Atomic K-shell binding energies of multiply charged neon ions studied by zero-degree Auger-electron spectroscopy

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In this work we report an improved experimental determination of K-shell binding energies from Be-like Ne^{6+}, B-like Ne^{5+}, and C-like Ne^{4+} ground-state multiply charged ions using high-resolution Ne-K Auger-electron spectroscopy. The derived energy differences, namely, $Ne^{6+}\,E(1s^22s^2)\,^1S$–$Ne^{7+}\,E(1s2s^2)^2S$, $Ne^{5+}\,E(1s^22s^22p)\,^2P^\circ$–$Ne^{6+}\,E(1s2s^22p)\,^3P^\circ$, and $Ne^{4+}\,E(1s^22s^22p^2)\,^3P$–$Ne^{5+}\,E(1s2s^22p^2(^3P))\,^4P$ are 1099.1, 1048.5, and 1001.8 eV, respectively. These energies are accurate to within ±0.1 eV. Theoretically, we have studied relativistic binding energies of Ne^{q+} ($q=6$, 5, and 4) by using the (i) saddle-point technique, (ii) $1/Z$ method, and (iii) multiconfiguration Dirac-Fock model. Excellent agreement with experiment is obtained.

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I. INTRODUCTION

K-shell binding energies of free atoms [1] and ions constitute important atomic data relevant to surface physics, fusion plasmas, x-ray laser design [2], astrophysics, and sophisticated ion sources such as the electron-cyclotron-resonance (ECR) source [3] and electron-beam ion trap (EBIT) [4]. These data are also of fundamental importance for a better understanding of electron correlation and relativistic interactions in autoionizing core-excited states which generally require computationally elaborate many-body theories [5–13]. Despite the fundamental importance of accurate inner-shell energy values, it was not until recently that free-atom K-shell binding energies of Be, B, and C have been studied both experimentally and theoretically [14–16]. Experimentally Bruch and coworkers applied the forward-angle (6.5°) projectile Auger-electron-spectroscopy method [14,15] to fast Be^+, B^+, and C^+ ion beams and Krause and Caldwell [16] made a study of the K-shell photoionization of atomic beryllium.

Highly accurate atomic data on binding energies of multiply charged ions are virtually nonexistent except for some recent results on the L, M, and N shells of multiply charged krypton ions by internal-conversion-electron spectroscopy [17].

Here we report K-shell binding energies for charge states 4+ (C-like Ne), 5+ (B-like Ne), and 6+ (Be-like Ne). To our knowledge these measurements represent the most accurate K-shell binding energies for multiply charged Ne ions. Furthermore we have calculated precise Ne K energy values and shifts as a function of the number of $2p$ orbitals by using relativistic many-body approaches. Our theoretical predictions are in excellent agreement with experimental results and may serve as benchmark calibration points. The determination of experimental K-binding energies is discussed in the following.

II. EXPERIMENTAL PROCEDURE

Zero-degree projectile Auger-electron spectroscopy [18–20] in conjunction with multiply charged energetic ion beams and light targets (H_2, He) has great potential for studying core-level binding energies, because (i) the excitation process is highly selective [21], similar to inner-shell photoionization [22–24], (i.e., mainly one inner-shell electron is removed), (ii) high-energy resolution is achieved due to drastic reduction of kinematic line broadening, and (iii) Auger spectra can be investigated individually, depending on the incident projectile charge state [25]. In this work Li-like, Be-like, and B-like core-excited configurations were selectively produced in 100-MeV Ne^{6+}+He, 100-MeV Ne^{5+}+He, and 70-MeV Ne^{4+}+He collisions (see Fig. 1). The experimental arrangement that has been used to study electron emission from selectively excited K-shell vacancy states of fast Ne ion beams has been described in detail previously [21] and will not be discussed here. However, the line assignment and absolute calibration for these Ne K Auger spectra have been considerably improved on the basis of refined theoretical computations using the saddle-point technique [26], the $1/Z$ method [13], and the multiconfiguration Dirac-Fock (MCDF) mode [6].

In particular the line assignment of the boronlike states [Fig. 1(c)] has been completely revised. Figure 1 presents the basic results of this experiment. It clearly demonstrates that discrete selective Auger transitions can be ob-

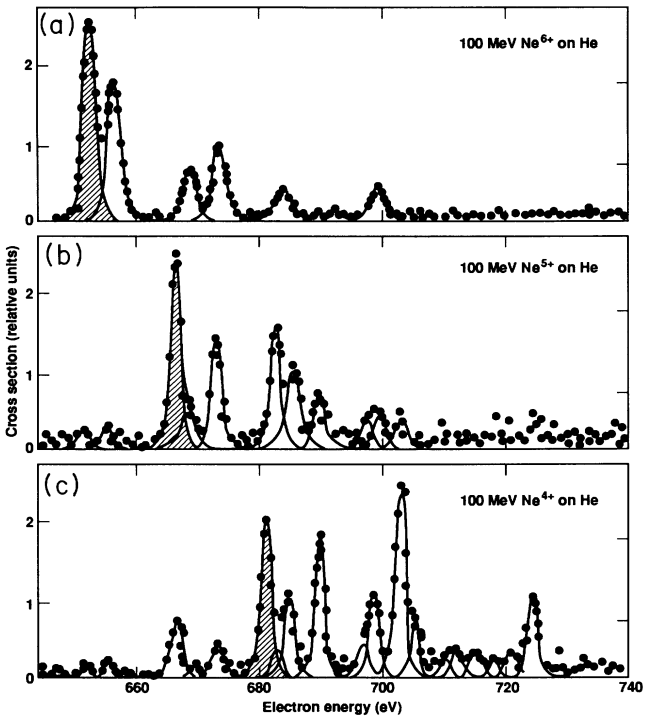

FIG. 1. High-resolution zero-degree electron spectra of neon, resulting from K-shell ionization following (a) 100-MeV $Ne^{6+}+He$, 100-MeV $Ne^{5+}+He$, and (c) 70-MeV $Ne^{4+}+He$ collisions. The spectra are displayed after background subtraction and transformation to the projectile emitter frame.

served in energetic $Ne^{q+}(q=6, 5, \text{and } 4)+He$ collisions. The majority of the Auger lines which are observed in Figs. 1(a) and 1(c) originate from Li-like, Be-like and B-like initial configurations. We have found striking evidence that the pronounced lines [see Figs. 1(a)–1(c)] can be uniquely identified as the

$$Ne^{7+}(1s2s^2)\,^2S \rightarrow (1s^2\epsilon s)\,^2S\ , \tag{1}$$

$$Ne^{6+}(1s2s^22p)\,^3P^0 \rightarrow (1s^22p\epsilon s \text{ or } \epsilon d)\,^3P^0\ , \tag{2}$$

$$Ne^{5+}[1s2s^22p^2(^3P)]\,^4P \rightarrow (1s^22p^2\,^3P\epsilon s \text{ or } \epsilon d)\,^4P \tag{3}$$

Auger transitions. A more detailed line identification and discussion of the branching ratios is given elsewhere [27].

According to Bisgaard *et al.* [14] we define the K-shell binding energies of Ne as the difference between the lowest-lying multiplet terms of the initial- and final-state configurations for the K-shell ionization process. For Be-, Be-, and C-like neon ions, the K-shell binding energies are therefore given as follows:

$$E^B_{1s} = \begin{cases} E(1s2s^2)\,^2S - E(1s^22s^2)\,^1S & \text{for } Ne^{6+} \quad (4) \\ E(1s2s^22p)\,^3P^0 - E(1s^22s^22p)\,^2P^0 & \text{for } Ne^{5+} \quad (5) \\ E[1s2s^22p^2(^3P)]\,^4P - E(1s^22s^22p^2)\,^3P & \text{for } Ne^{4+}. \quad (6) \end{cases}$$

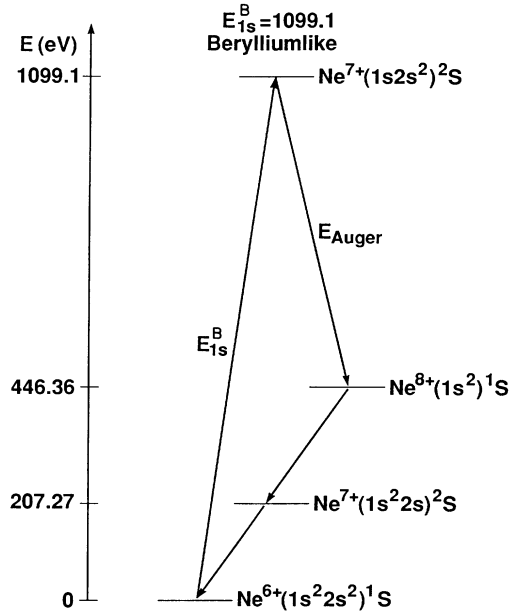

FIG. 2. Energy-level diagram for establishing the K-shell binding energy of berylliumike neon.

The procedure for extracting the berylliumlike, boronlike, and carbonlike K-shell binding energies is illustrated schematically in Figs. 2, 3, and 4, respectively. In these energy-level diagrams E_{Auger} is the experimentally determined Auger transition energy. In this connection we note that the necessary additional L-shell ionization energies of the Ne can be deduced with high accuracy from spectroscopic data [28]. The K-binding energies thus derived are summarized in Table I along with theoretical calculations which are discussed in the next section.

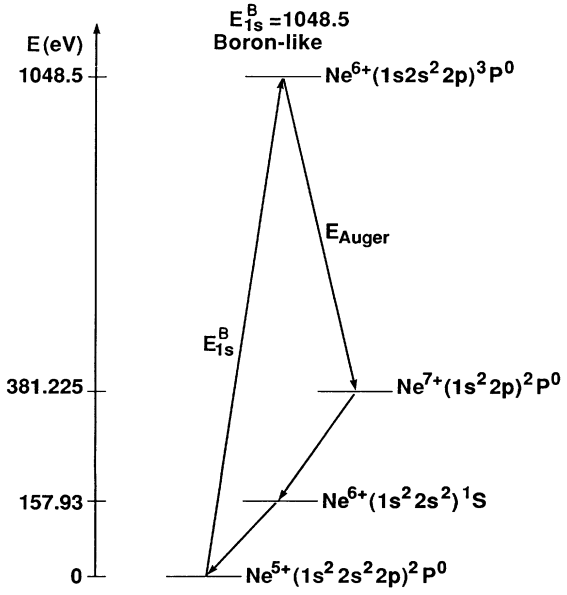

FIG. 3. Energy-level diagram for establishing the K-shell binding energy of boronlike neon.

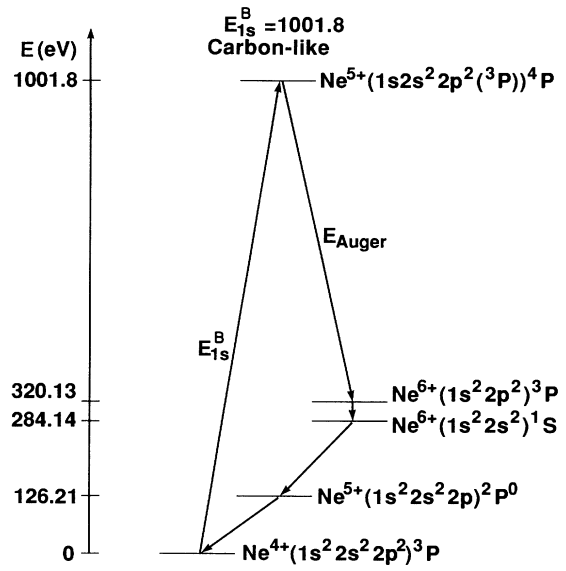

FIG. 4. Energy-level diagram for establishing the K-shell binding energy of carbonlike neon.

III. THEORETICAL COMPUTATION

In 1979, a saddle-point variation method was developed for dealing with resonances arising from inner-shell excitation [26]. This method has been applied to numerous two- and three-electron resonances. Here we have applied this technique to the lowest three-electron state, i.e., $(1s2s^2)\,^2S$ in Ne^{7+} and the lowest four-electron state, i.e., $(1s2s^22p)\,^3P^0$ in Ne^{6+}. The details of the calculations are reported by Chung and Bruch [7]. We note that the saddle-point method for a four-electron system [29] is very similar to that for a three-electron system. The nonrelativistic part of the calculation follows the same procedure as in Chung [30] in which an LS-coupling scheme was used. The relativistic corrections are calculated with the Breit-Pauli approximation [31] using first-order perturbation theory. The mass polarization effect is also included. The explicit forms of the operators are given by Chung [32].

The main advantage of this saddle-point method is the simplicity with which computations can be carried out to yield high-precision results, which can be used for calibration in high-resolution electron spectroscopy. Our theoretical predictions for K-shell binding energies deduced from the saddle-point method are listed in Table I.

Since the saddle-point method is limited so far to calculations of two-, three-, and a few four-electron systems, we have determined additional K-shell binding energies in beryllium and boronlike neon ions with $1s2s^22p$ and $1s2s^22p^2$ initial configurations. These calculations have been performed relativistically in terms of the multiconfiguration Dirac-Fock model in optimum-level

TABLE I. Experimental K-shell binding energies of Be-, B-, and C-like multiply charged neon ions in comparison with theoretical predictions.

System	Ionization process	Experimental		Theoretical		
		Projectile	Target	Saddle-point method	$1/Z$ expansion	MCDF model
Ne^{6+}	$(1s^22s^2)\,^1S\rightarrow(1s2s^2)\,^2S$	1099.1±0.1[a]	1099.4[b]	1099.02[c]		1099.26[d]
Be-like		1098.4±[e]	1098.8[f]			
			1098.4[g]			
Ne^{5+}	$(1s^22s^22p)\,^2P^0\rightarrow$ $(1s2s^22p)\,^3P^0$	1048.5±0.1[a]	1048.1[f]	1048.495[i]	1048.17[h]	1048.47[d]
B-like		1046.2±1[e]				1049.02[i]
Ne^{4+}	$(1s^22s^22p^2)\,^3P\rightarrow$ $[1s2s^22p^2(^3P)]\,^4P$	1001.8±0.1[a]	1002.0[f]		1001.95[h]	1001.87[d]
C-like						

Energy difference $Ne^{5+}(1s^22s^22p)\,^2P^0-Ne^{7+}(1s^22p)\,^2P^0$: 381.225 eV
Bashkin and Stoner (Ref. [28])
Energy difference $Ne^{4+}(1s^22s^22p^2)\,^3P-Ne^{6+}(1s^22p^2)\,^3P$: 320.13 eV
Bashkin and Stoner (Ref. [28])
Energy difference $Ne^{6+}(1s^22s^2)\,^1S-Ne^{8+}(1s^2)\,^1S$: 446.36 eV
Bashkin and Stoner (Ref. [28])

[a]Zero-degree projectile electron spectroscopy, this work.
[b]Target Auger-electron spectroscopy, Schneider, Moore, and Johnston (Ref. [37]).
[c]Saddle-point technique including relativistic corrections, this work.
[d]Multiconfiguration Dirac-Fock calculation, this work.
[e]Beam-foil Auger-electron spectroscopy, Schumann and co-workers (Refs. [35,36]).
[f]Target Auger-electron spectroscopy, Kádár *et al.* (Ref. [40]).
[g]Target Auger-electron spectroscopy, Stolterfoht *et al.* (Ref. [38]).
[h]$1/Z$-expansion method including relativistic corrections, this work (Ref. [13]).
[i]Multiconfiguration Dirac-Fock calculation, Schumann, Groeneveld, and Nolte (Ref. [35]).

scheme [33], where the Breit interaction and quantum-electrodynamic corrections are taken into account. In addition, the ground-state correlation corrections are also included [34].

In a third method we have applied the S-matrix formalism [13] as developed by Ivanov and Safronova to the nonrelativistic and relativistic energies of the $Ne^{6+}(1s2s^22p)\,^3P^0$ and $Ne^{5+}[1s2s^22p^2(^3P)]\,^4P$ states. This $1/Z$ expansion yields K-shell binding energies which are listed in Table I along with the MCDF values.

IV. RESULTS AND DISCUSSIONS

It is interesting to compare the experimental and theoretical K-binding energies for the different Ne charge states (see Table I). In the column labeled "Projectile" we compare our results with earlier beam-foil measurements of Schumann and co-workers [35,36]. It is evident that we have increased the accuracy of Ne K Auger energies by one order of magnitude. In this connection we note that for the Ne^{5+} case our projectile energy value deviates from the corresponding beam-foil result by 2.3 eV.

Complementary K-binding energies resulting from Ne K-target spectra following bombardment of fast multiply charged ions on Ne are also included in Table I (see column "Target"). The strong Coulomb field induced by the highly charged ions results in the removal of several electrons from the Ne L shell whenever a vacancy is produced in the K shell [37–40]. This causes the production of recoil charge states which correspond mainly to Li-, Be-, B-, and C-like electron configurations. As can be seen from Table I the K-shell binding energies derived from the work of Kádár *et al.* [40] agree within a few tenths of an eV with our experimental projectile results.

In our MCDF calculations of K-shell binding energies, the ground-state-correlation corrections which arise from the broken pairs in the ionization were estimated to be 1.17, 1.23, and 1.27 eV for Ne^{6+}, Ne^{5+}, and Ne^{4+}, respectively, by using the calculated nonrelativistic pair energies [41]. For Ne^{5+}, the present MCDF results differ slightly with the corresponding value given by Schumann, Groeneveld, and Nolte [35] due to the use of optimum-level scheme [33] and the inclusion of the ground-state-correlation correction in our calculation.

To our knowledge, the best theoretical data for K-shell binding energies are by Chung and Davis. Indeed, our experimental values for Ne^{6+} and Ne^{5+} are in excellent agreement with the saddle-point calculation. In the case of Ne^{5+} the $1/Z$-expansion method predicts K-binding energies outside our experimental uncertainty, whereas the saddle-point and MCDF calculations are in perfect agreement with our experimental value. For Ne^{4+} our MCDF result lies inside the experimental uncertainty quoted, whereas the $1/Z$ expansion predicts a binding energy which is slightly higher than our experimental energy.

There is another interesting point worth mentioning. It is apparent from Figs. 2–4 and Table I that the K-binding energies dramatically increase with decreasing number of $2p$ electrons. The corresponding binding-energy shifts derived from Table I are summarized in Table II. This effect can be explained qualitatively as a screening effect [22] of the nuclear potential owing to the $2p$ orbitals.

V. CONCLUSION

In summary, we have determined accurate K-binding energies for free neon ions of Be-, B-, and C-like configurations from high-resolution projectile-Auger-electron spectra. Our theoretical calculations agree very well with these data. In particular the present study provides insight into the role of $2p$ electron correlation and screening effects in the inner-shell ionization process of neon ions. The zero-degree projectile-Auger-electron-spectroscopy method can be extended to other studies of K-, L-, and M-shell binding energies along isoelectronic sequences, depending on the availability of intense fast-ion beams [42]. On the other hand, multiply charged inner-hole states can also be populated efficiently in slow collisions following selective multiple electron capture in ion-atom, ion-molecule, and ion-surface collisions [43]. The wealth of such Auger spectroscopic information may not only lead to a better understanding of the relativistic many-body problem in highly charged ions but may also help to unravel the complex physics in high-temperature dense plasmas as they are important for fusion, material processing, and x-ray laser research.

TABLE II. Ne K-shell binding-energy shifts in eV compared with theoretical calculations.

Charge state	Experimental		Theory		
	Projectile	Target	Saddle-point method	$1/Z$ expansion	MCDF model
5→6	50.6[a]	50.7[b]	50.53[c]		50.79[d]
	52.2[e]				
4→5	46.7[a]	46.1[b]		46.22[f]	46.60[d]

[a]Zero-degree projectile electron spectroscopy, this work.
[b]Target electron spectroscopy, Kádár *et al.* (Ref. [40]).
[c]Saddle-point technique including relativistic corrections, this work.
[d]Multiconfiguration Dirac-Fock calculation, this work.
[e]Beam-foil Auger-electron spectroscopy (Ref. [35]).
[f]$1/Z$-expansion method including relativistic corrections, Ivanov and Safronova (Ref. [13]), this work.

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