</sup>The intensity determined from line 8 (figure 1) for transition from initial state  $1s3p^3$  was shared between lines <sup>1</sup>D and <sup>3</sup>P according to calculations.

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