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Physics Division

**ELECTRON-IMPACT IONIZATION DATA
FOR THE NICKEL ISONUCLEAR SEQUENCE**

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ELECTRON-IMPACT IONIZATION DATA FOR THE NICKEL ISONUCLEAR SEQUENCE

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ABSTRACT

Atomic data for the electron impact ionization of ions in the nickel isonuclear sequence are reviewed. In 8 of the 28 ions of the nickel isonuclear sequence, experiment and theory are compared. In many of the ions, excitation-autoionization contributions to the total cross section are found to be quite important. For intermediate charge state ions a large fraction of the experimental cross section may be attributed to ionization from metastable levels of low-lying excited configurations. Maxwellian collisional rate coefficients are calculated from the cross section data and presented in tabular, graphical, and parametrized form.

1. INTRODUCTION

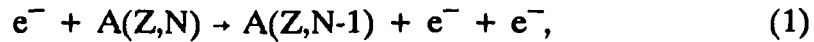
The principal ionization mechanism found in plasma transport modeling of impurities in magnetic fusion experiments is electron-impact ionization. Accurate ionization rate coefficients are thus needed for many transition series metals, due to their presence in containment vessels. Recently a joint theoretical and experimental research project to study the electron-impact ionization of atomic ions along the entire Fe isonuclear sequence was completed.¹⁻⁴ In this report we present the results of similar calculations and measurements for electron ionization of atomic ions in the Ni isonuclear sequence.

A number of collisional processes can contribute to the total electron-impact ionization of atomic ions. In addition to direct ionization from an initial ion with atomic number A and N bound electrons:

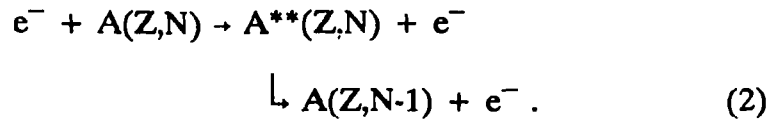
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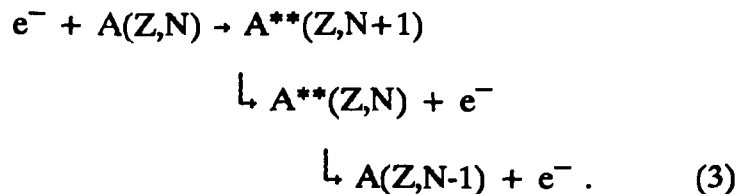


we can have inner-shell excitation followed by autoionization:



Studies over the past decade⁵ have shown that the contributions of excitation autoionization can dominate the total ionization cross section for ions in relatively low stages of ionization, when the doubly excited states resulting from $\Delta n=0$ inner-shell excitations are autoionizing. However, inner-shell excitations involving $\Delta n \geq 1$ excitations can also make significant contributions to the total ionization cross section, especially in higher stages of ionization. For a given isonuclear sequence, direct ionization cross sections decrease rather rapidly with ionization stage, while the magnitude of the $\Delta n \geq 1$ excitation cross sections tend to gradually increase; this, of course, results in a significant increase in the relative magnitude of the indirect contributions.

In addition to the ionization processes described in Eqs. (1) and (2), we can also have contributions from resonant recombination followed by double autoionization:



In order to determine whether this last process will contribute to the total ionization cross section, one must first determine the relative probability of sequential autoionization from the doubly excited state of the (N+1)-electron ion to all possible states of the (N-1)-electron ion versus the probability of all possible autoionizing and (or) radiative transitions to bound states of the (N+1)- or N-electron ions. In a complex ion, this typically involves many hundreds of transitions for a given (N+1)-electron level. For this reason this process is not well understood. As we shall see, comparisons of calculations which include only processes (1) and (2) with experimental cross sections indicate that this process does make contributions to the total ionization of several of the ions considered here.

In addition to ionization from the ground states of atomic ions, it is important to consider ionization from possible metastable states which might be heavily populated in a given plasma. One might expect that ionization from low-lying excited configurations to be important when the number of long-lived excited states (those that are forbidden to decay to the ground state because of J selection rules) is large in comparison to the number of relatively short-lived excited states plus the total number of states within the ground configuration. Thus when performing purely theoretical studies, we have normally included ionization from such low-lying excited configurations only when the ratio of metastable states to all states in the excited configuration and ground configuration is relatively large. However, extensive comparisons of theoretical calculations with cross section measurements in which the ECR ion source at Oak Ridge National Laboratory was employed indicate that this ion source preferentially populates some of the low-lying, long-lived states. Whether this is true in other laboratory and astrophysical plasmas is still an unanswered question.

The remainder of this report is arranged as follows. In the next section we briefly summarize the theoretical and calculational methods employed to determine the ionization cross section. In Sect. 3, we discuss the results of our cross section calculations for the Ni ions and compare them with available experimental data. Finally in Sect. 4, Maxwellian collisional rate coefficients are calculated from the cross section data and presented in tabular, graphical, and parametrized form.

2. THEORETICAL METHODS

The total single ionization cross section, ignoring interference effects between the direct ionization and excitation-autoionization processes, may be written as:

$$\sigma_{\text{tot}}(i) = \sum_f \sigma_{\text{ion}}(i \rightarrow f) + \sum_j \sigma_{\text{exc}}(i \rightarrow j) B_j^a, \quad (4)$$

where $\sigma_{\text{ion}}(i \rightarrow f)$ is the direct ionization cross section from the initial configuration to a particular level f within the ionized configurations and $\sigma_{\text{exc}}(i \rightarrow j)$ is the excitation cross section from the initial configuration to a particular level j within the core-excited configurations. The branching ratio for autoionization, B_j^a , from level j is given by:

$$B_j^a = \frac{\sum_m A_a(j \rightarrow m)}{\sum_m A_a(j \rightarrow m) + \sum_n A_T(j \rightarrow n)}, \quad (5)$$

where $A_a(j \rightarrow m)$ is the autoionizing rate from level j and $A_r(j \rightarrow n)$ is the radiative rate from level j . The further indirect ionization process of resonant-recombination double autoionization is not included in the calculations.

The direct ionization contributions, given by the first term of Eq. (4), may be obtained using distorted-wave methods.⁶⁻⁸ For the atomic ion of interest, a configuration-average collision cross section, $\bar{\sigma}_{\text{ion}}(n\ell)$, is calculated for each ionized subshell of the initial configuration which may contribute to single ionization. Cross sections for the other two or three subshells are needed for a typical nickel ion. The configuration-average cross sections, $\bar{\sigma}_{\text{ion}}(n\ell)$, are then statistically partitioned over all levels of the final ionized configurations. Finally the direct ionization cross sections are summed taking explicit account of the energy position of each ionized level calculated using the atomic structure package of Cowan.⁹

For ease in accessing the results of the numerical calculations, the direct ionization cross section for each subshell may be written in the following parameterized form:

$$\bar{\sigma}_{\text{ion}}(n\ell) = \frac{1}{IE} \left[A \left(1 - \frac{I}{E} \right) + B \left(1 - \frac{I}{E} \right)^2 + C \ln\left(\frac{E}{I}\right) + D \frac{I}{E} \ln\left(\frac{E}{I}\right) \right], \quad (6)$$

where E is the incident electron energy in eV, I is the subshell ionization potential in eV, and the cross section is in cm^2 . The parameters A , B , C , and D for the ground and certain excited configurations of all Ni ions are presented in Table 1.

The excitation-autoionization contributions, given by the second term of Eq. (4), may be obtained using distorted-wave methods.¹⁰⁻¹¹ For many atomic ions of interest, a configuration-average collision cross section, $\bar{\sigma}_{\text{exc}}(n\ell \rightarrow n' \ell')$, is calculated for each subshell excitation of the initial configuration which may contribute to single ionization. Cross sections for up to 40 excitations are needed for a typical nickel ion. The configuration-average cross sections, $\bar{\sigma}_{\text{exc}}(n\ell \rightarrow n' \ell')$, are then statistically partitioned over all levels of the final core-excited configurations. Finally the excitation cross sections are summed taking explicit account of both the energy position and branching ratio of each core-excited level calculated using the atomic structure package of Cowan.⁹ This method is a reasonable approximation when most of the levels within the final core-excited configuration are above the ionization limit, the branching ratios B_j^a are all close to one, and correlation in the initial and final states is small.

For certain atomic ions of interest, a level-to-level collision cross section, $\sigma_{\text{exc}}(i \rightarrow j)$, is calculated for transitions to each and every level of the final core-excited configurations. The excitation cross sections are then summed in the same

manner as the configuration-average method. The method is able to handle those cases where only a few levels are above the ionization limit and where branching ratios B_i^a are not close to one. In addition, correlation effects are easily incorporated into a level-to-level distorted-wave method. The major drawback of the method is that a full level-to-level cross section calculation for a single subshell excitation may take a couple of orders of magnitude more CPU time than the corresponding configuration-average calculation. The increase in time scales roughly as the average number of levels per final core-excited configuration. A worst case example is the $3p \rightarrow 4f$ excitation for the ground configuration of Ni^{5+} , resulting in a $3s^2 3p^5 3d^5 4f$ configuration with 2382 levels.

3. CROSS SECTIONS FOR Ni ATOMIC IONS

3.1 Ni^+ Results

In Fig. 1 the crossed-beams measurements of Montague and Harrison¹² for Ni^+ are compared with a configuration-average distorted-wave calculation for the $3s^2 3p^6 3d^9$ ground configuration. The calculation only includes direct ionization of the 3d subshell. Theory clearly overestimates the cross section in the threshold energy region.

3.2 Ni^{2+} Results

In Fig. 2 a configuration-average distorted-wave calculation for the $3s^2 3p^6 3d^8$ ground configuration of Ni^{2+} is presented. The calculation includes the $3p \rightarrow 3d$ excitation and direct ionization of the 3d subshell.

In Fig. 3 the configuration-average distorted-wave results are compared with the R-matrix LS close-coupling results of Burke, Fon, and Kingston.¹³ All 6 LS terms of the $3s^2 3p^5 3d^9$ configuration are included in the R-matrix calculation, while the distorted-wave calculation includes all 12 autoionizing levels. Reasonable agreement is found between the two calculations. The wavelike features in the R-matrix calculation are due to resonant-recombination followed by double autoionization. This additional indirect process is not included in the distorted-wave calculations.

3.3 Ni^{3+} Results

In Fig. 4 the crossed-beams measurements of Gregory and Howald¹⁴ for Ni^{3+} are compared with a configuration-average distorted-wave calculation for the

$3s^23p^63d^7$ ground configuration. The calculation includes the $3p \rightarrow 3d$ excitation and direct ionization of the 3d and 3p subshells. Almost half of the 3p direct ionization contributes to double ionization of Ni^{3+} , since 54 of the 110 levels of the $3s^23p^53d^7$ configuration are autoionizing. Theory clearly overestimates the cross section over much of the energy range.

In Fig. 5 experiment is compared with both the configuration-average distorted-wave results and the R-matrix LS close-coupling results of Burke, Fon, and Kingston.¹³ Only 6 of the 19 possible LS terms of the $3s^23p^53d^8$ configuration are included in the R-matrix calculation, while the distorted-wave calculation included all 45 autoionizing levels. The 6 LS terms included are expected, however, to contain the bulk of the $3p \rightarrow 3d$ excited collision strength. Reasonable agreement is found between the two calculations, although both overestimate the experimental cross section at the higher energies. The wave-like features in the R-matrix calculation are due to resonant-recombination processes.

3.4 Ni^{4+} Results

In Fig. 6 a configuration-average distorted-wave calculation for the $3s^23p^63d^6$ ground configuration of Ni^{4+} is presented. The calculation includes the $3p \rightarrow 3d$ excitation and direct ionization of the 3d and 3p subshells. The $3p \rightarrow 3d$ excitation is reduced significantly, since only 54 of the 110 levels of the $3s^23p^53d^7$ configuration are autoionizing.

3.5 Ni^{5+} Results

In Fig. 7 the crossed-beams measurements of Wang, Rinn, and Gregory¹⁵ for Ni^{5+} are compared with a configuration-average distorted-wave calculation for the $3s^23p^63d^5$ ground configuration. The calculation includes 41 excitations and direct ionization of the 3d, 3p, and 3s subshells. The largest excitations are $3p \rightarrow 4p$, in which 1190 of the 1208 levels of the $3s^23p^53d^54p$ configuration are autoionizing and $3s \rightarrow 3d$, in which all 63 levels of the $3s3p^63d^6$ configuration are autoionizing. Other important excitations are $3p \rightarrow 4d$, $3p \rightarrow 5p$, $3s \rightarrow 4s$, $3p \rightarrow 4s$, and $3p \rightarrow 4f$. The $3p \rightarrow 3d$ excitation is absent, since none of the 180 levels of the $3s^23p^53d^6$ configuration are autoionizing. An n^{-3} rule is used to estimate $3p \rightarrow n\ell$ and $3s \rightarrow n\ell$ excitation-autoionization contributions for $n \geq 9$. The agreement between theory and experiment is reasonable.

3.6 Ni⁶⁺ Results

In Fig. 8 the crossed-beams measurements of Wang, Rinn, and Gregory¹⁵ for Ni⁶⁺ are compared with a configuration-average distorted-wave calculation for the 3s²3p⁶3d⁴ ground configuration. The calculation includes 41 excitations and direct ionization of the 3d, 3p, and 3s subshells. The largest excitation is 3p → 4p, in which 450 of the 1038 levels of the 3s²3p⁵3d⁴4p configuration are autoionizing. Other important excitations are 3p → 5p, 3p → 4d, 3p → 4f, and 3s → 4s. The 3s → 3d excitation is greatly reduced, since only 6 of the 74 levels of the 3s3p⁶3d⁵ configuration are autoionizing. The n⁻³ rule is used to estimate n≥9 excitation-autoionization contributions. The agreement between theory and experiment is quite reasonable from threshold to around 700 eV.

3.7 Ni⁷⁺ Results

In Fig. 9 the crossed-beams measurements of Wang, Rinn, and Gregory¹⁵ for Ni⁷⁺ are compared with a configuration-average distorted-wave calculation for the 3s²3p⁶3d³ ground configuration. The calculation includes 39 excitations and direct ionization of the 3d, 3p, and 3s subshells. The largest excitations are 3p → 4f, in which 1169 of the 1180 levels of the 3s²3p⁵3d³4f configuration are autoionizing and 3p → 5p, in which all 613 levels of the 3s²3p⁵3d³5p configuration are autoionizing. Other important excitations are 3s → 4s and 3p → 5f. The 3p → 4p excitation is greatly reduced, since only 44 of the 613 levels of the 3s²3p⁵3d³4p configuration are autoionizing. The n⁻³ rule is used to estimate the n≥9 excitation-autoionization contributions. The agreement between theory and experiment is excellent from threshold to around 500 eV.

3.8 Ni⁸⁺ Results

In Fig. 10 the crossed-beams measurements of Wang, Rinn, and Gregory¹⁵ for Ni⁸⁺ are compared with a configuration-average distorted-wave calculation for the 3s²3p⁶3d² ground configuration. The calculation includes 38 excitations and direct ionization of the 3d, 3p, and 3s subshells. The largest excitations are 3p → 5p, in which 184 of the 256 levels of the 3s²3p⁵3d²5p configuration are autoionizing, and 3p → 5f in which all 472 levels of the 3s²3p⁵3d²5f configuration are autoionizing. Other important excitations are 3p → 6p and 3p → 6f. The n≥9 excitation-autoionization contributions for 3p → nℓ and 3s → nℓ, estimated by the n⁻³ rule, increase the total cross section by about 8%. The agreement between theory and experiment is excellent from threshold to around 500 eV.

3.9 Ni⁹⁺ Results

In Fig. 11 a configuration-average distorted-wave calculation for the $3s^23p^63d$ ground configuration of Ni^{9+} is presented. The calculation includes 34 excitations and direct ionization of the 3d, 3p, and 3s subshells. The largest excitation is $3p \rightarrow 5f$ in which all 113 levels of the $3s^23p^53d5f$ configuration are autoionizing. Other important excitations are $3p \rightarrow 6p$, $3p \rightarrow 6f$, and $2p \rightarrow 3d$. The $n \geq 9$ excitation-autoionization contributions for $3p \rightarrow n\ell$ and $3s \rightarrow n\ell$, estimated by the n^{-3} rule, increase the total cross section by about 12%.

3.10 Ni¹⁰⁺ Results

In Fig. 12 a configuration-average distorted-wave calculation for the $3s^23p^6$ ground configuration of Ni^{10+} is presented. The calculation includes the $2p \rightarrow 3d$ and $2p \rightarrow 4\ell$ ($\ell = 0,1,2,3$) excitations and direct ionization of the 3p and 3s subshells.

In Fig. 13 a configuration-average distorted-wave calculation for the $3s^23p^53d$ excited configuration of Ni^{10+} is presented. The calculation includes the $3s \rightarrow 4d$, $3s \rightarrow 5\ell$ ($\ell = 0,1,2$), $2p \rightarrow 3p$, $2p \rightarrow 3d$, and $2p \rightarrow 4\ell$ ($\ell = 0,1,2,3$) excitations and direct ionization of the 3d, 3p, and 3s subshells. The largest excitation is $2p \rightarrow 3d$. The $3s \rightarrow 4d$ excitation is reduced, since only 31 of the 192 levels of the $3s3p^53d4d$ configuration are autoionizing. The ratio of metastable states in the $3s^23p^53d$ excited configuration to all states in the excited and ground configurations is 0.84. The difference between the total and direct ionization cross sections in Fig. 13 from threshold to about 835 eV is due solely to the $3s \rightarrow n\ell$ excitations.

3.11 Ni¹¹⁺ Results

In Fig. 14 a configuration-average distorted-wave calculation for the $3s^23p^5$ ground configuration of Ni^{11+} is presented. The calculation includes the $2p \rightarrow 3p$, $2p \rightarrow 3d$, $2p \rightarrow 4\ell$ ($\ell = 0,1,2,3$), $2s \rightarrow 3p$, and $2s \rightarrow 3d$ excitations and direct ionization of the 3p and 3s subshells.

In Fig. 15 a configuration-average distorted-wave calculation for the $3s^23p^43d$ excited configuration of Ni^{11+} is presented. The calculation includes the $3s \rightarrow 4d$, $3s \rightarrow n\ell$ ($n = 5,6$ and $\ell = 0,1,2$), $2p \rightarrow 3p$, $2p \rightarrow 3d$, $2p \rightarrow 4\ell$ ($\ell = 0,1,2,3$), $2p \rightarrow 3p$, and $2s \rightarrow 3d$ excitations and direct ionization of the 3d, 3p, and 3s subshells. The largest excitation is $2p \rightarrow 3d$. The $3s \rightarrow 4d$ excitation is greatly reduced, since only 9 of the 452 levels of the $3s3p^43d4d$ configuration are autoionizing; in addition, 73 of the 107 levels of the $3s3p^43d5s$ configuration and 254 of the 303 levels of the

$3s3p^43d5p$ configuration are autoionizing. The ratio of metastable states in the $3s^23p^43d$ excited configuration to all states in the excited and ground configurations is 0.38. The 2s and 2p excitations appear in Fig. 15 only above 835 eV.

3.12 Ni¹²⁺ Results

In Fig. 16 the crossed-beams measurements of Wang, Rinn, and Gregory¹⁵ for Ni¹²⁺ are compared with a configuration-average distorted-wave calculation for the $3s^23p^4$ ground configuration. The calculation includes the $2p \rightarrow 3p$, $2p \rightarrow 3d$, $2p \rightarrow 4\ell$ ($\ell = 0,1,2,3$), $2s \rightarrow 3p$, and $2s \rightarrow 3d$ excitations and direct ionization of the 3p and 3s subshells. As can be seen, the experimental measurements are noticeably higher than the calculated cross section and the experimental ionization threshold appears to occur at about 50 to 60 eV below the calculated ground state threshold.

In Fig. 17 the crossed-beams measurements of Wang, Rinn, and Gregory¹⁵ for Ni¹²⁺ are compared with a configuration-average distorted-wave calculation for the $3s^23p^33d$ excited configuration. The calculation includes the $3s \rightarrow n\ell$ ($n = 5,6$ and $\ell = 0,1,2$), $2p \rightarrow 3p$, $2p \rightarrow 3d$, $2p \rightarrow 4\ell$ ($\ell = 0,1,2,3$), $2s \rightarrow 3p$, and $2s \rightarrow 3d$ excitations and direct ionization of the 3d, 3p, and 3s subshells. The largest excitation is $2p \rightarrow 3d$. The ratio of metastable states in the $3s^23p^33d$ excited configuration to all states in the excited and ground configuration is 0.26. Experiment and theory agree quite well from threshold to an energy of approximately 750 eV. The lowest level of the $3s^23p^33d$ configuration lies about 55 eV above the ground state. The discrepancy from 750 eV to about 1080 eV may be at least partially due to the process of resonant recombination followed by double autoionization which is not included in these calculations. Nevertheless, the overall agreement between theory and experiment has improved, indicating that the initial population of the $3s^23p^33d$ excited configuration is quite high.

3.13 Ni¹³⁺ Results

In Fig. 18 a configuration-average distorted-wave calculation for the $3s^23p^3$ ground configuration of Ni¹³⁺ is presented. The calculation includes the $2p \rightarrow 3p$, $2p \rightarrow 3d$, $2p \rightarrow 4\ell$ ($\ell = 0,1,2,3$), $2s \rightarrow 3p$, and $2s \rightarrow 3d$ excitations and direct ionization of the 3p and 3s subshells.

In Fig. 19 a configuration-average distorted-wave calculation for the $3s^23p^23d$ ground configuration of Ni¹³⁺ is presented. The calculation includes the $3s \rightarrow n\ell$ ($n = 5,6$ and $\ell = 0,1,2$), $2p \rightarrow 3p$, $2p \rightarrow 3d$, $2p \rightarrow 4\ell$ ($\ell = 0,1,2,3$), $2s \rightarrow 3p$, and $2s \rightarrow 3d$ excitations and direct ionization of the 3d, 3p, and 3s subshells. The largest

excitation is $2p \rightarrow 3d$. The ratio of metastable states in the $3s^23p^23d$ excited configuration to all states in the excited and ground configurations is 0.12.

3.14 Ni¹⁴⁺ Results

In Fig. 20 the crossed-beams measurements of Wang, Rinn, and Gregory¹⁵ for Ni¹⁴⁺ are compared with a configuration-average distorted-wave calculation for the $3s^23p^2$ ground configuration. The calculation includes the $2p \rightarrow 3p$, $2p \rightarrow 3d$, $2p \rightarrow n\ell$ ($n = 4,5$ and $\ell = 0,1,2,3$), $2s \rightarrow 3p$, and $2p \rightarrow 3d$ excitations and direct ionization of the 3p and 3s subshells. Although the agreement between experiment and theory is not bad, the experimental onset of ionization appears to occur before the ionization threshold, and the measurements are consistently above the calculated cross section.

In Fig. 21 the crossed-beams measurements of Wang, Rinn, and Gregory¹⁵ for Ni¹⁴⁺ are compared with a configuration-average distorted-wave calculation for the $3s^23p3d$ excited configuration. The calculation includes the $3s \rightarrow 6\ell$ ($\ell = 0,1,2$), $2p \rightarrow 3p$, $2p \rightarrow 3d$, $2p \rightarrow n\ell$ ($n = 4,5$ and $\ell = 0,1,2,3$), $2s \rightarrow 3p$, and $2s \rightarrow 3d$ excitations and direct ionization of the 3d, 3p, and 3s subshells. The largest excitation is $2p \rightarrow 3d$. The ratio of the metastable state 3F_4 in the $3s^23p3d$ excited configuration to all states in the excited and ground configuration is 0.12. The agreement between experiment and theory is now much better. The theory is inside the error bars for the majority of the measurements. The two noticeably high points at 1034 and 1085 eV may be due to the process of resonant recombination followed by double autoionization. The comparison of the experimental measurements with theory in the case of Ni¹⁴⁺ may give the clearest evidence so far that the ECR ion source tends to populate metastable states, even for cases where theory predicts a very low metastable population on the basis of statistics alone.

3.15 Ni¹⁵⁺ Results

In Fig. 22 a configuration-average distorted-wave calculation for the $3s^23p$ ground configuration of Ni¹⁵⁺ is shown. The calculation includes the $2p \rightarrow 3p$, $2p \rightarrow 3d$, $2p \rightarrow n\ell$ ($n = 4,5$ and $\ell = 0,1,2,3$), $2s \rightarrow 3p$, and $2s \rightarrow 3d$ excitations and direct ionization of the 3p and 3s subshells. As can be seen, the excitation-autoionization contributions more than double the cross section by this stage of ionization.

3.16 Ni¹⁶⁺ Results

In Fig. 23 a distorted-wave calculation for the $3s^2$ ground configuration of Ni¹⁶⁺ is presented. The important $2p \rightarrow 3\ell$ ($\ell = 1,2$) excitations are calculated using a multiconfiguration level-to-level method; while the $2p \rightarrow n\ell$ ($n = 4,5$ and $\ell = 0,1,2,3$), $2s \rightarrow 3p$, $2s \rightarrow 3d$, and $2s \rightarrow 4\ell$ ($\ell = 0,1,2$) excitations and direct ionization of the $3s$ and $2p$ subshells are calculated using a configuration-average method. Correlation effects on excitation cross sections and branching ratios are significant for the $2p \rightarrow 3\ell$ excitations.

In Fig. 24 a distorted-wave calculation for the $3s3p$ excited configuration of Ni¹⁶⁺ is presented. The important $2p \rightarrow 3\ell$ ($\ell = 0,1,2$) excitations are calculated using a multiconfiguration level-to-level method; while the $2p \rightarrow n\ell$ ($n = 4,5$ and $\ell = 0,1,2,3$) and $2s \rightarrow n\ell$ ($n = 3,4$ and $\ell = 0,1,2$) excitations and direct ionization of the $3p$, $3s$, $2p$, and $2s$ subshells are calculated using a configuration-average method. As can be seen, in Figs. 23 and 24, the contributions from excitation-autoionization are now quite sizeable; near threshold the total cross section is about 4 times the direct cross section for $3s^2$, while this factor is about 3.5 in the case of $3s3p$.

3.17 Ni¹⁷⁺ Results

In Fig. 25 the multiconfiguration level-to-level distorted-wave results of Griffin, Pindzola, and Bottcher¹¹ for the $3s$ ground configuration of Ni¹⁷⁺ are presented. The calculation includes the $2p \rightarrow 3\ell$ ($\ell = 0,1,2$), $2p \rightarrow n\ell$ ($n = 4,5$ and $\ell = 1,2,3$), $2s \rightarrow 3\ell$ ($\ell = 0,1,2$), and $2s \rightarrow 4\ell$ ($\ell = 0,1,2,3$) excitations and direct ionization of the $3s$, $2p$, and $2s$ subshells. As can be seen, the ratio of the total ionization cross section to the direct ionization contribution is about 7 to 1 near threshold.

3.18 Ni¹⁸⁺ through Ni²⁶⁺ Results

For Ni¹⁸⁺ through Ni²⁶⁺ the contributions of excitation-autoionization to the total ionization cross section from the ground configuration should be less than 5%. For electron ionization from the ground configuration, the direct configuration-average cross section results of Table 1 should give a reasonable estimate of the total cross section and rate coefficient. Work is in progress on cross sections and rates from excited configurations of these same ions.

4. RATE COEFFICIENTS FOR Ni ATOMIC IONS

Rate coefficients for Ni⁺ through Ni¹⁷⁺ were calculated using the theoretical and experimental cross section data discussed in the previous section. The theoretical results are presented in Tables 2-4 and Figs. 26-28, while the experimental results are presented in Table 5 and Fig. 29. The experimental cross section measurements were extrapolated to high energies in order to provide data over a sufficient energy range for these rate coefficient calculations.

In addition to the tabulated values and figure curves, a set of fitting parameters A₀ through A₈ are included in Tables 2-5. The natural logarithms of the rate coefficients are fitted to a Chebyshev polynomial expansion following the method of Cox and Hayes.¹⁶ One can then obtain the rate coefficients for any temperature kT from E_{min} to E_{max} using the equation

$$\alpha(kT) = \exp \left[\frac{A_0}{2} + \sum_{n=1}^8 A_n T_n(x) \right] , \quad (7)$$

where α is in units of cm³/sec, T_n(x) are the Chebyshev polynomials of the first kind,¹⁷ and x is defined by the equation

$$x = \ln \left[\frac{(kT)^2}{E_{\min} E_{\max}} \right] / \ln \left[\frac{E_{\max}}{E_{\min}} \right] , \quad (8)$$

with kT, E_{min}, and E_{max} in units of eV.

Our recommendation for Ni isonuclear rate coefficients is to use the experimental results for Ni⁺, Ni³⁺, Ni⁵⁺, Ni⁶⁺, Ni⁷⁺, Ni⁸⁺, Ni¹²⁺, and Ni¹⁴⁺; the ground configuration theoretical results for Ni²⁺, Ni⁴⁺, Ni⁹⁺, Ni¹⁵⁺, and Ni¹⁷⁺; excited configuration theoretical results for Ni¹⁰⁺, Ni¹¹⁺, Ni¹³⁺, and Ni¹⁶⁺; and the ground configuration direct only theoretical results from Table 1 for Ni¹⁸⁺ through Ni²⁶⁺. These recommended rates are incorporated in a subroutine called NIRATE (Q,TEMP), which will return the rate coefficient in cm³/sec for any ionic charge Q and Temperature, TEMP, in electron volts. It will be available as a library function in directory /256/ATOMIC at the National Magnetic Fusion Energy Computer Center in Livermore, California. A listing of a program, written in BASIC, that produces rates using the given Chebyshev coefficients is found in Table 6.

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Table 1. Direct ionization cross section parameters for ground and excited configurations in units of 10^{-14} ($\text{eV}^2 \cdot \text{cm}^2$)

Ion	Configuration	Subshell	I(eV)	A	B	C	D
Ni ⁺	3s ² 3p ⁶ 3d ⁹	3d	18.15	-3.65	-23.20	25.08	-4.48
Ni ²⁺	3s ² 3p ⁶ 3d ⁸	3d	36.16	5.25	-22.73	32.27	-23.78
Ni ³⁺	3s ² 3p ⁶ 3d ⁷	3d	54.90	55.67	-43.21	31.58	-71.45
		3p	126.52	114.04	-56.05	8.90	-108.80
Ni ⁴⁺	3s ² 3p ⁶ 3d ⁶	3d	79.08	67.81	-39.17	28.85	-75.70
		3p	149.27	86.76	-33.94	10.07	-81.76
Ni ⁵⁺	3s ² 3p ⁶ 3d ⁵	3d	104.21	52.69	-23.15	22.80	-52.98
		3p	173.87	68.58	-20.77	10.88	-61.32
		3s	221.53	14.35	-1.79	2.65	-11.73
Ni ⁶⁺	3s ² 3p ⁶ 3d ⁴	3d	131.35	38.07	-12.40	16.38	-32.16
		3p	200.15	63.13	-17.65	11.35	-52.65
		3s	248.55	13.77	-1.46	2.65	-10.07
Ni ⁷⁺	3s ² 3p ⁶ 3d ³	3d	160.39	29.92	-8.59	10.68	-21.18
		3p	228.02	62.39	-18.22	11.54	-48.89
		3s	277.13	14.99	-2.49	2.64	-10.36
Ni ⁸⁺	3s ² 3p ⁶ 3d ²	3d	191.25	22.05	-6.37	6.09	-13.89
		3p	257.38	62.34	-19.01	11.51	-46.43
		3s	307.18	16.99	-4.05	2.62	-11.62
Ni ⁹⁺	3s ³ 3p ⁶ 3d	3d	223.90	11.83	-3.43	2.58	-6.87
		3p	288.19	62.22	-19.42	11.33	-44.43
		3s	338.64	17.69	-4.81	2.60	-11.79
Ni ¹⁰⁺	3s ² 3p ⁶	3p	320.39	59.96	-18.39	10.01	-4.07
		3s	371.45	17.82	-5.18	2.57	-11.53

Table 1 (Continued)

Ion	Configuration	Subshell	I(eV)	A	B	C	D
Ni ¹⁰⁺	3s ² 3p ⁵ 3d	3d	256.10	12.80	-3.82	2.10	-7.21
		3p	320.34	50.17	-15.40	9.15	-34.07
		3s	368.42	15.94	-4.14	2.55	-9.75
Ni ¹¹⁺	3s ² 3p ⁵	3p	353.67	54.81	-18.06	8.85	-3.76
		3s	402.25	16.73	-4.74	2.51	-10.25
Ni ¹¹⁺	3s ² 3p ⁴ 3d	3d	289.43	12.85	-3.74	1.77	-6.82
		3p	353.46	43.97	-14.50	7.06	-30.13
		3s	399.02	15.73	-4.18	2.48	-9.30
Ni ¹²⁺	3s ² 3p ⁴	3p	387.90	44.35	-14.59	6.80	-2.97
		3s	433.85	14.28	-3.51	2.45	-7.64
Ni ¹²⁺	3s ² 3p ³ 3d	3d	323.87	12.78	-3.60	1.51	-6.43
		3p	387.52	33.40	-11.02	5.09	-22.39
		3s	430.42	14.17	-3.44	2.41	-7.57
Ni ¹³⁺	3s ² 3p ³	3p	423.04	32.29	-10.25	4.89	-2.07
		3s	466.24	16.17	-4.84	2.38	-9.35
Ni ¹³⁺	3s ² 3p ² 3d	3d	359.39	12.87	-3.60	1.29	-6.30
		3p	422.50	21.73	-6.95	3.25	-1.40
		3s	462.62	16.15	-4.86	2.35	-9.37
Ni ¹⁴⁺	3s ² 3p ²	3p	459.11	21.43	-6.70	3.12	-13.38
		3s	499.42	18.67	-6.48	2.31	-11.71
Ni ¹⁴⁺	3s ² 3p3d	3d	396.00	12.91	-3.59	1.12	-6.17
		3p	458.41	10.79	-3.39	1.56	-6.76
		3s	495.61	18.94	-6.66	2.28	-12.02
Ni ¹⁵⁺	3s ² 3p	3p	496.08	11.53	-3.75	1.49	-7.36
		3s	533.36	20.27	-7.75	2.25	-13.16
Ni ¹⁶⁺	3s ²	3s	568.08	17.81	-6.28	2.19	-10.73

Table 1 (Continued)

Ion	Configuration	Subshell	I(eV)	A	B	C	D
Ni ¹⁶⁺	3s3p	3p	530.80	9.56	-2.63	1.40	-5.24
		3s	572.17	8.97	-3.16	1.11	-5.40
Ni ¹⁷⁺	2s ² 2p ⁶ 3s	3s	607.48	9.06	-3.23	1.08	-5.47
		2p	1495.1	74.33	-24.32	10.70	-48.50
		2s	1642.9	16.35	-5.09	3.62	-11.70
Ni ¹⁸⁺	2s ² 2p ⁶	2p	1546.4	71.69	-23.19	10.71	-45.63
		2s	1692.1	16.33	-5.04	3.52	-11.47
Ni ¹⁹⁺	2s ² 2p ⁵	2p	1655.5	61.24	-19.16	7.78	-38.09
		2s	1786.4	16.49	-5.11	3.44	-11.41
Ni ²⁰⁺	2s ² 2p ⁴	2p	1667.6	49.29	-15.28	5.77	-30.11
		2s	1882.9	16.36	-4.97	3.35	-11.09
Ni ²¹⁺	2s ² 2p ³	2p	1882.5	37.12	-11.41	4.02	-22.30
		2s	2179.8	16.08	-4.74	3.26	-10.62
Ni ²²⁺	2s ² 2p ²	2p	2000.3	24.76	-7.54	2.50	-14.64
		2s	2082.6	15.74	-4.47	3.18	-10.13
Ni ²³⁺	2s ² 2p	2p	2121.0	13.41	-3.76	1.16	-7.24
		2s	2185.6	15.52	-4.27	3.09	-9.74
Ni ²⁴⁺	2s ²	2s	2290.9	15.46	-4.18	3.01	-9.52
Ni ²⁵⁺	1s ² 2s	2s	2401.2	7.82	-2.13	1.48	-4.77
		1s	10150	23.37	-9.12	4.02	-19.82
Ni ²⁶⁺	1s ²	1s	10299	23.27	-8.97	3.92	-19.55

Table 2. Theoretical electron-impact ionization rate coefficients for Ni^+ through Ni^{9+} in ground configurations. A_0 through A_8 are Chebyshev fitting parameters which can be used to calculate rate coefficients at any value of kT between E_{\min} and E_{\max} (in eV).

kT (eV)	Ni^+	Ni^{2+}	Ni^{3+}	Ni^{4+}	Ni^{5+}
4	0.377E-09				
7	0.339E-08	0.912E-10			
10	0.837E-08	0.508E-09	0.588E-10		
20	0.252E-07	0.436E-08	0.133E-08	0.433E-09	0.706E-10
40	0.460E-07	0.144E-07	0.698E-08	0.313E-08	0.116E-08
70	0.608E-07	0.253E-07	0.151E-07	0.791E-08	0.403E-08
100	0.683E-07	0.320E-07	0.209E-07	0.118E-07	0.674E-08
200	0.772E-07	0.423E-07	0.310E-07	0.194E-07	0.125E-07
400	0.788E-07	0.470E-07	0.371E-07	0.249E-07	0.168E-07
700	0.760E-07	0.472E-07	0.386E-07	0.269E-07	0.185E-07
1000	0.727E-07	0.459E-07	0.382E-07	0.270E-07	0.187E-07
2000	0.646E-07	0.416E-07	0.352E-07	0.254E-07	0.177E-07
4000	0.555E-07	0.360E-07	0.307E-07	0.224E-07	0.156E-07
7000	0.480E-07	0.312E-07	0.266E-07	0.195E-07	0.136E-07
10000	0.434E-07	0.283E-07	0.241E-07	0.177E-07	0.122E-07
20000	0.351E-07	0.229E-07	0.194E-07	0.142E-07	0.982E-08
A_0	-3.66635E+01	-3.76460E+01	-3.79681E+01	-3.85750E+01	-3.91743E+01
A_1	2.25401E+00	2.27280E+00	2.22173E+00	2.15972E+00	2.01676E+00
A_2	-2.43707E+00	-2.35146E+00	-2.29010E+00	-2.19591E+00	-2.13163E+00
A_3	1.19271E+00	1.08800E+00	1.05141E+00	9.68002E-01	9.64536E-01
A_4	-5.65630E-01	-4.56723E-01	-4.42409E-01	-3.90634E-01	-3.96441E-01
A_5	2.55951E-01	1.77111E-01	1.77389E-01	1.54522E-01	1.54723E-01
A_6	-1.05624E-01	-6.33619E-02	-6.77278E-02	-6.05860E-02	-5.56487E-02
A_7	3.58266E-02	1.96560E-02	2.24215E-02	2.10912E-02	1.64365E-02
A_8	-9.19214E-03	-4.98623E-03	-6.04353E-03	-6.22187E-03	-3.25822E-03
E_{\min}	2.34823E+00	5.02809E+00	7.79442E+00	1.00463E+01	1.47345E+01
E_{\max}	1.00000E+05	1.00000E+05	1.00000E+05	1.00000E+05	1.00000E+05

Table 2 (Continued)

kT (eV)	Ni ⁶⁺	Ni ⁷⁺	Ni ⁸⁺	Ni ⁹⁺
20	0.130E-11	0.241E-11		
40	0.411E-09	0.155E-09	0.461E-10	0.145E-10
70	0.189E-08	0.945E-09	0.401E-09	0.179E-09
100	0.352E-08	0.197E-08	0.961E-09	0.491E-09
200	0.740E-08	0.470E-08	0.270E-08	0.162E-08
400	0.107E-07	0.722E-08	0.451E-08	0.298E-08
700	0.121E-07	0.845E-08	0.548E-08	0.380E-08
1000	0.125E-07	0.880E-08	0.580E-08	0.413E-08
2000	0.121E-07	0.866E-08	0.581E-08	0.435E-08
4000	0.108E-07	0.781E-08	0.529E-08	0.418E-08
7000	0.945E-08	0.687E-08	0.468E-08	0.389E-08
10000	0.858E-08	0.624E-08	0.426E-08	0.368E-08
20000	0.695E-08	0.505E-08	0.346E-08	0.322E-08
A ₀	-3.97758D+01	-4.11488D+01	-4.18260D+01	-4.21495D+01
A ₁	1.90654D+00	2.54999D+00	2.45873D+00	2.59824D+00
A ₂	-2.00215D+00	-2.45092D+00	-2.35509D+00	-2.19817D+00
A ₃	8.99513D-01	1.14157D+00	1.08660D+00	1.04048D+00
A ₄	-3.63967D-01	-4.80538D-01	-4.48140D-01	-4.30821D-01
A ₅	1.38502D-01	1.87510D-01	1.70502D-01	1.56374D-01
A ₆	-4.88968D-02	-6.60528D-02	-5.91575D-02	-5.40717D-02
A ₇	1.44073D-02	1.91574D-02	1.71917D-02	1.72057D-02
A ₈	-2.91663D-03	-3.92451D-03	-3.40225D-03	-3.62183D-03
E _{min}	1.94347D+01	1.83878D+01	2.29468D+01	2.75983D+01
E _{max}	1.00000D+05	1.00000D+05	1.00000D+05	1.00000D+05

Table 3. Theoretical electron-impact ionization rate coefficients for Ni^{10+} through Ni^{17+} in ground configurations. A_0 through A_8 are Chebyshev fitting parameters which can be used to calculate rate coefficients at any value of kT between E_{\min} and E_{\max} (in eV).

kT (eV)	Ni^{10+} ($3p^6$)	Ni^{11+} ($3p^5$)	Ni^{12+} ($3p^4$)	Ni^{13+} ($3p^3$)
70	0.147E-10	0.671E-11	0.299E-11	0.119E-11
100	0.667E-10	0.353E-10	0.183E-10	0.866E-11
200	0.417E-09	0.265E-09	0.167E-09	0.102E-09
400	0.109E-08	0.777E-09	0.542E-09	0.387E-09
700	0.165E-08	0.124E-08	0.908E-09	0.695E-09
1000	0.192E-08	0.148E-08	0.110E-08	0.867E-09
2000	0.219E-08	0.174E-08	0.132E-08	0.107E-08
4000	0.216E-08	0.174E-08	0.133E-08	0.110E-08
7000	0.199E-08	0.162E-08	0.125E-08	0.104E-08
10000	0.185E-08	0.151E-08	0.117E-08	0.975E-09
20000	0.154E-08	0.127E-08	0.978E-09	0.825E-09
A_0	-4.34929D+01	-4.38220E+01	-4.42682E+01	-4.45804E+01
A_1	2.37145D+00	2.29690E+00	2.22281E+00	2.18514E+00
A_2	-2.11061D+00	-2.02628E+00	-1.96603E+00	-1.90788E+00
A_3	8.92249D-01	8.37964E-01	8.03011E-01	7.69567E-01
A_4	-3.32325D-01	-3.02312E-01	-2.82754E-01	-2.60756E-01
A_5	1.12536D-01	9.81709E-02	8.66540E-02	7.17096E-02
A_6	-3.59692D-02	-3.10159E-02	-2.52266E-02	-1.70567E-02
A_7	1.10547D-02	1.02622E-02	8.19505E-03	4.98693E-03
A_8	-3.38784D-03	-3.97595E-03	-3.95725E-03	-3.56403E-03
E_{\min}	4.54271D+01	5.26554E+01	5.99177E+01	6.94518E+01
E_{\max}	1.00000D+05	1.00000E+05	1.00000E+05	1.00000E+05

Table 3 (Continued)

kT (eV)	Ni ¹⁴⁺ (3p ²)	Ni ¹⁵⁺ (3p)	Ni ¹⁶⁺ (3s ²)	Ni ¹⁷⁺ (2s ² 2p ⁶ 3s)
70	0.473E-12	0.167E-12		
100	0.413E-11	0.180E-11	0.614E-12	0.223E-12
200	0.625E-10	0.378E-10	0.206E-10	0.104E-10
400	0.276E-09	0.197E-09	0.138E-09	0.818E-10
700	0.531E-09	0.400E-09	0.312E-09	0.204E-09
1000	0.680E-09	0.522E-09	0.424E-09	0.294E-09
2000	0.860E-09	0.677E-09	0.581E-09	0.445E-09
4000	0.896E-09	0.718E-09	0.638E-09	0.532E-09
7000	0.854E-09	0.692E-09	0.624E-09	0.552E-09
10000	0.806E-09	0.657E-09	0.596E-09	0.545E-09
20000	0.684E-09	0.563E-09	0.516E-09	0.499E-09
A ₀	-4.58933E+01	-4.62552E+01	-4.63945E+01	-4.65892E+01
A ₁	3.00409E+00	2.97346E+00	2.92112E+00	2.28453E+00
A ₂	-2.42796E+00	-2.38466E+00	-2.32119E+00	-2.39389E+00
A ₃	1.00956E+00	9.95441E-01	9.63562E-01	1.14118E+00
A ₄	-3.46325E-01	-3.39889E-01	-3.29972E-01	-4.86274E-01
A ₅	9.35175E-02	8.28793E-02	7.94690E-02	1.84636E-01
A ₆	-2.27503E-02	-9.86203E-03	-4.06391E-03	-5.65652E-02
A ₇	8.17149E-03	-6.46052E-04	-6.27780E-03	1.06504E-02
A ₈	-6.58973E-03	-2.14704E-03	2.54280E-03	2.92630E-03
E _{min}	5.77462E+01	6.57106E+01	7.90307E+01	9.10000E+01
E _{max}	1.00000E+05	1.00000E+05	1.00000E+05	1.00000E+06

Table 4. Theoretical electron-impact ionization rate coefficients for Ni^{10+} through Ni^{14+} and Ni^{16+} in excited configuration. A_0 through A_8 are Chebyshev fitting parameters which can be used to calculate rate coefficients at any value of kT between E_{\min} and E_{\max} (in eV).

kT (eV)	Ni^{10+} ($3p^33d$)	Ni^{11+} ($3p^43d$)	Ni^{12+} ($3p^33d$)	Ni^{13+} ($3p^33d$)
40	0.135E-11			
70	0.303E-10	0.172E-11	0.741E-11	0.307E-11
100	0.113E-09	0.699E-10	0.343E-11	0.170E-10
200	0.568E-09	0.394E-09	0.231E-10	0.145E-09
400	0.134E-08	0.100E-09	0.656E-09	0.473E-09
700	0.194E-08	0.150E-08	0.104E-08	0.798E-09
1000	0.222E-08	0.174E-08	0.124E-08	0.972E-09
2000	0.246E-08	0.198E-08	0.145E-08	0.116E-08
4000	0.238E-08	0.194E-08	0.144E-08	0.117E-08
7000	0.218E-08	0.178E-08	0.134E-08	0.109E-08
10000	0.201E-08	0.165E-08	0.125E-08	0.102E-08
20000	0.167E-08	0.137E-08	0.104E-08	0.857E-09
A_0	-4.33524E+01	-4.36978E+01	-4.42060E+01	-4.45228E+01
A_1	2.40505E+00	2.35247E+00	2.28880E+00	2.21252E+00
A_2	-2.15144E+00	-2.09190E+00	-2.01518E+00	-1.94726E+00
A_3	9.02842E-01	8.65733E-01	8.12960E-01	7.77841E-01
A_4	-3.27903E-01	-3.11149E-01	-2.79648E-01	-2.58932E-01
A_5	1.06287E-01	1.01562E-01	8.53762E-02	7.15809E-02
A_6	-3.16805E-02	-3.24382E-02	-2.69842E-02	-1.96727E-02
A_7	8.90980E-03	1.06369E-02	1.01666E-02	7.56180E-03
A_8	-2.19098E-03	-3.35400E-03	-4.57564E-03	-4.75867E-03
E_{\min}	3.84743E+01	4.29800E+01	4.98190E+01	5.88219E+01
E_{\max}	1.00000E+05	1.00000E+05	1.00000E+05	1.00000E+05

Table 4 (Continued)

kT (eV)	Ni ¹⁴⁺ (3p3d)	Ni ¹⁶⁺ (3s3p)
70	0.133E-11	
100	0.867E-11	0.885E-12
200	0.922E-10	0.244E-10
400	0.346E-09	0.153E-09
700	0.623E-09	0.344E-09
1000	0.777E-09	0.470E-09
2000	0.952E-09	0.655E-09
4000	0.970E-09	0.731E-09
7000	0.914E-09	0.723E-09
10000	0.857E-09	0.694E-09
20000	0.720E-09	0.605E-09
A ₀	-4.57567E+01	-4.62547E+01
A ₁	2.98174E+00	3.06484E+00
A ₂	-2.43670E+00	-2.36139E+00
A ₃	1.00131E+00	9.54352E-01
A ₄	-3.38721E-01	-3.15891E-01
A ₅	9.43743E-02	7.26676E-02
A ₆	-2.85781E-02	-3.27672E-03
A ₇	1.31372E-02	-5.30048E-03
A ₈	-8.53298E-03	9.61339E-04
E _{min}	4.98190E+01	7.34060E+01
E _{max}	1.00000E+05	1.00000E+05

Table 5. Experimental electron-impact ionization rate coefficients for various Ni ions. A_0 through A_8 are Chebyshev fitting parameters used to calculate the rate coefficient at any kT from E_{\min} to E_{\max} (in eV).

kT (eV)	Ni ⁺	Ni ³⁺	Ni ⁵⁺	Ni ⁶⁺	Ni ⁷⁺
10	0.666E-08	0.693E-10	0.365E-12	0.157E-13	0.816E-15
20	0.199E-07	0.112E-08	0.661E-10	0.119E-10	0.224E-11
30	0.302E-07	0.309E-08	0.399E-09	0.116E-09	0.358E-10
40	0.380E-07	0.533E-08	0.101E-08	0.369E-09	0.146E-09
70	0.532E-07	0.115E-07	0.350E-08	0.171E-08	0.907E-09
100	0.620E-07	0.162E-07	0.595E-08	0.325E-08	0.192E-08
150	0.705E-07	0.219E-07	0.924E-08	0.548E-08	0.351E-08
200	0.751E-07	0.257E-07	0.117E-07	0.720E-08	0.480E-08
300	0.793E-07	0.303E-07	0.148E-07	0.957E-08	0.663E-08
400	0.805E-07	0.329E-07	0.166E-07	0.111E-07	0.777E-08
700	0.786E-07	0.358E-07	0.185E-07	0.130E-07	0.921E-08
1000	0.751E-07	0.361E-07	0.185E-07	0.135E-07	0.945E-08
1500	0.699E-07	0.353E-07	0.177E-07	0.132E-07	0.912E-08
2000	0.658E-07	0.342E-07	0.169E-07	0.126E-07	0.860E-08
3000	0.598E-07	0.319E-07	0.154E-07	0.114E-07	0.771E-08
A_0	-3.45059E+01	-3.76222E+01	-4.11200E+01	-4.31480E+01	-4.51200E+01
A_1	1.29314E+00	2.61866E+00	4.39480E+00	5.53320E+00	6.57760E+00
A_2	-8.35410E-01	-1.37880E+00	-2.45420E+00	-3.06310E+00	-3.70010E+00
A_3	2.05560E-01	4.09000E-01	8.40810E-01	1.10400E+00	1.34790E+00
A_4	-6.43491E-02	-1.28846E-01	-2.82720E-01	-3.82580E-01	-4.47220E-01
A_5	2.79552E-02	3.95767E-02	8.78700E-02	1.03060E-01	1.08590E-01
A_6	-6.04574E-03	-7.30130E-03	-1.45300E-02	-1.77800E-02	-4.83000E-03
A_7	3.68188E-04	-3.22187E-04	1.44000E-03	4.86000E-03	-3.67000E-03
A_8	-1.07925E-03	1.06608E-05	-2.37000E-03	-1.70000E-03	9.80000E-04
E_{\min}	7.00000E+00	1.00000E+01	1.00000E+01	1.00000E+01	1.00000E+01
E_{\max}	3.00000E+03	3.00000E+03	3.00000E+03	3.00000E+03	3.00000E+03

Table 5 (Continued)

kT (eV)	Ni ⁸⁺	Ni ¹²⁺	Ni ¹⁴⁺
10	0.254E-15		
20	0.446E-12		
30	0.990E-11		
40	0.499E-10		
70	0.413E-09	0.621E-11	0.834E-12
100	0.980E-09	0.318E-10	0.669E-11
150	0.197E-08	0.120E-09	0.360E-10
200	0.283E-08	0.241E-09	0.870E-10
300	0.413E-08	0.500E-09	0.218E-09
400	0.500E-08	0.729E-09	0.348E-09
700	0.637E-08	0.118E-08	0.619E-09
1000	0.694E-08	0.141E-08	0.752E-09
1500	0.718E-08	0.156E-08	0.832E-09
2000	0.703E-08	0.160E-08	0.839E-09
3000	0.655E-08	0.155E-08	0.799E-09
A ₀	-4.66390E+01	-4.46378E+01	-4.68830E+01
A ₁	7.30100E+00	3.13794E+00	3.91127E+00
A ₂	-3.82440E+00	-1.36974E+00	-1.77077E+00
A ₃	1.28820E+00	3.25212E-01	4.27401E-01
A ₄	-3.09730E-01	-7.66653E-02	-9.63996E-02
A ₅	-1.92400E-02	1.75100E-02	2.75672E-02
A ₆	6.31500E-02	-3.79199E-03	-8.64076E-03
A ₇	-3.70500E-02	5.90838E-04	2.79192E-03
A ₈	1.44800E-02	7.40489E-04	4.98384E-04
E _{min}	1.00000E+01	5.50000E+01	5.50000E+01
E _{max}	3.00000E+03	3.00000E+03	3.00000E+03

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Table 6. Sample BASIC program to calculate rate coefficients from Chebyshev fitting parameters

```
10  REM PROGRAM CHEBFE
20  REM CHBFIT PROGRAM IS A BASIC PROGRAM DERIVED FROM A PROGRAM IN
30  REM "ELEMENTARY NUMERICAL ANALYSIS: AN ALGORITHMIC APPROACH",S.D. CONTE
40  REM AND C. DE BOOR, MCGRAW-HILL, INC., P 254, 1972.
50  DIM D(9)
60  NTERMS=9
70  INPUT"ENTER Emin (eV) ",EMIN:INPUT"ENTER Emax (eV) ",EMAX
80  EMINL=LOG(EMIN)
90  EMAXL=LOG(EMAX)
100 PRINT USING "ENTER # COEFFICIENTS A0 THROUGH A8; NTERMS
110 FOR J=1 TO NTERMS
120 INPUT D(J):NEXT J
130 PRINT USING "INPUT ENERGY (eV) BETWEEN ###.# AND ##.#... FOR THE RATE COEF.
CALCULATION";EMIN;EMAX
140 REM GET ENERGY FOR CALCULATION AND USE THREE TERM RECURRENCE RELATION
150 INPUT X
160 K=NTERMS
170 CHEB=D(K)
180 IF X<0 THEN END
190 X=LOG(X)
200 K=K-1
210 IF K=0 THEN END
220 XNORM=(X-EMINL-(EMAXL-X))/(EMAXL-EMINL)
230 TWOX=2*XNORM
240 PREV2=0
250 PREV=CHEB
260 IF K=1 GOTO 310
270 CHEB=D(K)+TWOX*PREV-PREV2
280 PREV2=PREV
290 K=K-1
300 GOTO 250
310 CHEB=.5*D(1)+XNORM*PREV-PREV2
320 PRINT USING "###.#... = RATE CHEB=EXP(CHEB) COEFFICIENT (CM3/S)";CHEB
330 GOTO 130
340 END
```

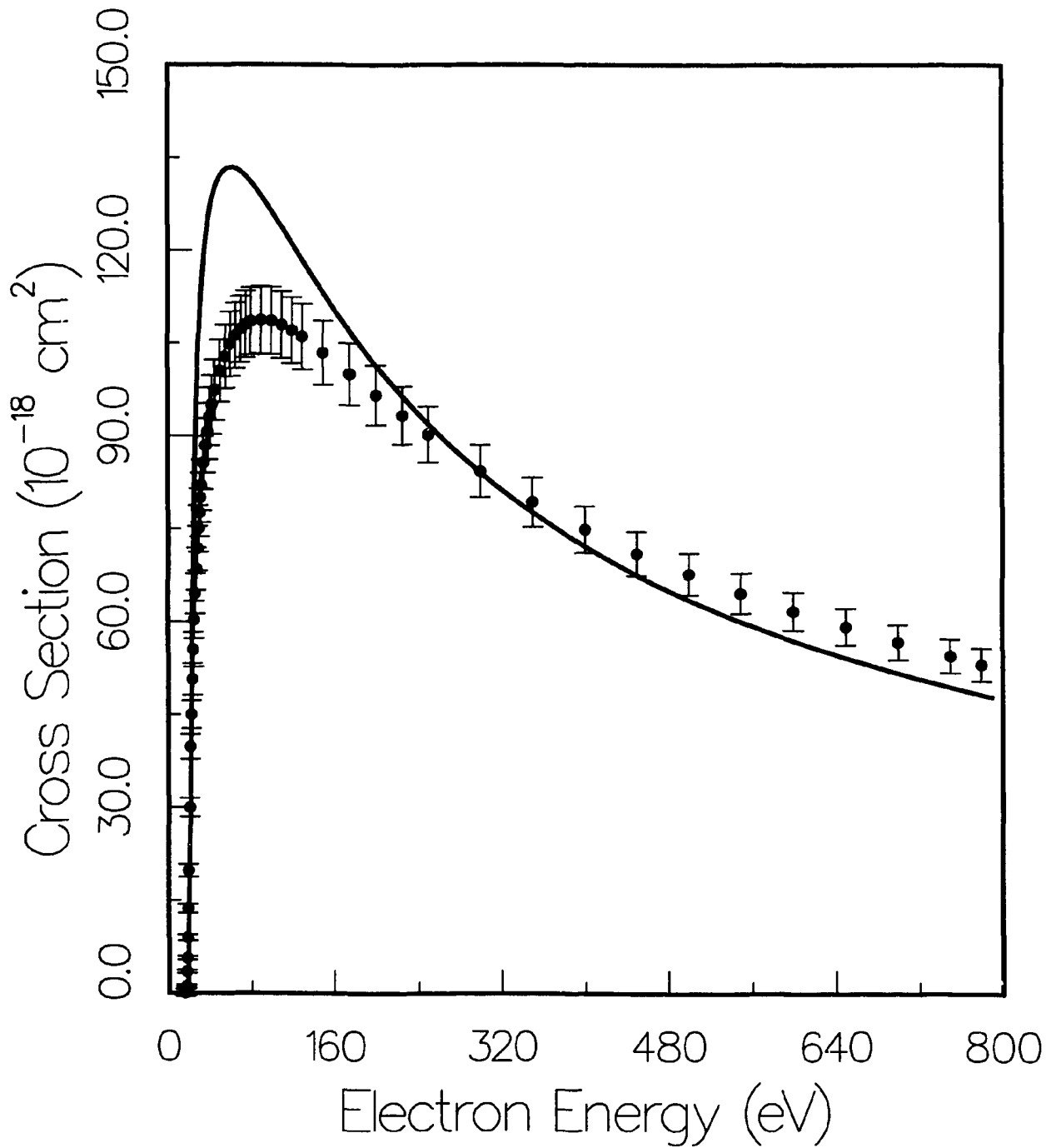
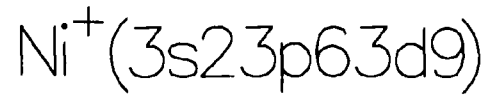


Fig. 1. Electron-impact ionization of Ni⁺. Full curve, configuration-average direct ionization cross section from the 3d⁹ ground configuration; experimental points (ref. 12).

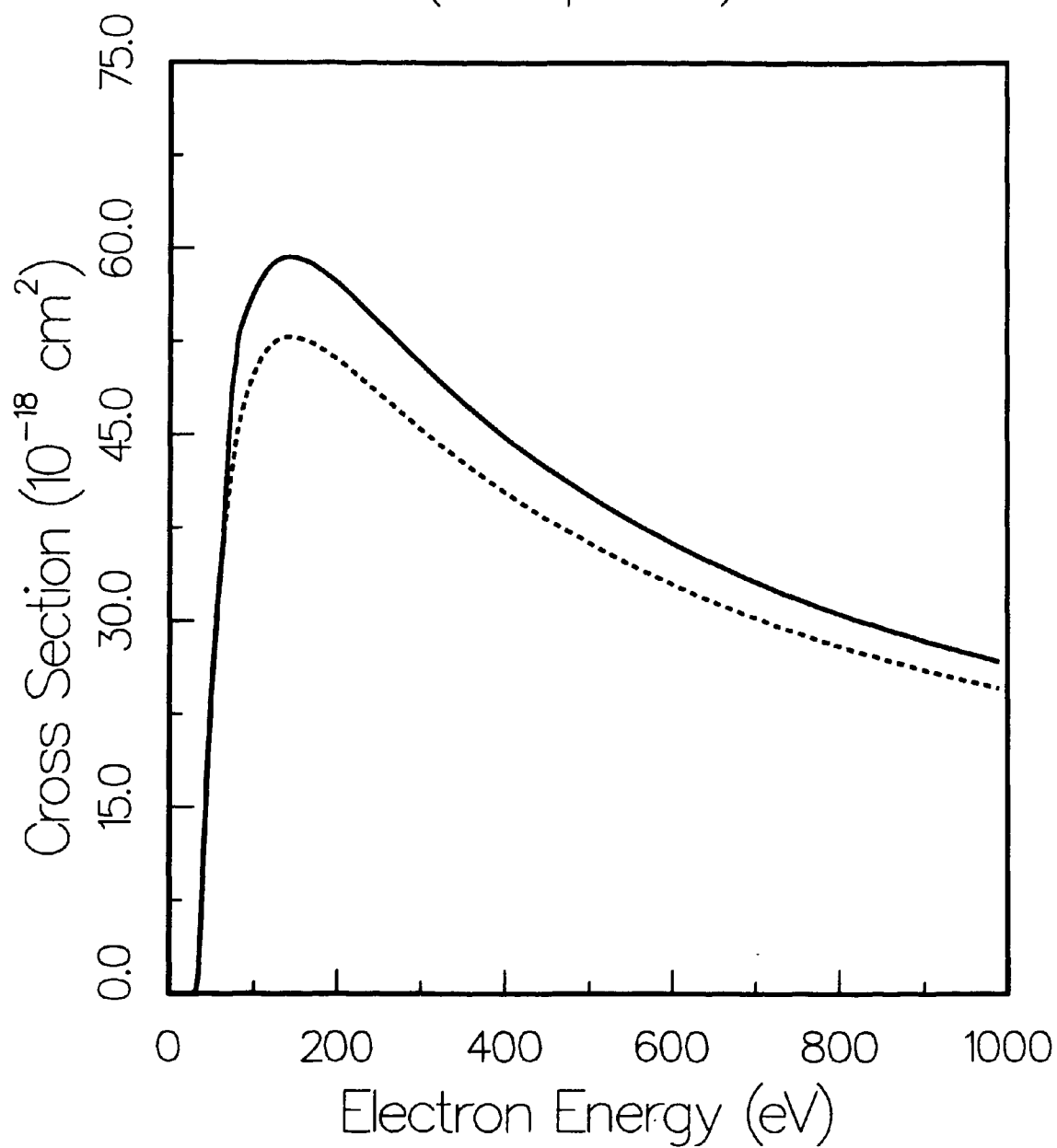
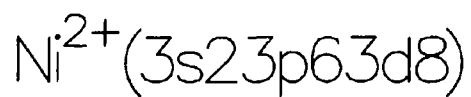


Fig. 2. Electron-impact ionization of Ni^{2+} . Full curve, configuration-average total ionization cross section from the $3d^8$ ground configuration; dashed curve, direct ionization cross section only.

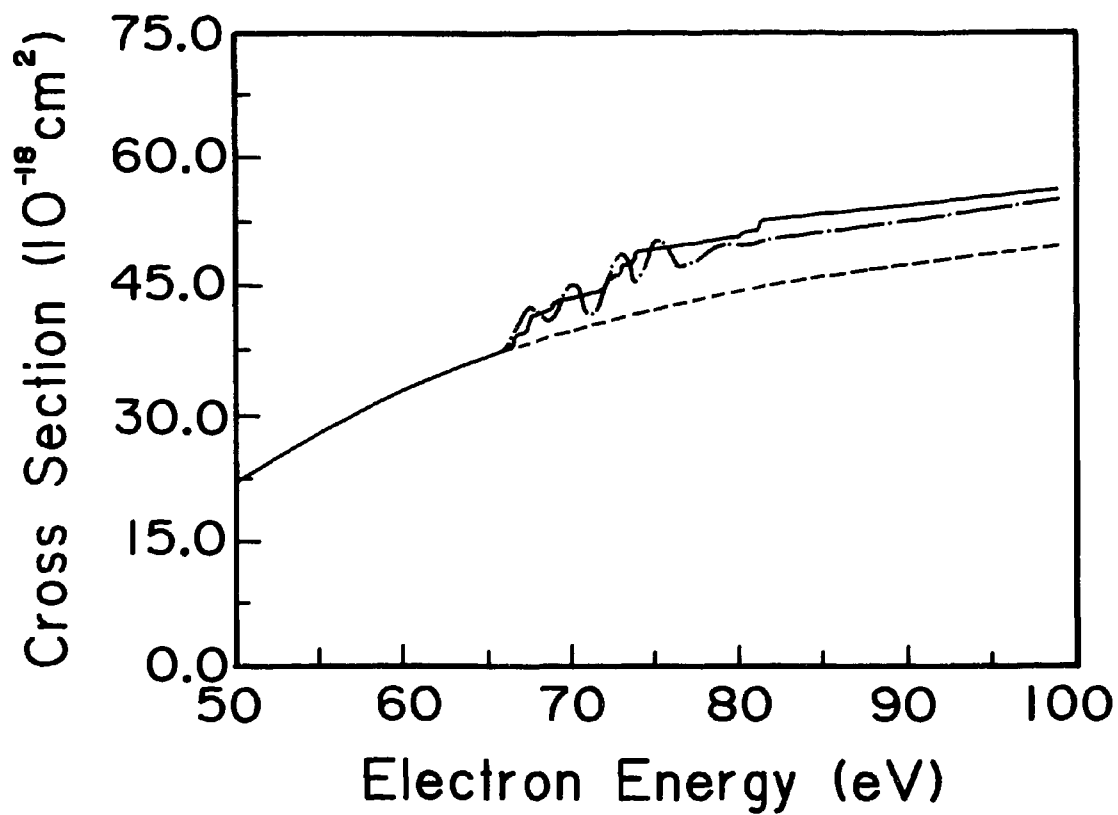


Fig. 3. Electron-impact ionization of Ni^{2+} below 100 eV. Full curve, configuration-average total ionization cross section from the $3d^8$ ground configuration; chained curve, R-matrix calculation (ref. 13); dashed curve, direct ionization cross section only.

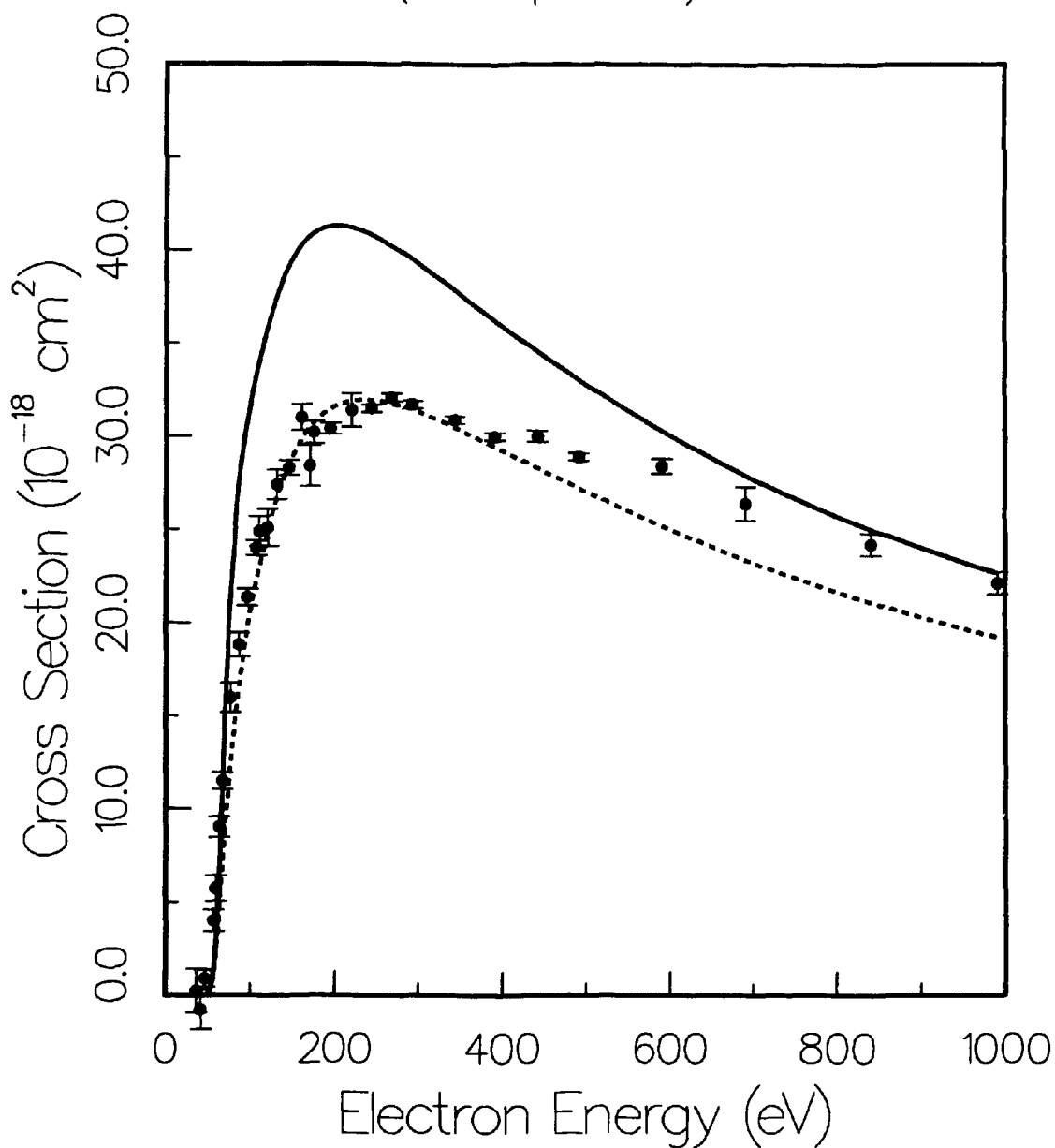
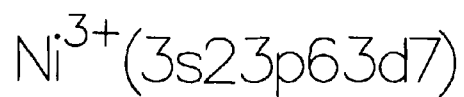


Fig. 4. Electron-impact ionization of Ni^{3+} . Full curve, configuration-average total ionization cross section from the $3d^7$ ground configuration; dashed curve, direct ionization cross section only; experimental points (ref. 14).

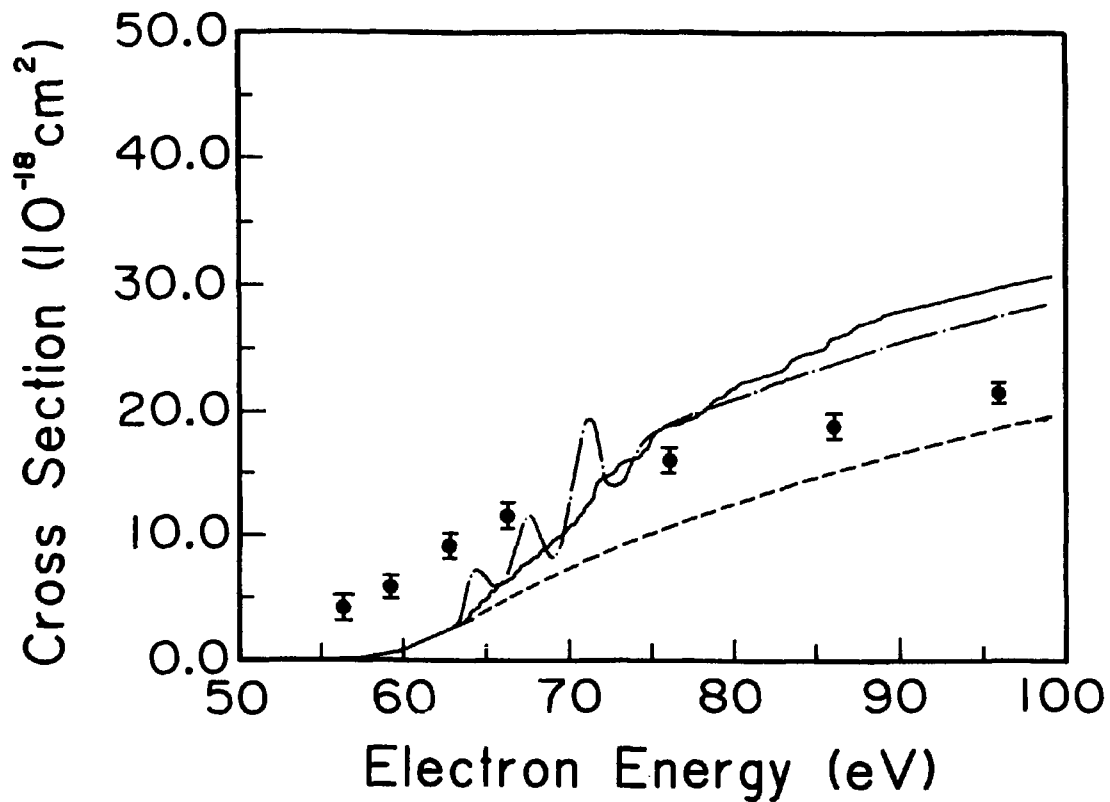


Fig. 5. Electron-impact ionization of Ni^{3+} below 100 eV. Full curve, configuration-average total ionization cross section from the $3d^7$ ground configuration; chained curve, R-matrix calculation (ref. 13); dashed curve, direct ionization cross section only; experimental points (ref. 14).

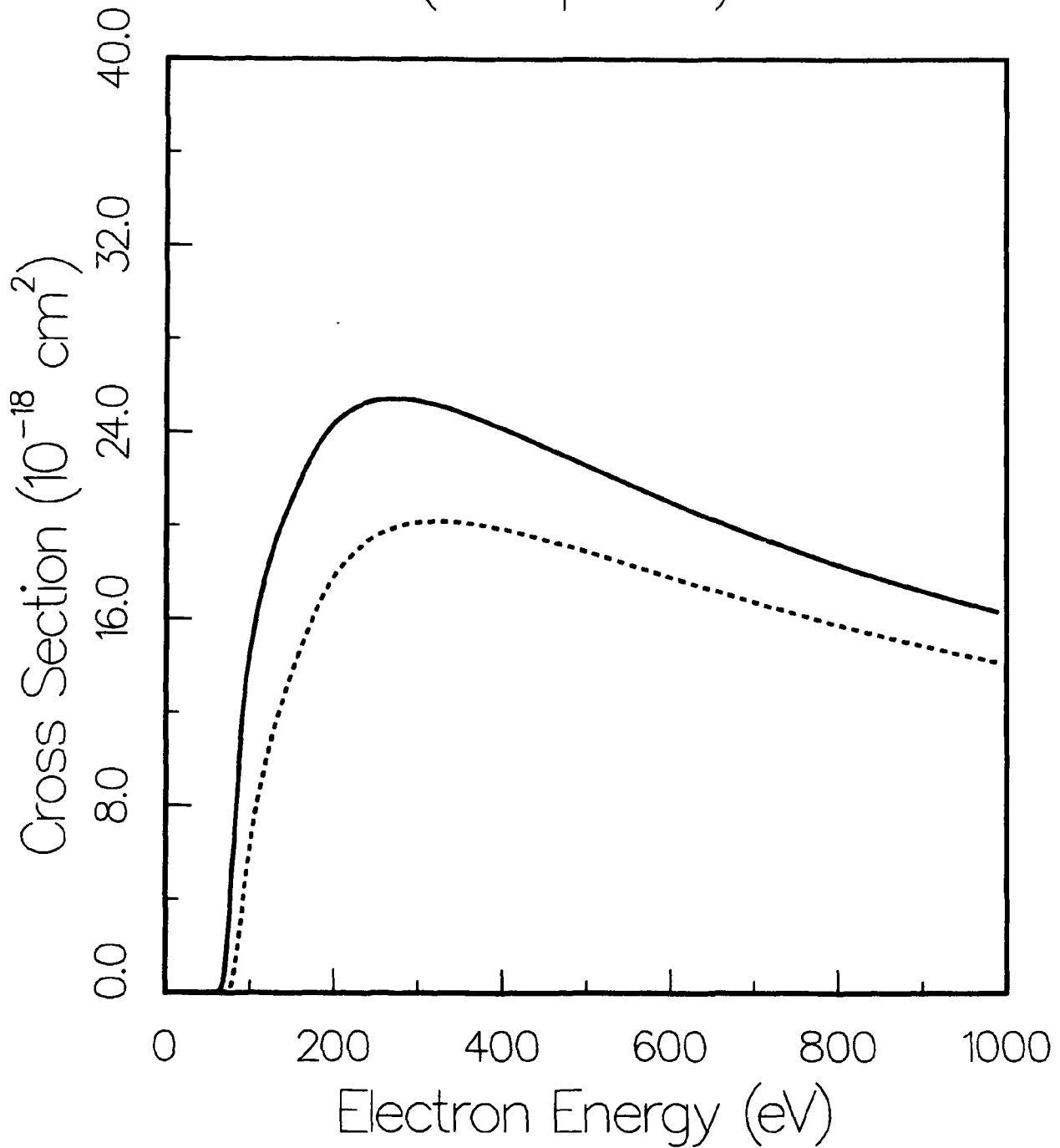
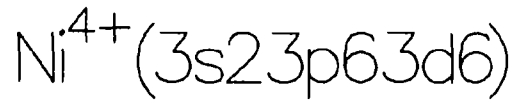


Fig. 6. Electron-impact ionization of Ni^{4+} . Full curve, configuration-average total ionization cross section from the $3d^6$ ground configuration; dashed curve, direct ionization cross section only.

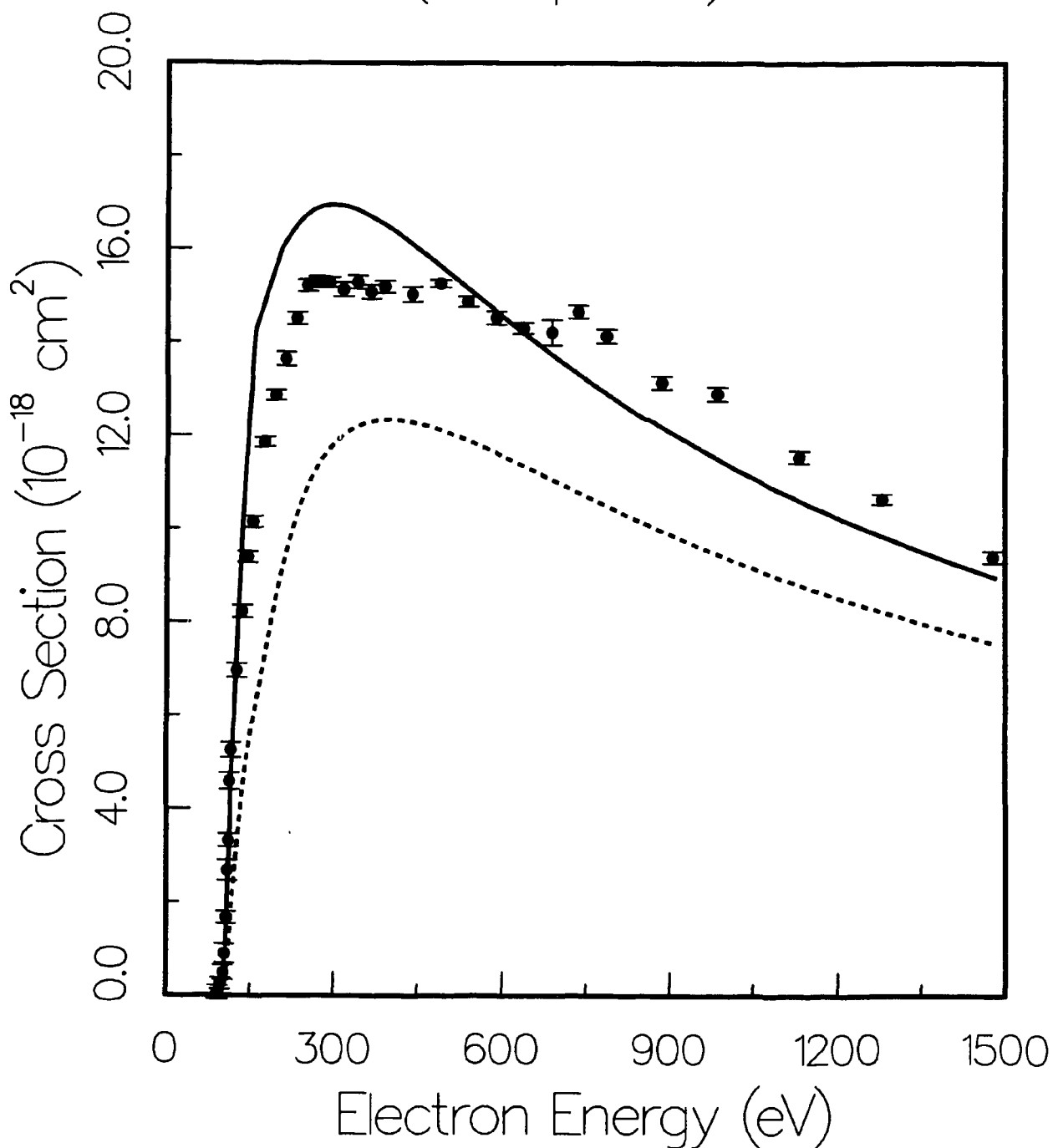
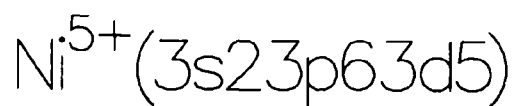


Fig. 7. Electron-impact ionization of Ni^{5+} . Full curve, configuration-average total ionization cross section from the $3d^5$ ground configuration; dashed curve, direct ionization cross section only; experimental points (ref. 15).

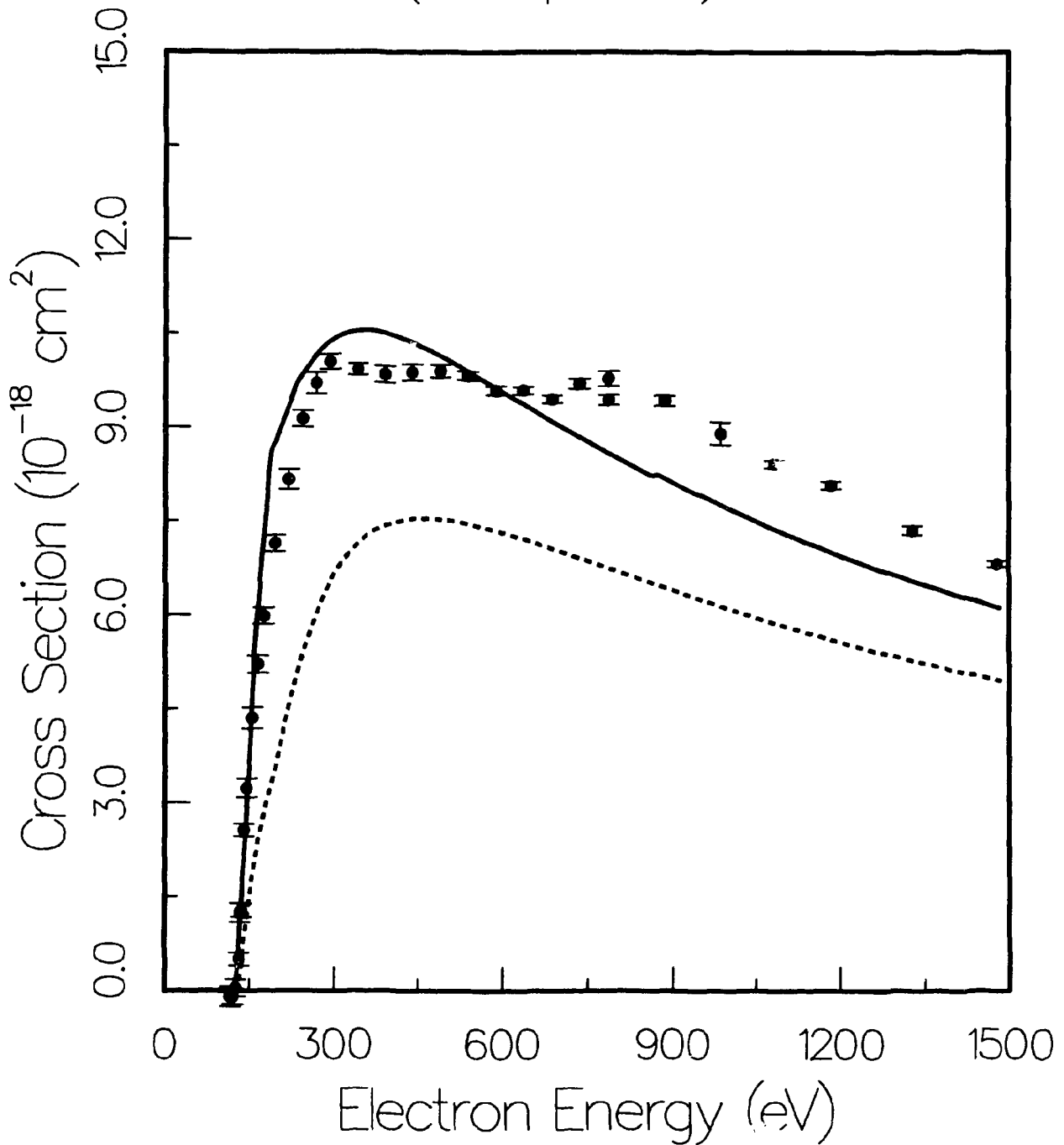
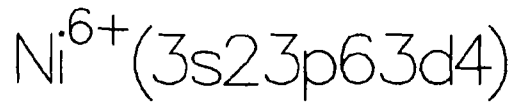


Fig. 8. Electron-impact ionization of Ni^{6+} . Full curve, configuration-average total ionization cross section from the $3d^4$ ground configuration; dashed curve, direct ionization cross section only; experimental points (ref. 15).

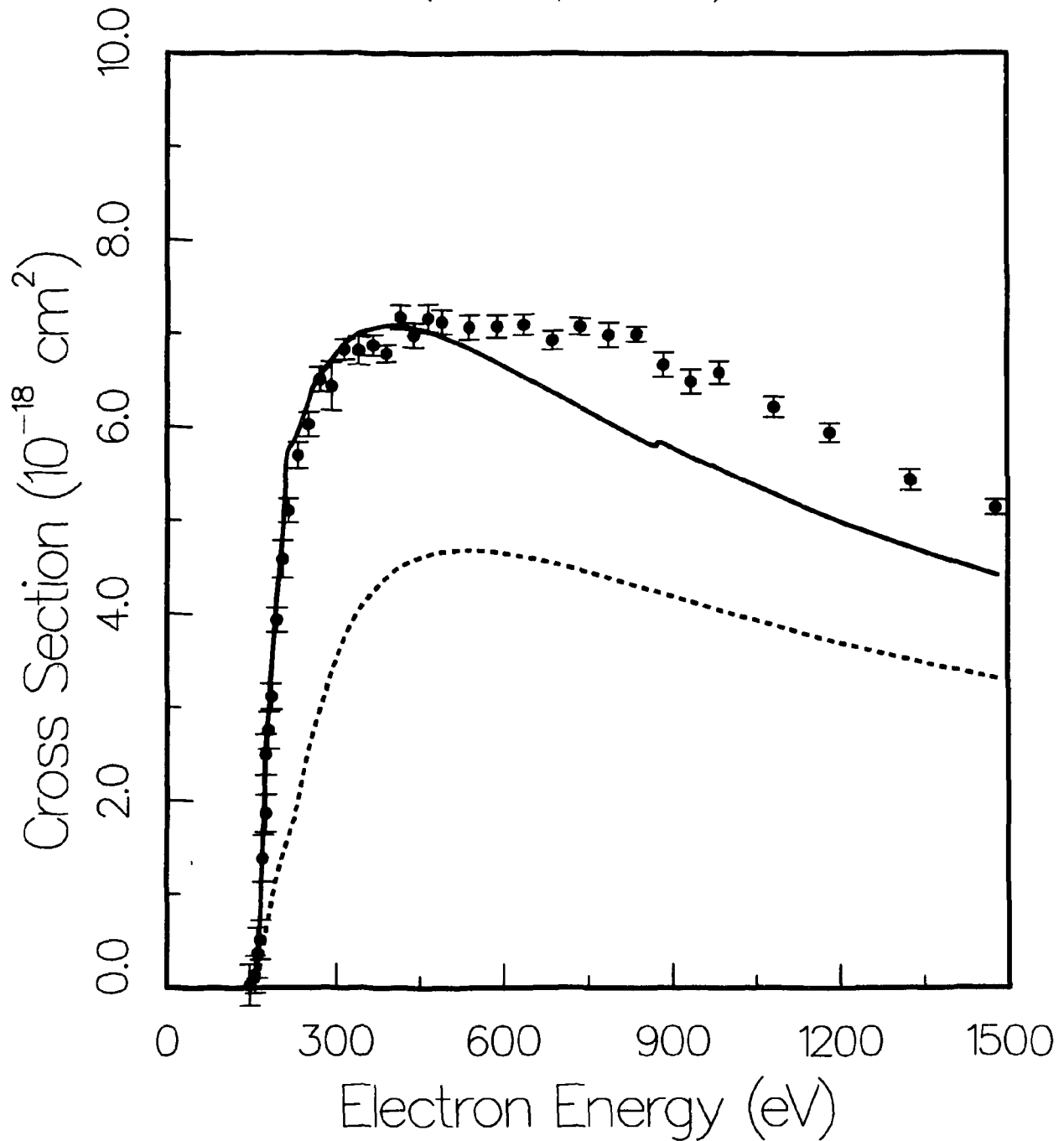
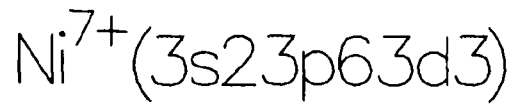


Fig. 9. Electron-impact ionization of Ni^{7+} . Full curve, configuration-average total ionization cross section from the $3d^3$ ground configuration; dashed curve, direct ionization cross section only; experimental points (ref. 15).

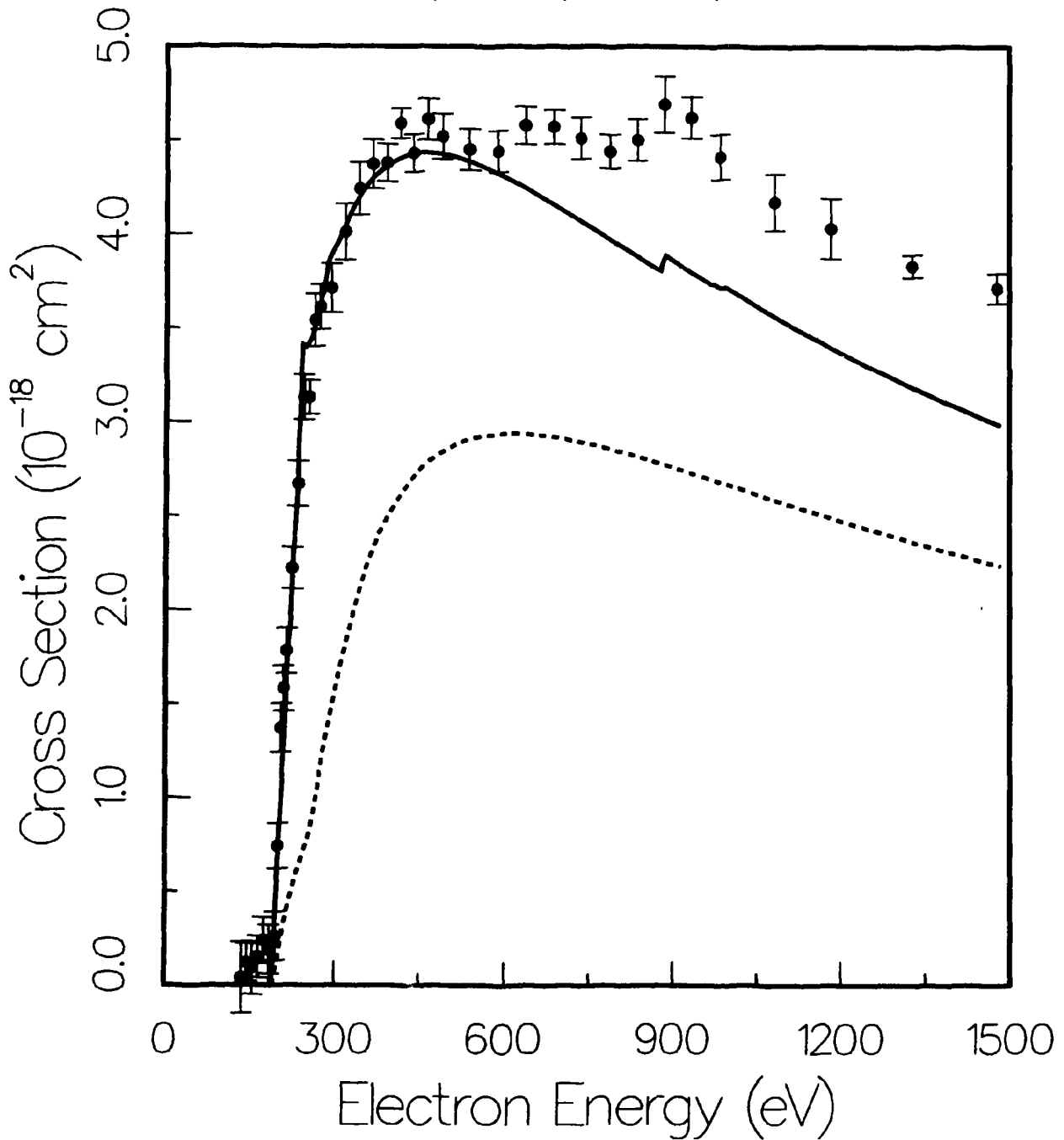
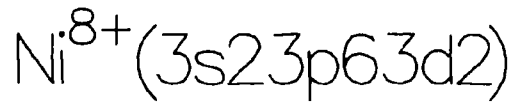


Fig. 10. Electron-impact ionization of Ni^{8+} . Full curve, configuration-average total ionization cross section from the $3d^2$ ground configuration; dashed curve, direct ionization cross section only; experimental points (ref. 15).

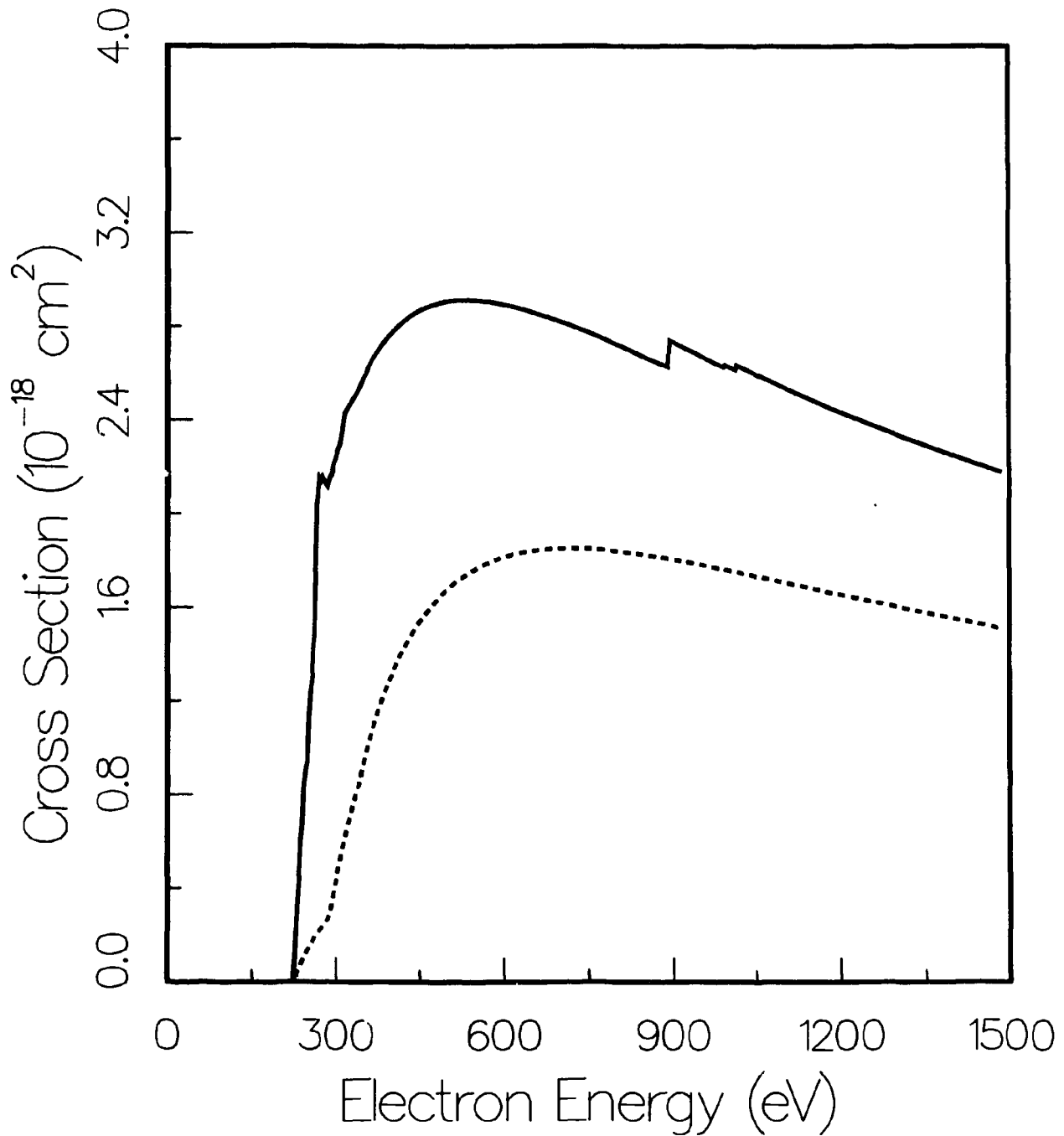
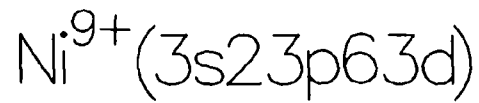


Fig. 11. Electron-impact ionization of Ni^{9+} . Full curve, configuration-average total ionization cross section from the 3d ground configuration; dashed curve, direct ionization cross section only.

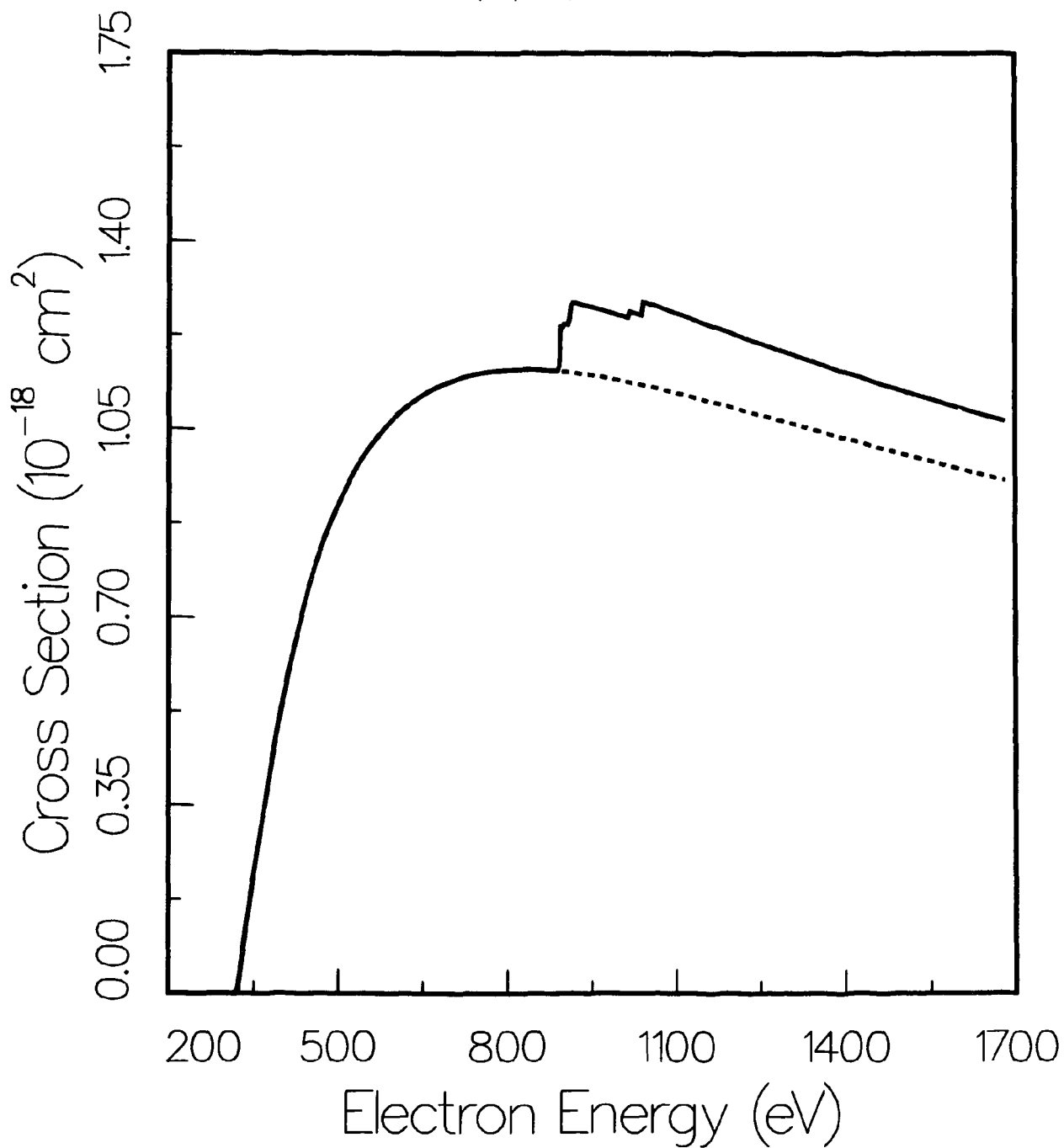
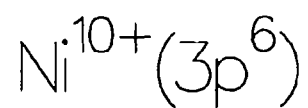


Fig. 12. Electron-impact ionization of Ni^{10+} . Full curve, configuration-average total ionization cross section from the $3p^6$ ground configuration; dashed curve, direct ionization cross section only.

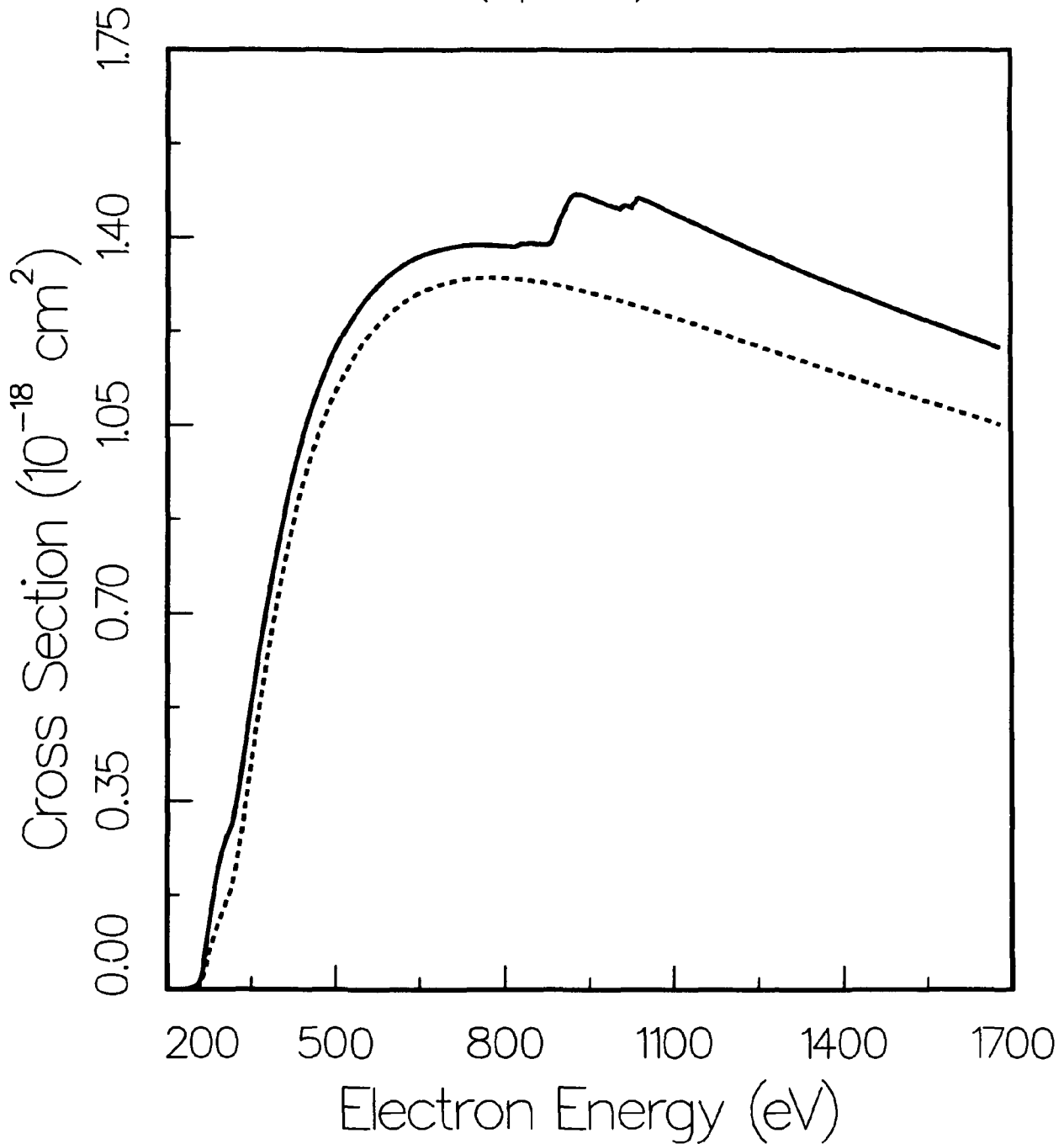
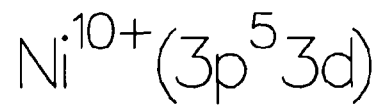


Fig. 13. Electron-impact ionization of Ni^{10+} . Full curve, configuration-average total ionization cross section from the $3p^5 3d$ excited configuration; dashed curve, direct ionization cross section only.

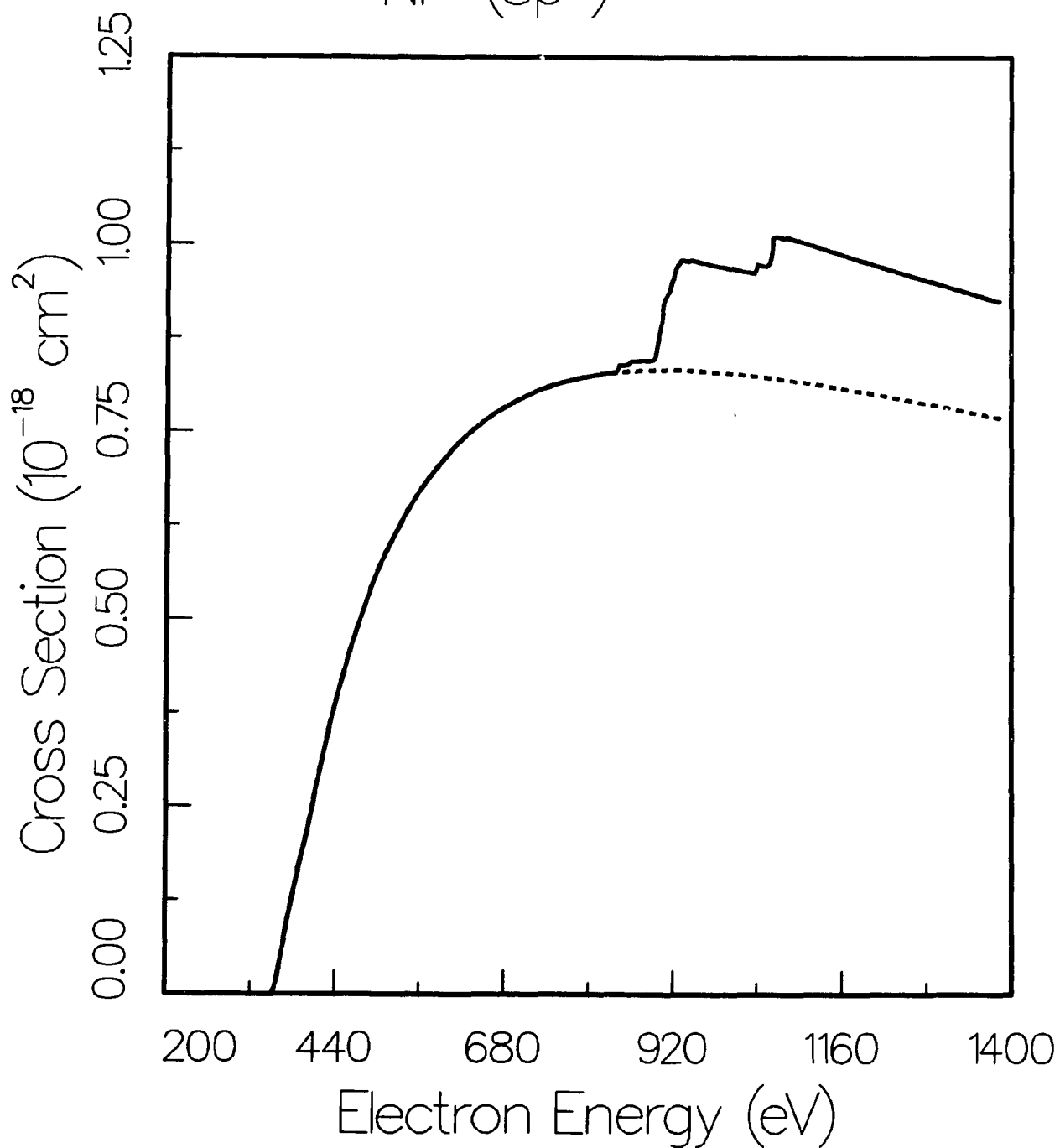
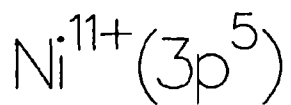


Fig. 14. Electron-impact ionization of Ni^{11+} . Full curve, configuration-average total ionization cross section from the $3p^5$ ground configuration; dashed curve, direct ionization cross section only.

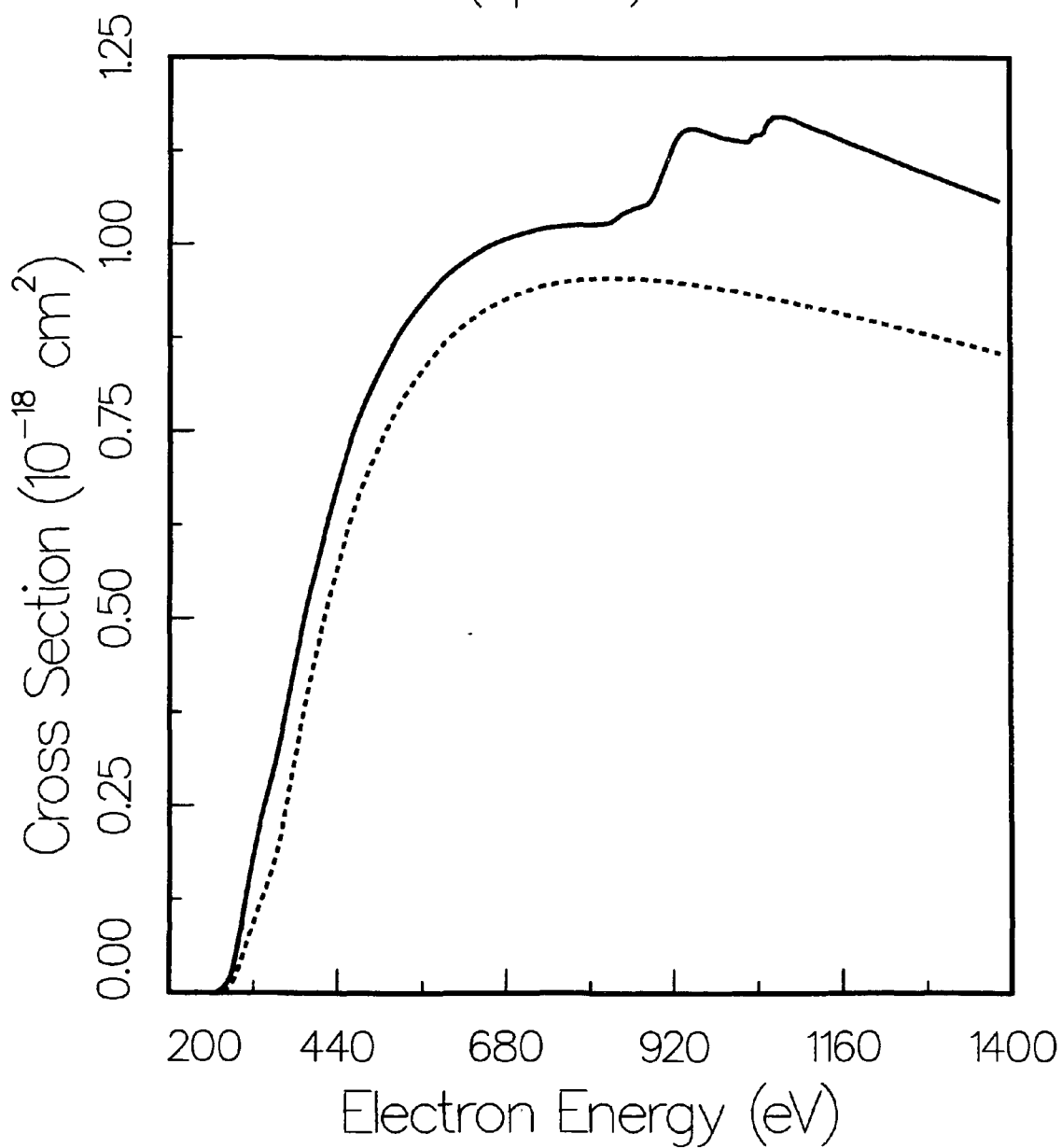
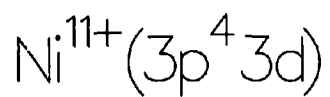


Fig. 15. Electron-impact ionization of Ni^{11+} . Full curve, configuration-average total ionization cross section from the $3p^4 3d$ excited configuration; dashed curve, direct ionization cross section only.

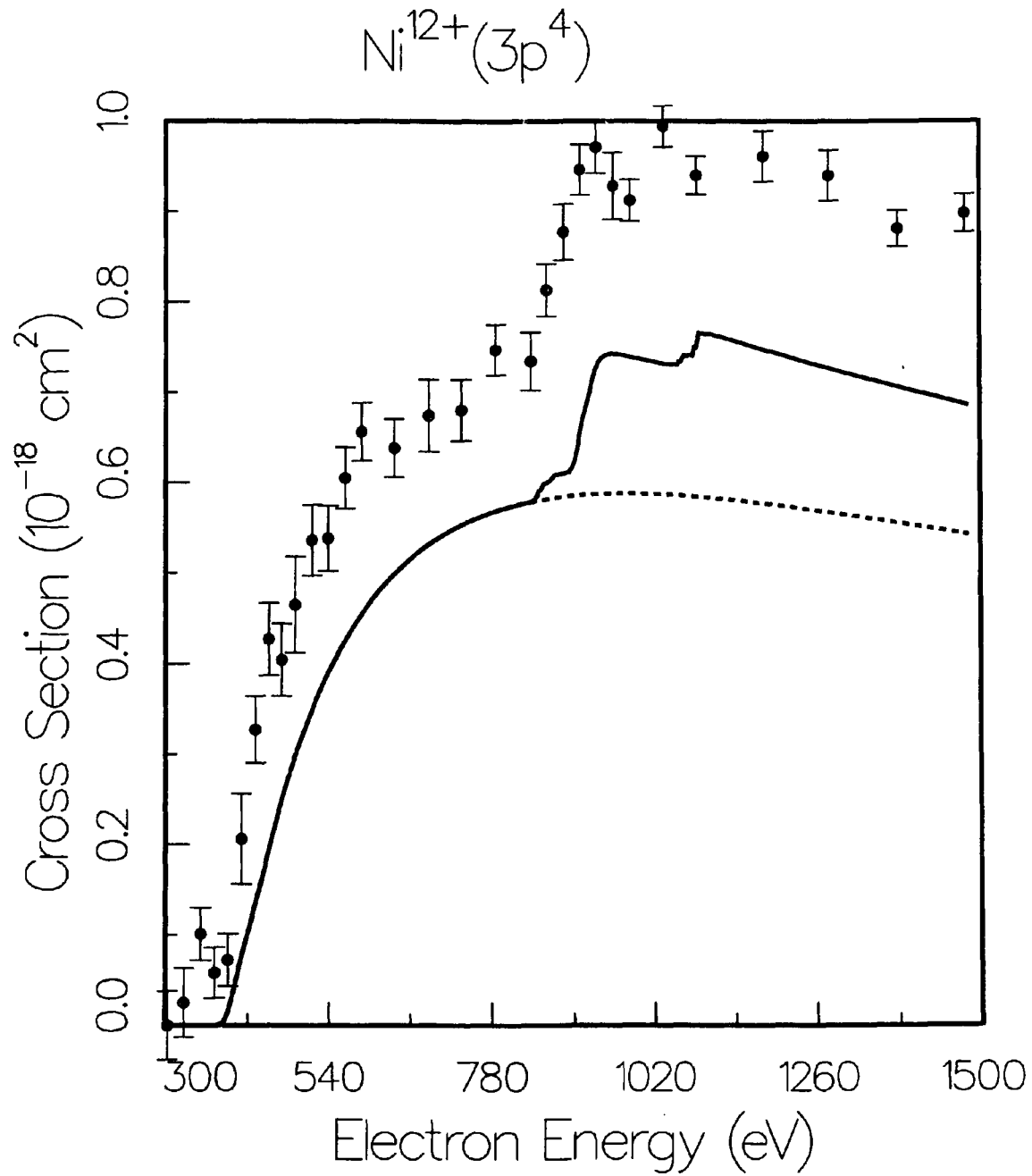


Fig. 16. Electron-impact ionization of Ni^{12+} . Full curve, configuration-average total ionization cross section from the $3p^4$ ground configuration; dashed curve, direct ionization cross section only; experimental points (ref. 15).

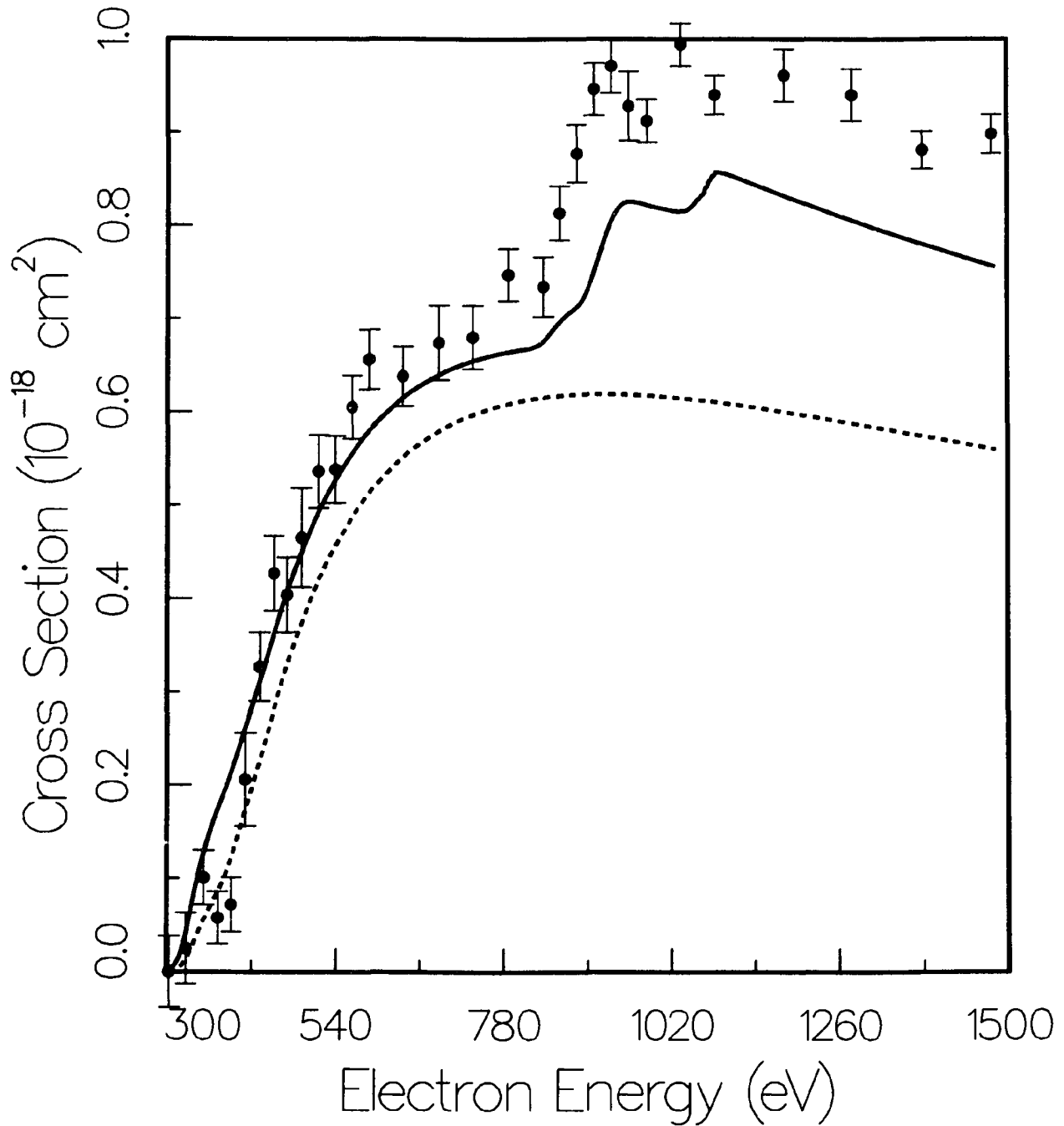
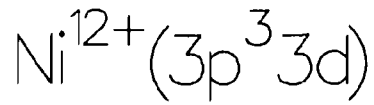


Fig. 17. Electron-impact ionization of Ni^{12+} . Full curve, configuration-average total ionization cross section from the $3p^3 3d$ excited configuration; dashed curve, direct ionization cross section only; experimental points (ref. 15).

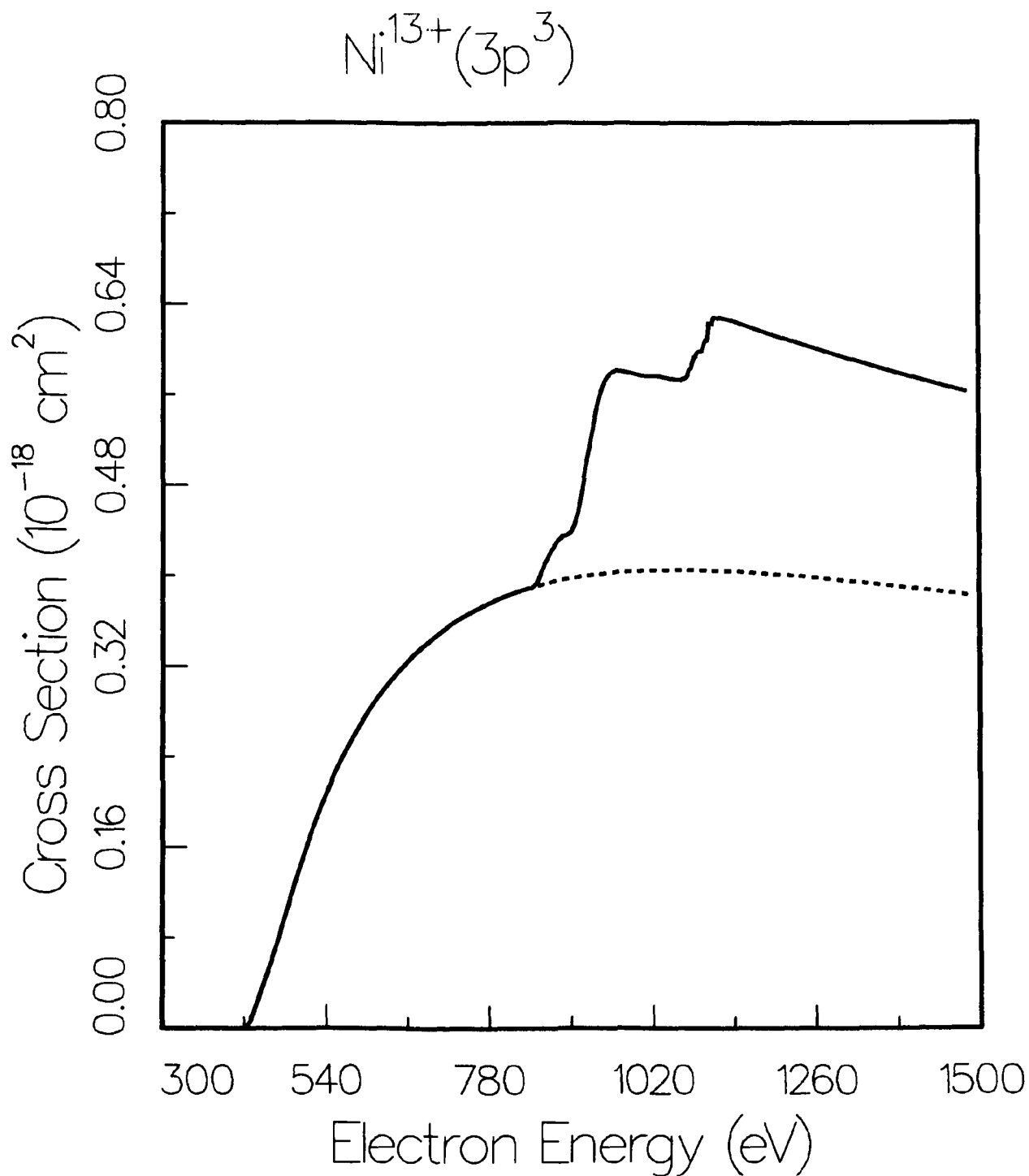


Fig. 18. Electron-impact ionization of Ni^{13+} . Full curve, configuration-average total ionization cross section from the $3p^3$ ground configuration; dashed curve, direct ionization cross section only.

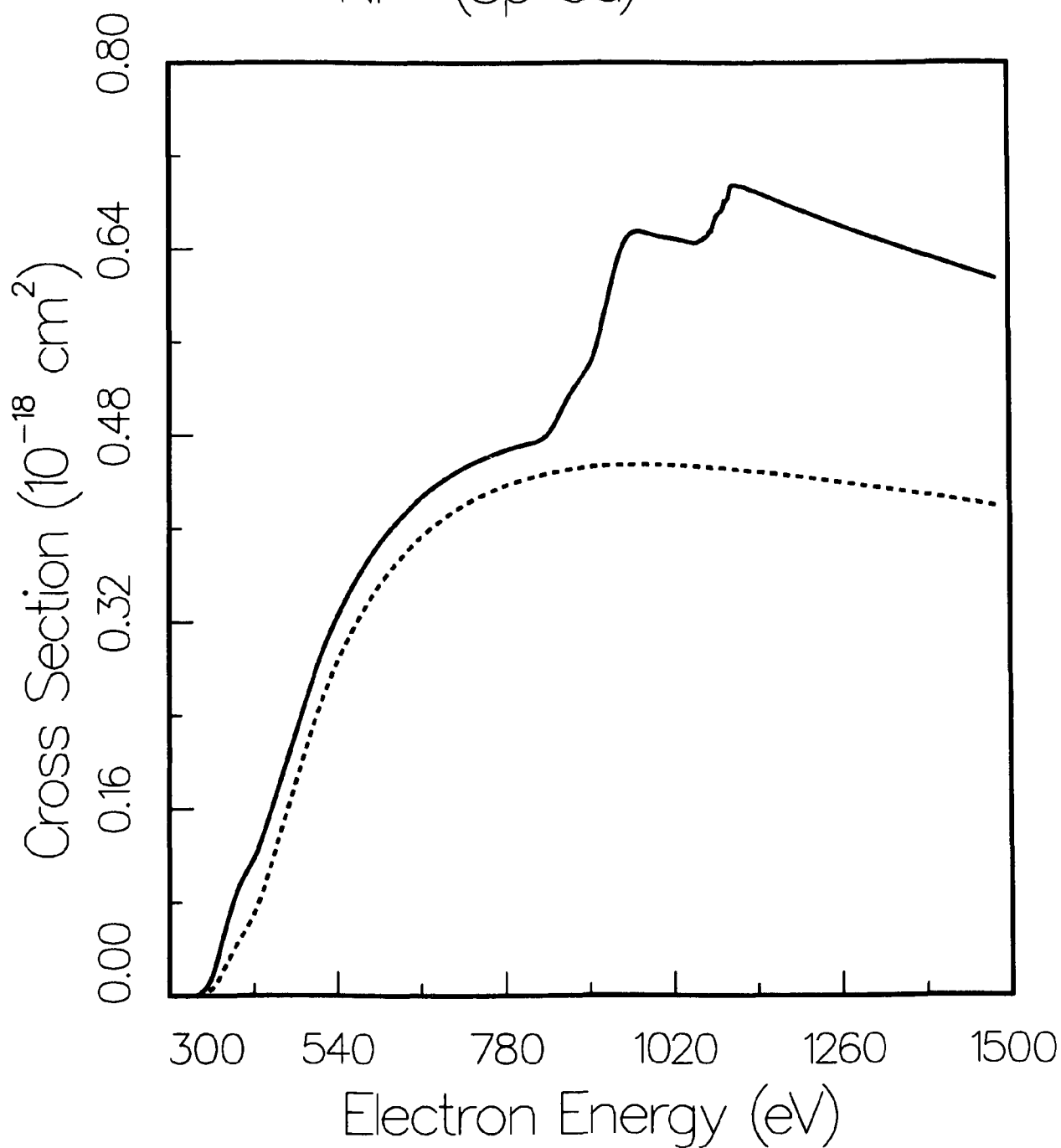
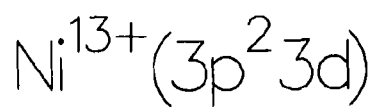


Fig. 19. Electron-impact ionization of Ni^{13+} . Full curve, configuration-average total ionization cross section from the $3p^2 3d$ excited configuration; dashed curve, direct ionization cross section only.

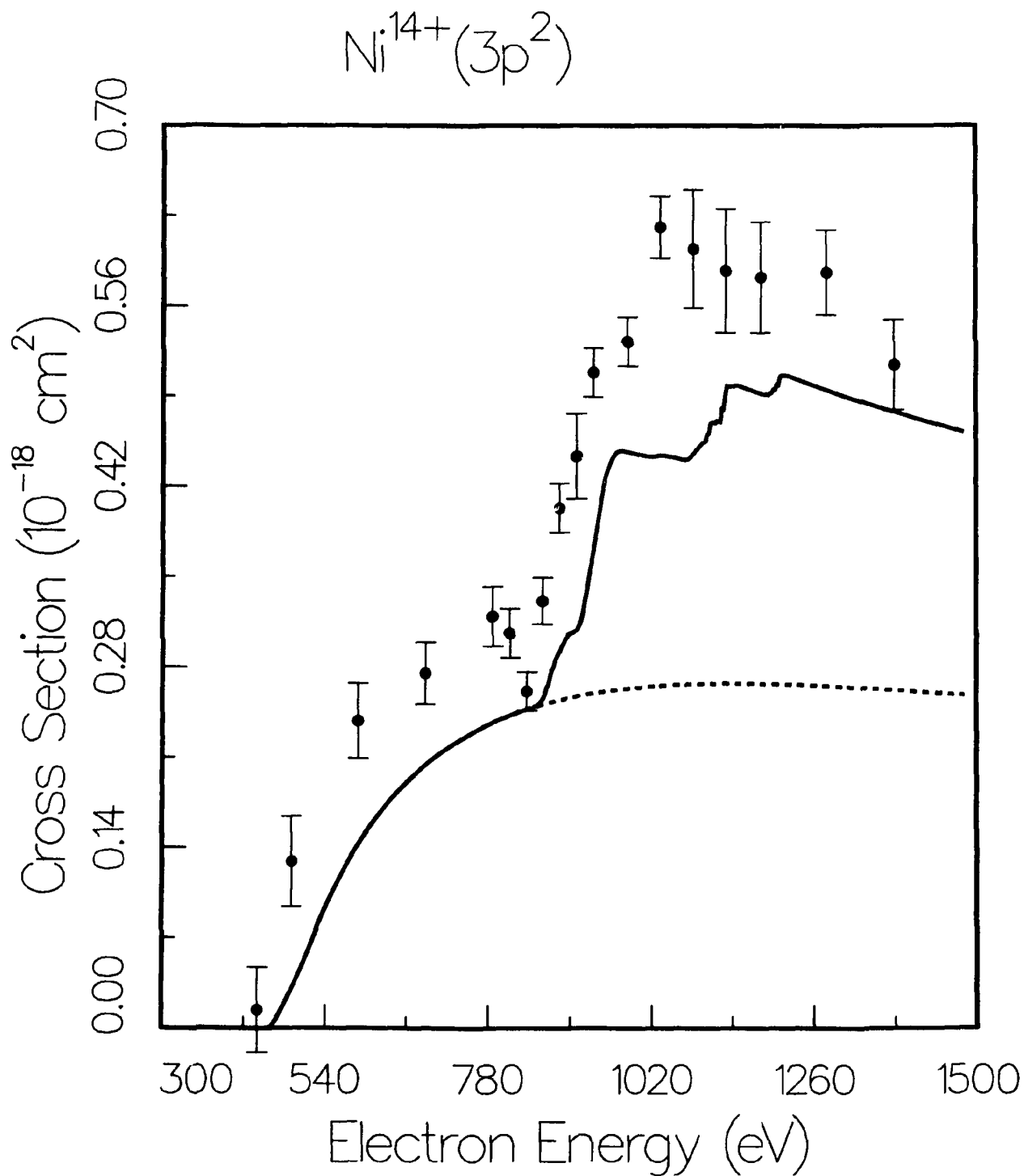


Fig. 20. Electron-impact ionization of Ni^{14+} . Full curve, configuration-average total ionization cross section from the $3p^2$ ground configuration; dashed curve, direct ionization cross section only; experimental points (ref. 15).

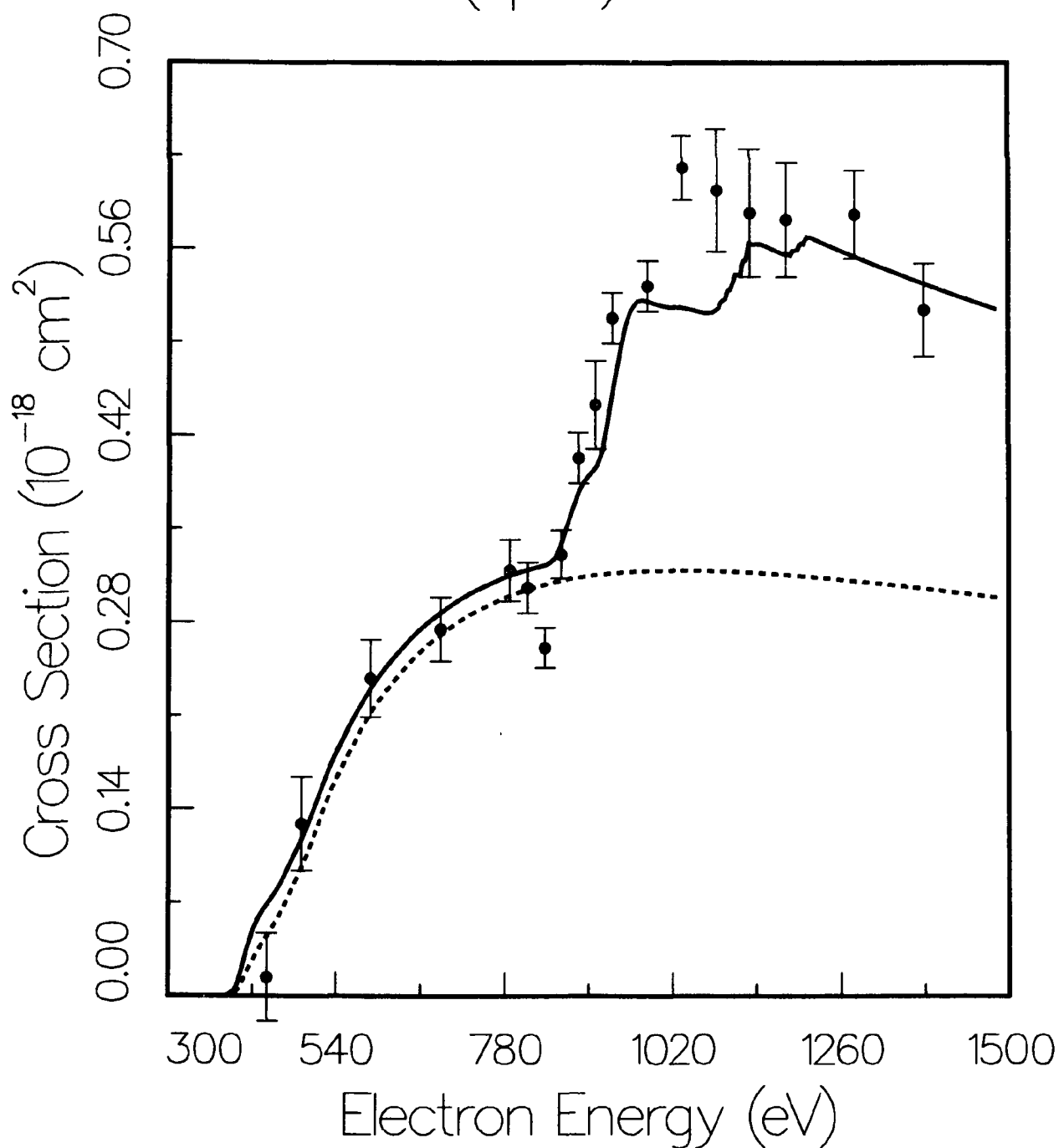
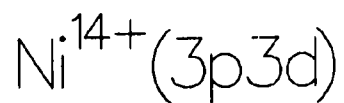


Fig. 21. Electron-impact ionization of Ni^{14+} . Full curve, configuration-average total ionization cross section from the 3p3d excited configuration; dashed curve, direct ionization cross section only; experimental points (ref. 15).

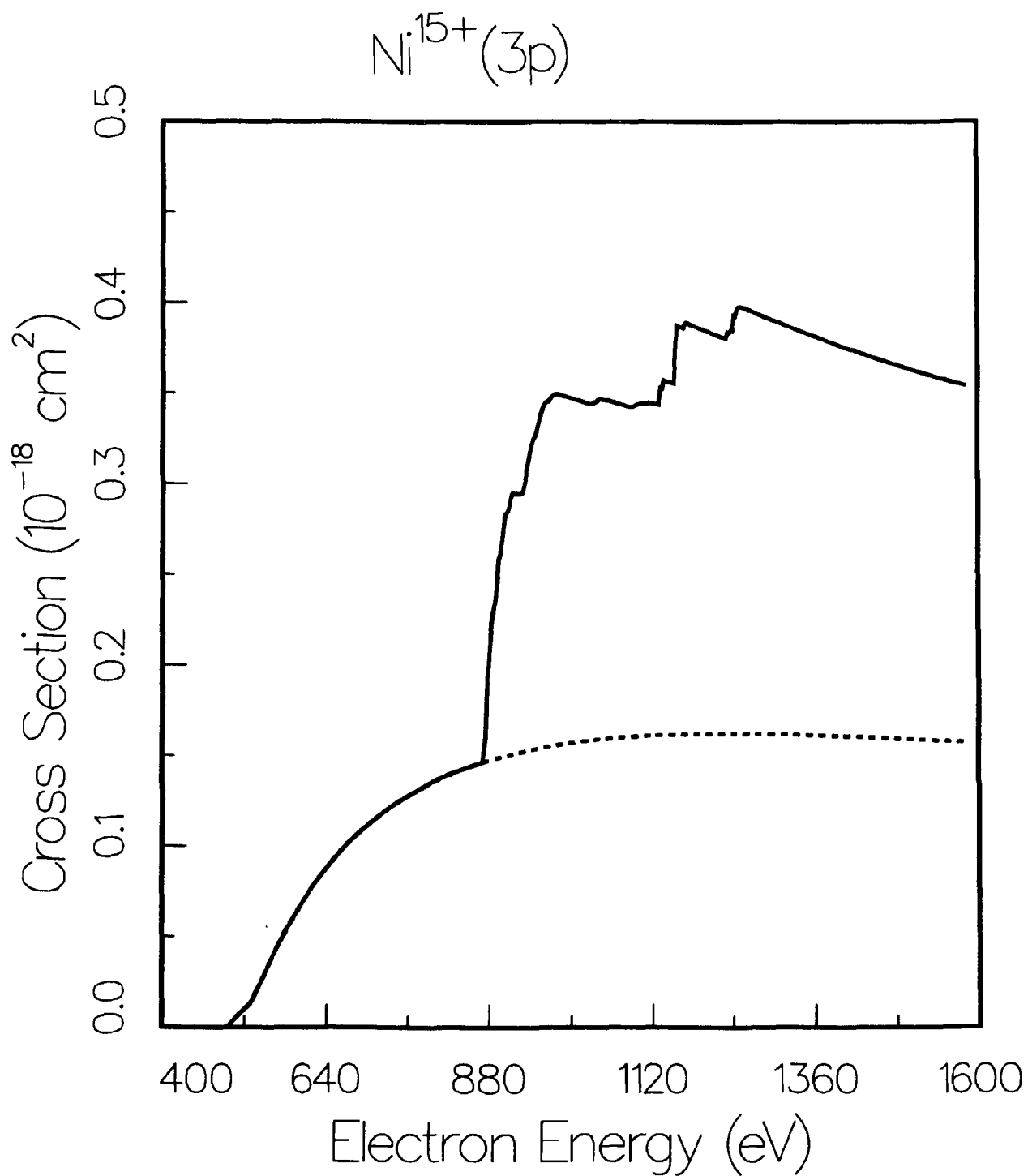


Fig. 22. Electron-impact ionization of Ni^{15+} . Full curve, configuration-average total ionization cross section from the $3p$ ground configuration; dashed curve, direct ionization cross section only.

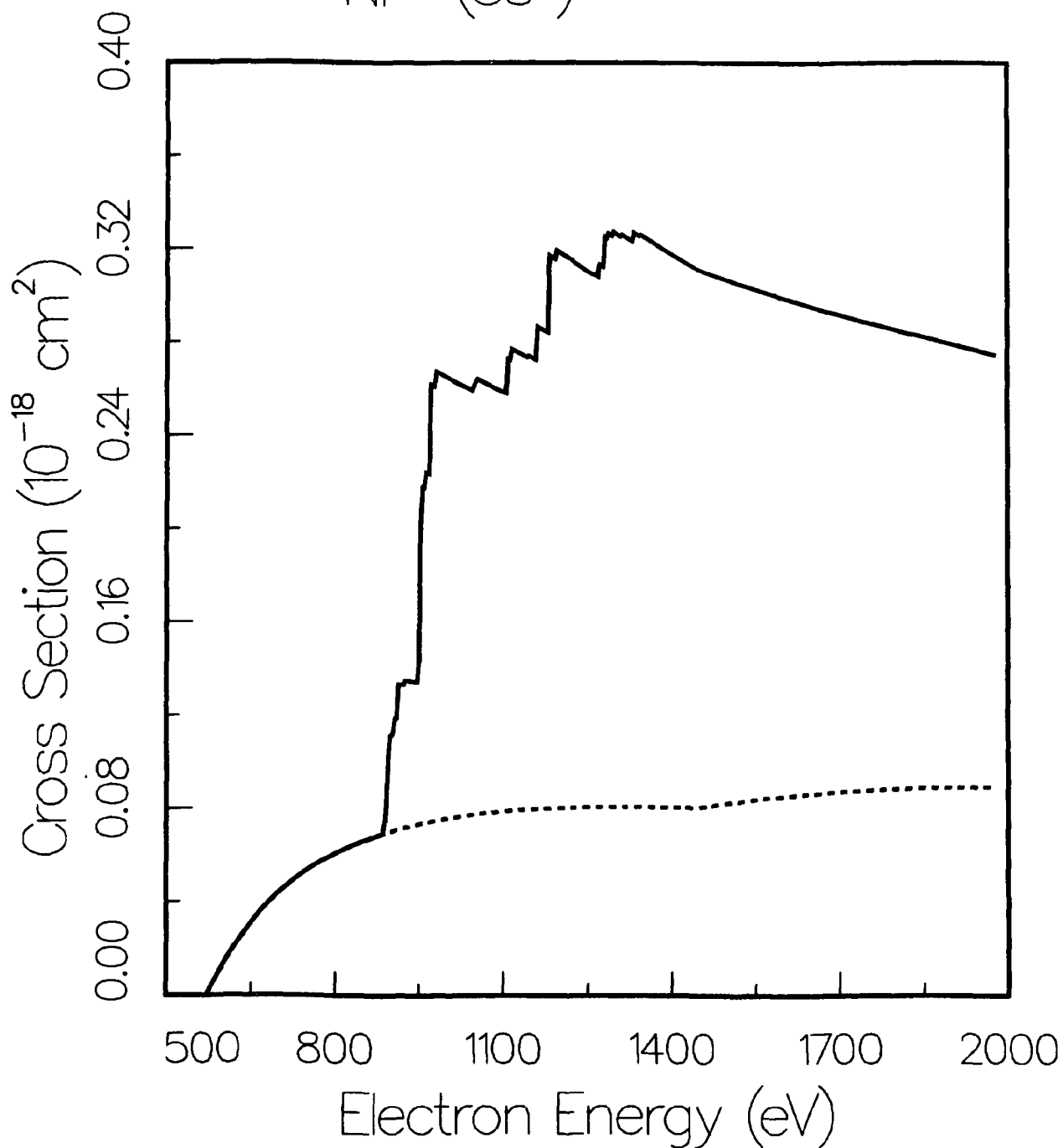
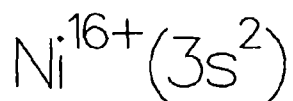


Fig. 23. Electron-impact ionization of Ni^{16+} . Full curve, level-to-level and configuration-average total ionization cross section from the $3s^2$ ground configuration; dashed curve, direct ionization cross section only.

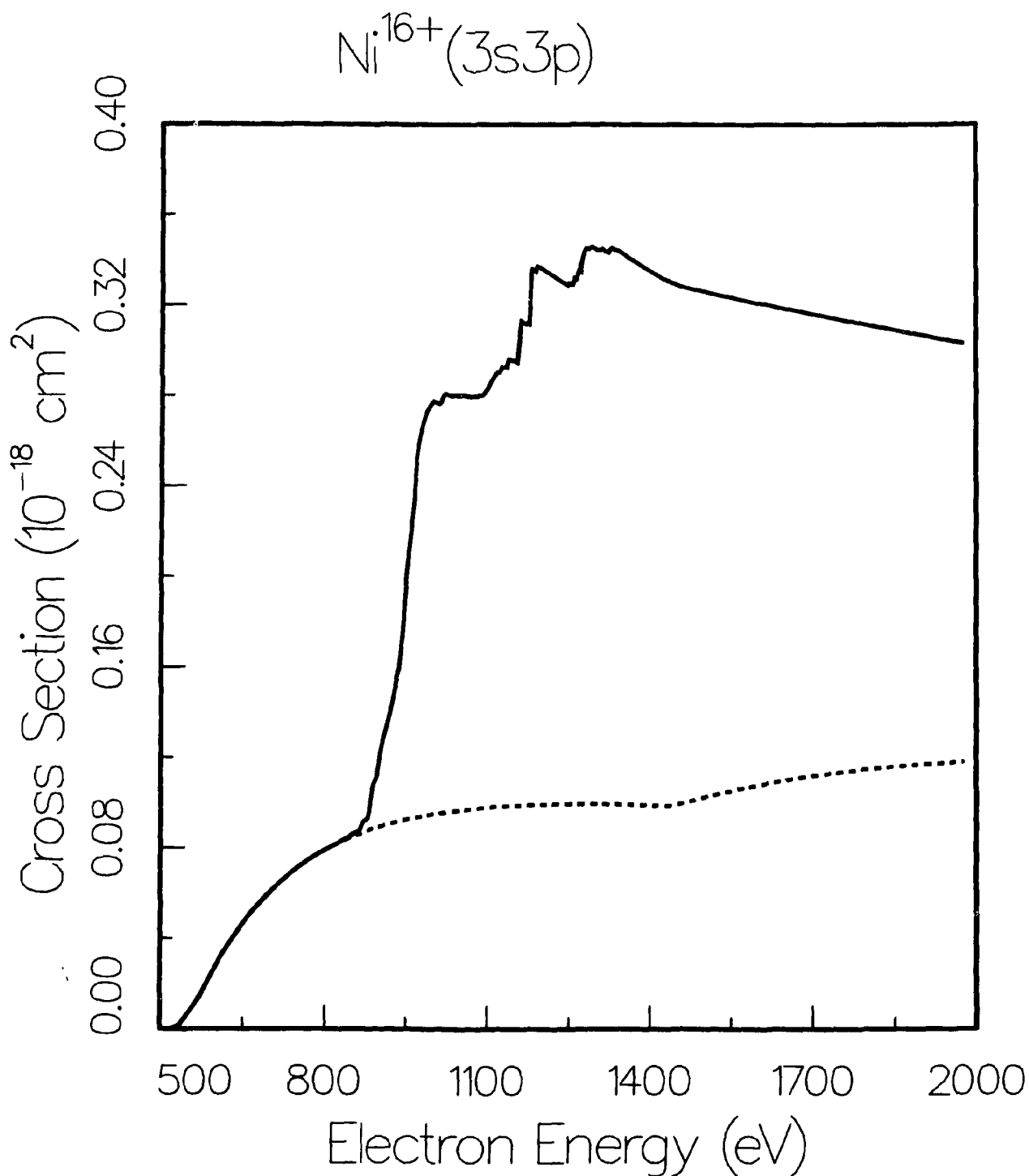


Fig. 24. Electron-impact ionization of Ni^{16+} . Full curve, level-to-level and configuration-average total ionization cross section from the $3s3p$ excited configuration; dashed curve, direct ionization cross section only.

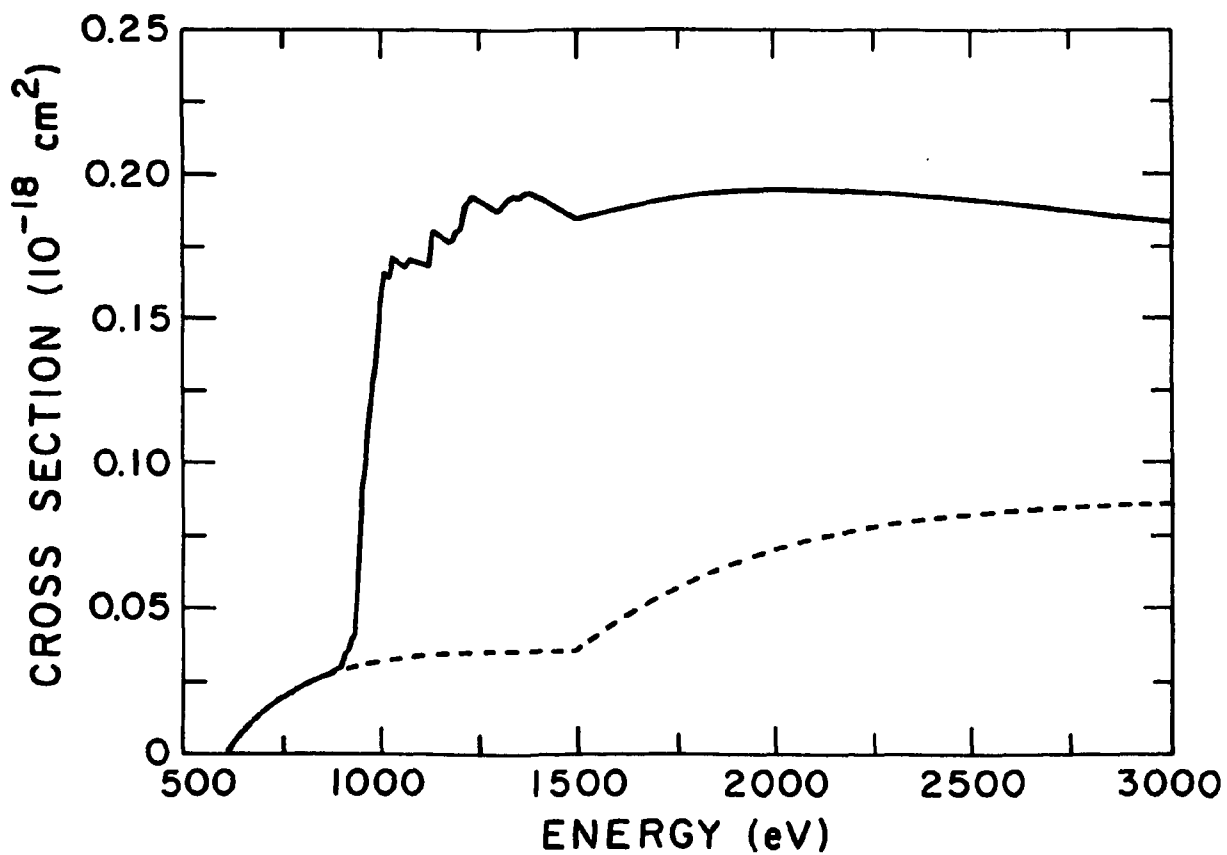


Fig. 25. Electron-impact ionization of Ni^{17+} . Full curve, level-to-level total ionization cross section from the 3s ground configuration; dashed curve, direct ionization cross section only.

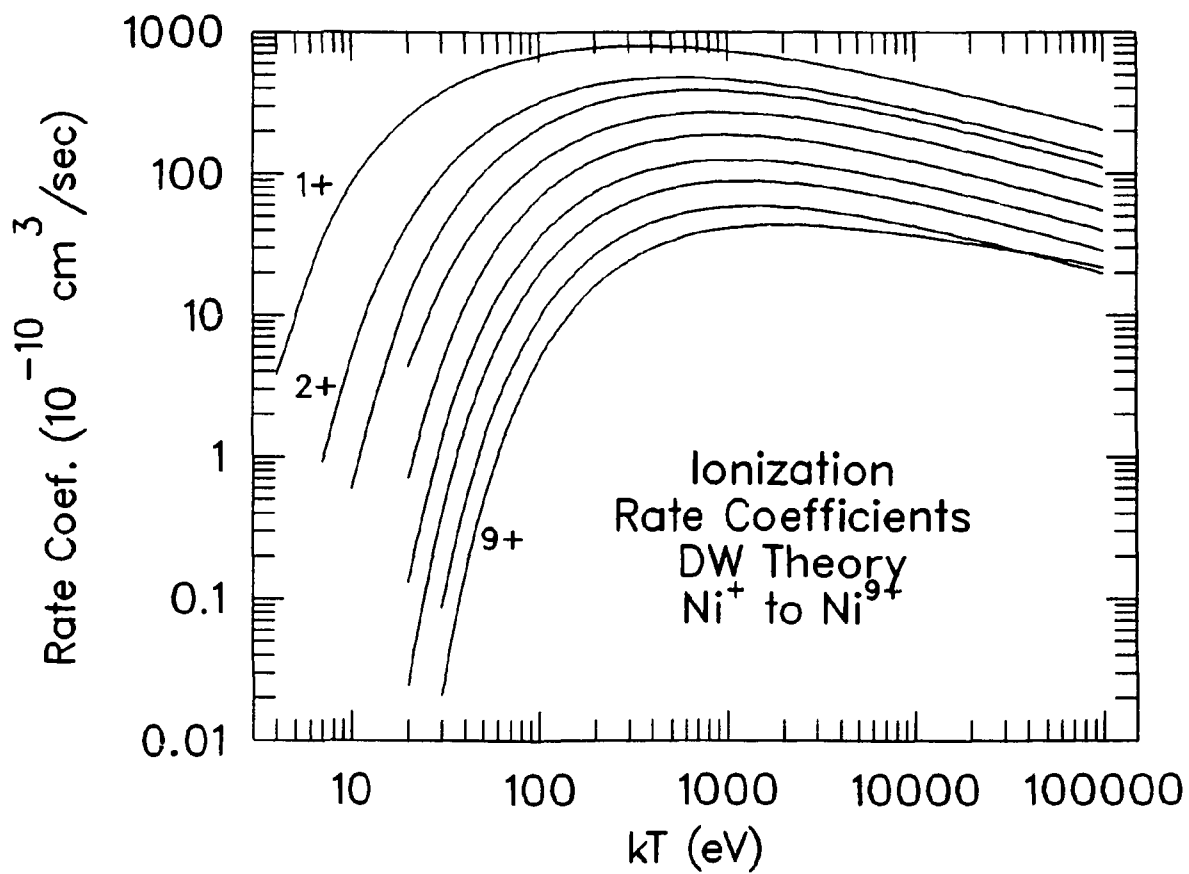


Fig. 26. Theoretical rate coefficients for Ni⁺ through Ni⁹⁺ in ground configuration.

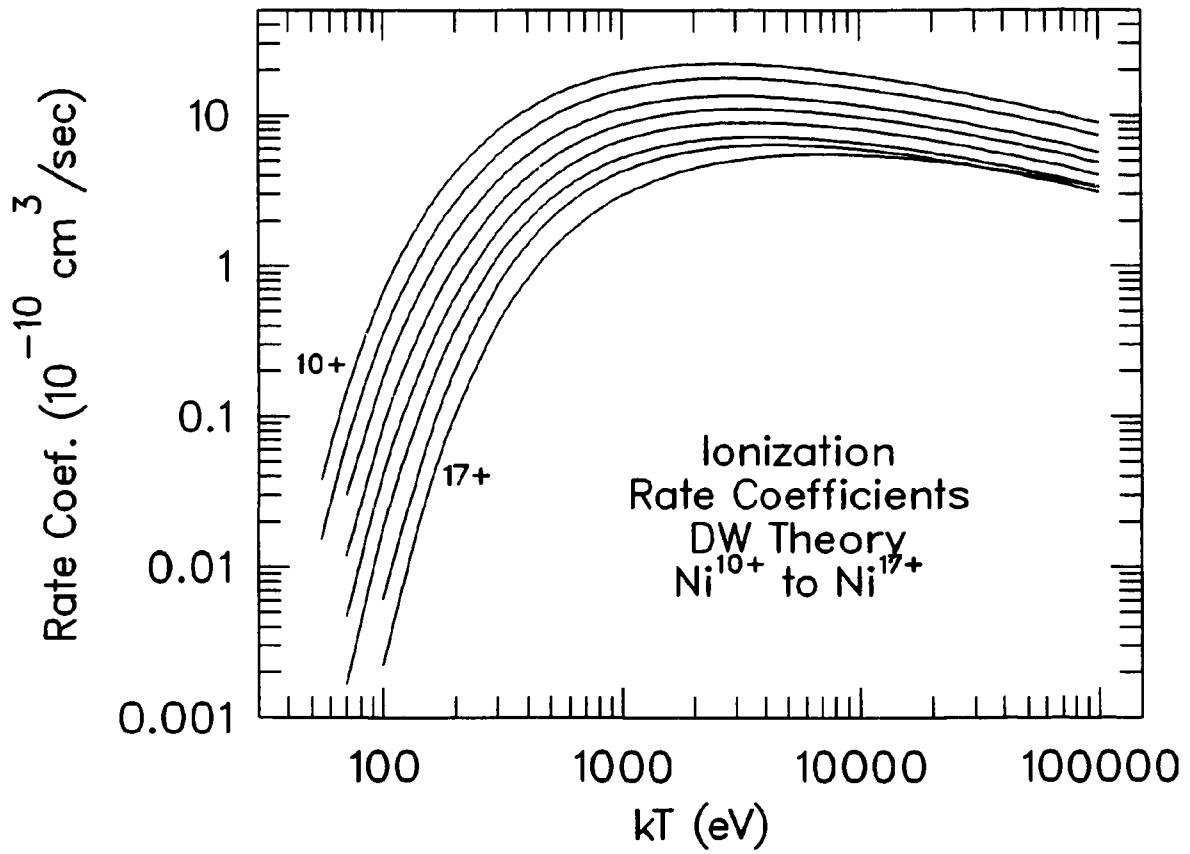


Fig. 27. Theoretical rate coefficients for Ni¹⁰⁺ through Ni¹⁷⁺ in ground configuration.

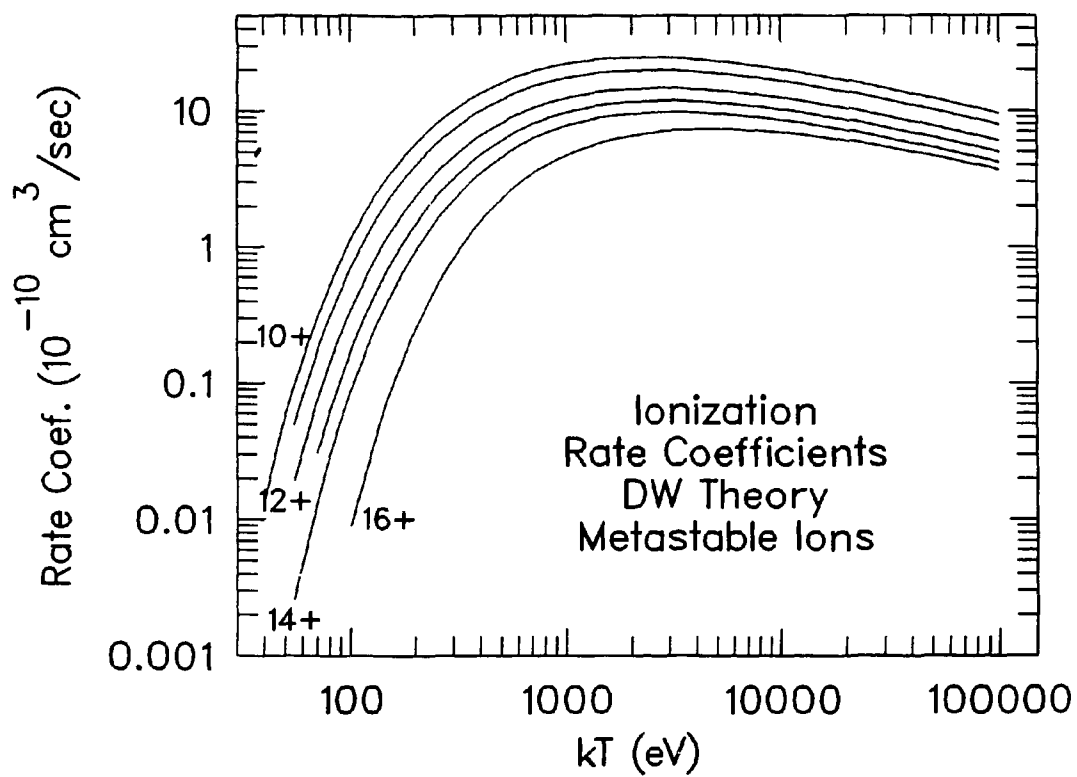


Fig. 28. Theoretical rate coefficients for Ni^{10+} through Ni^{14+} and Ni^{16+} in excited configuration.

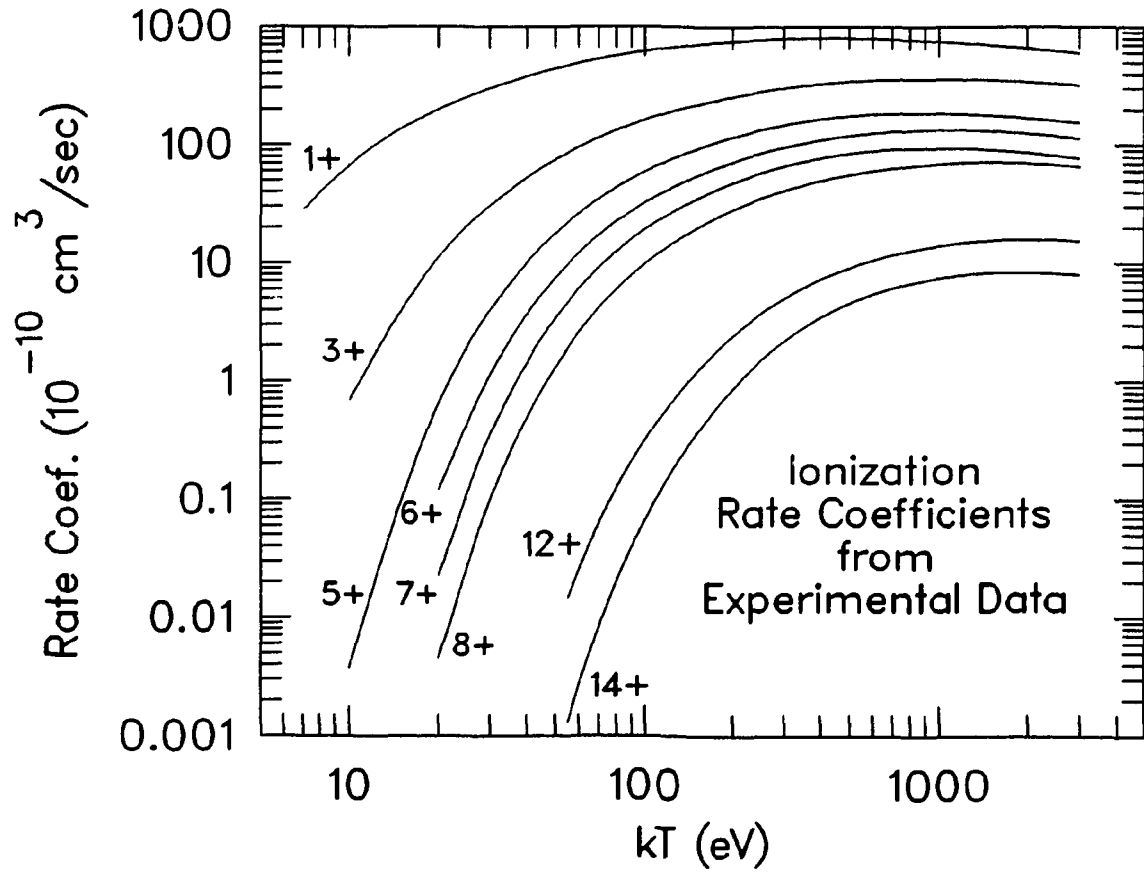


Fig. 29. Experimental rate coefficients for various Ni ions.