J. Phys. B: At. Mol. Opt. Phys. **30** (1997) L665–L669. Printed in the UK PII: S0953-4075(97)86542-X

LETTER TO THE EDITOR

K-shell photoionization of atomic boron

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Received 11 August 1997

Abstract. The direct and conjugate shake-up cross sections for the $2p \rightarrow 3p, 3s$ and $2s \rightarrow 2p, 3s$ transitions are calculated for atomic boron in a close-coupling approximation using the *R*-matrix method. In the photon energy interval 17–45 Ryd we find that the total cross section for these secondary processes represents about 30% of the single inner-shell photoionization cross section. The $2s \rightarrow 3s$ excitation gives the dominant contribution (80% of the total), while the $2p \rightarrow 3p$ and $2s \rightarrow 2p$ excitation contributions are broadly comparable with each other in this energy range. The contribution from the $2p \rightarrow 3s$ transition is negligible. It is then probable that the 2s shake-off excitation dominates the 2p one, giving rise mostly to terms of the 1s2s2p configuration. Our results suggest that the ionization equilibrium of multiply charged B, C, Na, Mg, Al and Si in a low-density soft-x-ray photoionized plasma will be perturbed strongly by such processes.

Much experimental and theoretical effort has been devoted to the study of secondary processes following single inner-shell 1s photoionization (shake-up and shake-off processes) both as a probe of our understanding of higher-order quantum mechanical processes and because of the efficiency of such processes in producing highly charged ions in cool photoionized plasmas. However, results are scarce for low-Z atoms and ions despite the global importance of these processes (Åberg 1969) and the fact that they increase rapidly with decreasing Z, relative to the total inner-shell photoionization process. For example, in the early 1970s Krause and his collaborators analysed the Auger and photoelectron spectra of Ne following irradiation (see Krause 1971, Krause *et al* 1971, Carlson *et al* 1971). They found that the direct shake-up and the KL shake-off processes represented about 8% and 13.8% of the total 1s photoionization processes, respectively. The shake-up processes in this case are dominated by the $2p \rightarrow 3p$ excitation. In the case of Be, Krause and Caldwell (1987a, b) reported cross sections above the K-edge where the $2s \rightarrow 3s$ transition and the $2s \rightarrow 2p$ transition represented about 19% and 10.5% of the total 1s photoionization cross section, respectively.

Close-coupling calculations of inner-shell photoionization (including shake-up) with (necessarily) extensive multiconfiguration wavefunctions are demanding even for Be. Complex calculations for Be have been performed by VoKy *et al* (1992) using the *R*-matrix method, following earlier work by Bely-Dubau *et al* (1977) that used only a small number of configurations. VoKy *et al* reproduced accurately all of the features that were observed in the photoelectron spectrum by Krause and Caldwell (1987a, b) and confirmed the

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0953-4075/97/190665+05$19.50

importance of the conjugate shake-up process at low energies, i.e. near the photoionization thresholds. However, they did not calculate cross sections for the direct 2s $\rightarrow$ 3s shake-up transition in the same low-energy interval or for the direct and conjugate shake-up processes at higher energies, where the 2s $\rightarrow$ 3s excitation is expected to largely dominate the other excitations.

In this letter we examine the importance of the direct and conjugate shake-up processes following the 1s photoionization of boron, the first atom starting to fill-in a p-type orbital in the ground configuration ($1s^2 2s^2 2p$). If shake-up of the 2p electron is large, then there is also the possibility that there will be a strong shake-up of the 2s electron due to weak screening by the 2p electron. The only existing calculation on boron was performed by Le Dourneuf (1974) in the close-coupling approximation, using the *R*-matrix method, but taking into account only a few target configurations which did not allow for shake-up. To the best of our knowledge no realistic calculation exists for the inner-shell photoionization of boron, until now. In particular, we have calculated cross sections for the 2p $\rightarrow$ 3p, 3s and 2s $\rightarrow$ 2p, 3s shake-up transitions. We used the *R*-matrix method (Berrington *et al* 1987, 1995) and covered the photon energy interval 17–45 Ryd, where all electron channels are open. We used the SUPERSTRUCTURE code originated by Eissner *et al* (1974) to describe the electron target (i.e. B^+). We chose the following two categories of configurations: (i) closed K-shell: $1s^2 2s^2$, $1s^2 2s2p$, $1s^2 2p^2 ({}^1S)$, $1s^2 2s3s$ and (ii) open K-shell: $1s2s^2 2p$, $1s2s2p^2$, $1s2s^2 3s$, $1s2s^2 3p$, $1s2p^3 ({}^3P^o, {}^1P^o)$ and 1s2s2p3s. The latter case gives rise to 20 terms over a range of 2 Ryd starting at 14.6 Ryd (above the ground ^1S state), since neither the quintet nor the $^3S^o$, $^3D^o$, $^1D^o$ terms are required. The values of the λ_{nl} scaling parameters occurring in the Thomas–Fermi potential that we used to produce the 1s, 2s, 2p, 3s and 3p orbitals are 1.3972, 1.2055, 1.1520, 2.4040 and 1.9149, respectively. A correlation configuration $1s^2 2p3d$ was also introduced (with $\lambda_{3d} = 9.5$) to improve the description of the target. We obtained close agreement between the length and velocity forms of the 2s–2p weighted oscillator strength (1.0086 and 1.0078, respectively), while for the 1s–3p values the agreement is 20% or better, except for the weakest transition which differs by a factor of three. The agreement between our calculated energies and the experimental values was within 1% for the lowest terms and 2% for the 1s-hole terms, for which data is available. For the $^2P^o$ symmetry 41 closed channels occur. For the ^2S, ^2P and ^2D symmetries, representing the diffusion of the ejected electron by the B^+ ion, we have 23, 21 and 43 channels, respectively. From the *R*-matrix calculation, we obtained an ionization energy for boron of 0.609 Ryd, which is very close to the experimental one of 0.612 Ryd (Moore 1966). We used an *R*-matrix radius of 18.8 au and included 50 continuum basis orbitals in order to obtain smooth converged cross sections at the highest photon energy considered (45 Ryd). Solutions in the 'outer region' were obtained using Seaton's asymptotic codes STGB, STGF, STGBF (see Berrington *et al* 1987) and numerical difficulties can occur here (VoKy *et al* 1992). In STGB, closed-channel radial solutions arising from $1s2s^2 2p + e^-$, for example, can become vanishingly small (i.e. unrepresentable on a computer) at values of *r* for which other closed channels (to which they are coupled) e.g. $1s^2 2s^2 + e^-$, have yet to reach their exponentially decaying asymptotic behaviour. We solved this problem as follows: if a closed-channel radial solution is vanishingly small ($< 10^{-70}$ was found to be sufficient) then we set it to zero and move inwards until it is large enough (but still 'small') such that the inward numerical integration proceeds in a stable manner. Since coupling is treated as a perturbation, only the offending channel is affected by this operation. Similar changes are necessary in STGBF where the outer-region solutions are regenerated.

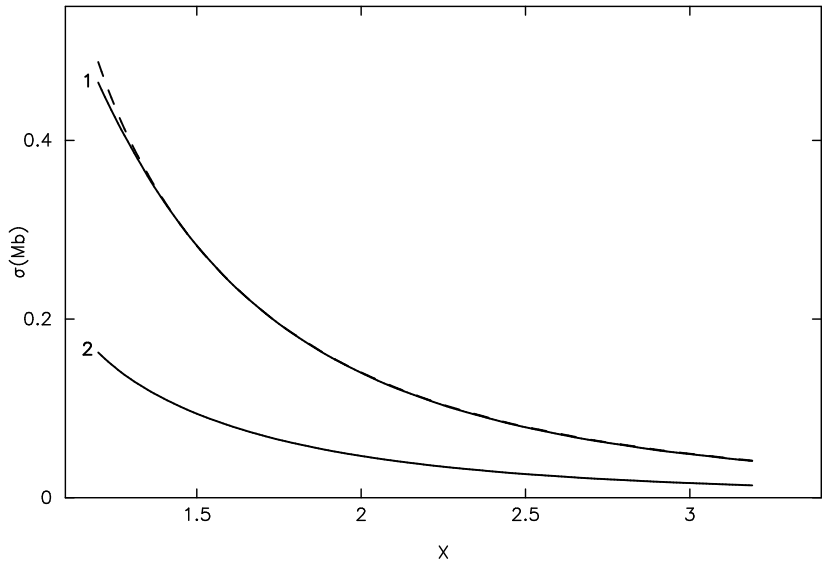

Figure 1. Single inner-shell photoionization cross sections (in Mb) versus $X = E_{h\nu}/E_{1s}$. $E_{h\nu}$ and E_{1s} represent the photon and 1s ionization energies, respectively. ——, $1s^22s^22p \rightarrow 1s2s^22p(^3P^o)$ (curve 1) and $1s^22s^22p \rightarrow 1s2s^22p(^1P^o)$ (curve 2); - - - -, $1s^22s^22p \rightarrow 1s2s^22p(^1P^o)$ multiplied by a spin statistical weight of 3. All results from this work.

In figure 1 we present our cross sections for the 1s photoionization versus energy in threshold units X: $X = E_{h\nu}/E_{1s}$, where $E_{h\nu}$ and E_{1s} are the photon and 1s ionization energies, respectively ($E_{1s} = 15$ Ryd). The values of X shown correspond to the photon energy interval 17–45 Ryd. We see that the ratio of cross sections for the transitions $1s^22s^22p \rightarrow 1s2s^22p\ ^3P$ and $1s^22s^22p \rightarrow 1s2s^22p\ ^1P$ is very close to statistical (3:1) for values of $X > 1.25$. In figure 2 we present the total shake-up cross section (curve 5) and the partial shake-up cross sections corresponding to the transitions $2s \rightarrow 3s$ (curve 4), $2p \rightarrow 3p$ (curve 3), $2s \rightarrow 2p$ (curve 2) and $2p \rightarrow 3s$ (curve 1), all relative to the 1s single-photoionization cross section. We note that the total shake-up cross section represents about 30% of the 1s single-photoionization cross section, which shows the importance of the shake-up processes in the case of boron. The direct shake-up $2s \rightarrow 3s$ transition (curve 4) gives the dominant contribution, while the conjugate shake-up $2p \rightarrow 3s$ transition (curve 1) is negligible. The dominant effect of the direct shake-up $2s \rightarrow 3s$ excitation cannot be explained by configuration mixing. Indeed, the $1s2s^22p$ configuration does not mix significantly with either the 1s2s2p3s or $1s2s^23p$ configurations according to our calculations. An argument in favour of a strong contribution given by this transition is the larger number of terms (five) associated with the 1s2s2p3s configuration compared to the (three of the) $1s2s^23p$ configuration. Another possible explanation could be a stronger correlation between the 2s and 3s electrons as compared to the correlation between the 2p and 3p electrons, which makes the direct shake-up $2s \rightarrow 3s$ excitation more probable. Furthermore, we observe that the contribution of the $2p \rightarrow 3p$ and $2s \rightarrow 2p$ transitions are close to each other in magnitude. This can be understood in terms of the long-range potential channel-coupling occurring in the close-coupling approximation. This coupling connects target terms of different parity. At low energy, collisional excitation due to the ejected electron is more efficient compared to the effect due to the change in the central field.

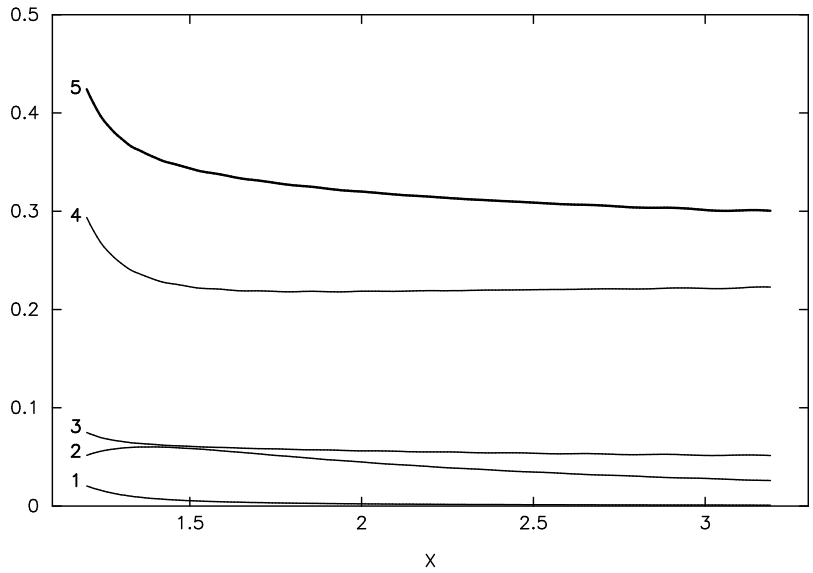

Figure 2. Shake-up cross sections, relative to the 1s photoionization cross section, versus X. Curve 5 represents the total relative shake-up cross section. The other curves represent the relative shake-up cross sections for the transitions: 2s $\rightarrow$ 3s (curve 4), 2s $\rightarrow$ 2p (curve 2), 2p $\rightarrow$ 3p (curve 3) and 2p $\rightarrow$ 3s (curve 1). Curve 1 was obtained by multiplying the actual values for the 2p $\rightarrow$ 3s cross section by a factor of 5. Curve 3 refers to the excitations to terms of the $1s2s^2 3p$ and $1s2p^3$ configurations. All results from this work.

As the ejected electron energy increases such collisional effects decrease, but they remain important for transitions involving no change in the principal quantum number. Finally, as a check on the sensitivity to open K-shell correlation we looked at the effect of adding the 1s2s2p3d configuration, using the 3d orbital that we determined previously. This only changed the total shake-up cross section by less than 2% of the 1s single-photoionizaton cross section.

In conclusion, we have calculated cross sections for the shake-up processes accompanying the photoionization of boron in a close-coupling approximation using the R-matrix method. We covered the 17–45 Ryd photon energy interval and found that the total cross section for these processes reaches about 30% of the single inner-shell photoionization cross section. The full shake-up regime is reached for $X > 4$ due to the strong 2s $\rightarrow$ 2p conjugate shake-up transition. In contrast to the case of Ne, the 2s $\rightarrow$ 3s excitation is strong and gives the dominant contribution since the 2p screening is weak and this favours the 2s excitation. This feature is possibly unique, and the case of carbon is of interest for future studies as a limiting case for a substantial 2s shake-up. This result also suggests a strong shake-off process leading to the $1s2s^2$ and 1s2s2p terms in B^{2+} and to a similar conclusion for the first ions of the boron isoelectronic series. These features, strong 2s and 2p excitations, are of interest in astrophysical plasmas undergoing soft-x-ray irradiation (Petrini and Da Silva 1996).

More experimental and theoretical work is needed, especially to confirm the strong 2s $\rightarrow$ 3s excitation and to obtain accurate relative shake-up probabilities for the $1s^2 2s^2 2p^n$ second row atoms and ions. Moreover, this work, together with the results of some preliminary calculations, suggests that the shake-up process of an outer 2p-subshell electron

is important for atoms like Na and Mg following K-shell photoionization, or for 3s excitation following 2s or 2p ionization of atomic Al and Si, for example. (In the latter case, the L-shell edge is at $\lesssim$100 eV.) These processes (including shake-off and double Auger process) are of great importance in low-density astrophysical plasmas since highly ionized species are produced, perturbing the ionization equilibrium and giving rise directly to excited states. This will be critical for diagnosing spectra from the next-generation high-resolution x-ray satellites XMM and AXAF, for example.

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