Electron collisions with copper atoms: Elastic scattering and electron-impact excitation of the $(3d^{10}4s)^2S \rightarrow (3d^{10}4p)^2P$ resonance transition

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We report on a theoretical investigation of elastic electron scattering from the $(3d^{10}4s)^2S$ ground state and electron-impact excitation of the $(3d^{10}4s)^2S \rightarrow (3d^{10}4p)^2P$ resonance transition in copper atoms. The calculations were performed using a semirelativistic and a fully relativistic B-spline R-matrix (close-coupling) approach. The results for the angle-integrated and angle-differential cross sections are generally in good agreement with those obtained in previous calculations and with numerous experimental data. Where discrepancies with experiment in the differential cross sections remain, the present work generally supports the previous calculations.

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I. INTRODUCTION

Electron collisions with copper atoms are of interest for both fundamental reasons and the need for accurate atomic data in modeling applications such as the copper-vapor laser (CVL), which has become a well-established source of high-power visible light [1]. As summarized in a recent paper on electron-impact excitation of the $(3d^{10}4s)^2S \rightarrow (3d^{10}4p)^2P$ resonance transition [2], a significant amount of effort, both experimentally and theoretically, has been devoted over the last several decades to this particular collision process, due to its importance in the understanding of the CVL laser.

In another recent paper [3], our newly developed fully relativistic B-spline R-matrix (close-coupling) approach [4] was used to calculate angle-integrated cross sections for the $(3d^{10}4s)^2S \rightarrow (3d^9 4s^2)^2D$ forbidden transition. Although much weaker, a detailed knowledge of this transition is also very important, since the ^2D state is part of the three-level system (^2S ground state, ^2P upper laser state, ^2D lower laser state) for pulsed-laser operation. Consequently, the cross sections for these excitation processes are among the most important parameters needed in modeling the CVL [5].

As mentioned in Ref. [3], copper is a very difficult target to describe theoretically in a fully *ab initio* manner, due to the alkali-like characteristics of its $3d^{10}nl$ valence states being strongly perturbed by the $3d^9nln'l'$ states involving the open $3d^9$ doubly ionized core. This leads to a strong term dependence of the $3d$ core and all valence orbitals. The term dependence can become a serious problem in close-coupling calculations when both of these sets of target states are included in the expansion of the total scattering-wave function. If one is interested only in the excitation of the $(3d^{10}4s)^2S \rightarrow (3d^{10}4p)^2P$ resonance transition, or generally transitions involving $(3d^{10}nl)^2L$ states with a filled $3d^{10}$ subshell, the problem can be reduced by using model potentials to simulate the effect of the core. This was done, for example, in second-order distorted-wave calculations carried out by Madison *et al.* [6] and in convergent close-coupling (CCC) [7] and close-coupling with optical potential (CCO) [2,7] calculations.

The present study was motivated by several factors. First, comparison with experimental data and other theoretical predictions provided the opportunity for another independent check of our new program. Second, plasma modelers very much like internally consistent input data from a single source, and the straightforward way to provide such data is to perform a close-coupling calculation and produce all relevant cross sections using the same model. Hence, we now supplement our published results for electron-impact excitation of the $(3d^{10}4s)^2S \rightarrow (3d^9 4s^2)^2D$ forbidden transition [3] by providing angle-integrated cross sections for excitation of the $(3d^{10}4s)^2S \rightarrow (3d^{10}4p)^2P$ resonance transition, as well as results for elastic scattering, including the momentum-transfer cross section. Finally, we will show results for angle-differential cross sections (DCS), both for elastic scattering and again for excitation of the $(3d^{10}4p)^2P$ state. There is significant disagreement between two experimental data sets, obtained by Trajmar *et al.* [8] and Ismail and Teubner [9]. Even after renormalizing these data to theoretical predictions at small scattering angles, discrepancies between experiment and theory remained regarding the shape and the relative magnitude of the DCS at scattering angles larger than about 40°. Since the DCS values are relatively small in this angular regime, it is likely that theoretical predictions are very sensitive to details of the numerical treatment. Hence, it seemed worthwhile to produce another independent data set for comparison.

Since the details of our theoretical approach were given in Ref. [3], only the most important aspects will be briefly summarized in the next section. This is followed by the presentation and discussion of our results for angle-integrated and angle-differential cross sections. We finish with a brief conclusion.

II. COMPUTATIONAL METHOD

The B-spline R-matrix (BSR) method [4,10,11] has proven to be a highly accurate tool for solving the close-coupling equations for electron collisions with atoms and ions. Compared to the well-known R-matrix package RMATRX-I developed by the Belfast group [12], the key aspects of the BSR code [13] include (1) the ability to use term-dependent, and hence nonorthogonal, sets of one-electron orbitals in the target description and (2) B-splines as the underlying, effectively complete basis to expand the wave function of the projectile. Like RMATRX-I, it is an all-electron approach, and hence core-valence correlation effects (such as the core polarization) can, in principle, be described *ab initio*.

A major advantage of using term-dependent orbitals is the fact that accurate structure descriptions can be obtained with relatively small configuration interaction expansions and, if the core is not frozen, in a fully *ab initio* way. A detailed illustration for the present case of interest is given in Tables I and II of Ref. [3]. In particular, the resulting target excitation energies agreed with the experimental values to much better than 0.1 eV, and we also obtained close agreement with experiment for the oscillator strength of the $(3d^{10}4s)^2S \rightarrow (3d^{10}4p)^2P$ resonance transition.

Specifically, our scattering calculations were performed in a 20-state nonrelativistic approximation (which we will refer to as BSR20) and in the corresponding 34-state fully relativistic (DBSR34) model, closely coupling all states with principal configurations $3d^{10}4s$, $3d^{10}4p$, $3d^{10}4d$, $3d^{10}5s$, $3d^{10}5p$, $3d^{10}6s$, $3d^{9}4s^2$, and $3d^{9}4s4p$. Although the semirelativistic Breit-Pauli approach is generally expected to be sufficiently accurate for neutral Cu, we performed calculations using both the semirelativistic and a fully relativistic Dirac-based (DBSR) version. Not surprisingly, the biggest differences between the results from these two models were previously found in the near-threshold resonance region for excitation of the $(3d^{9}4s^2)^2D_{5/2,3/2}$ states [3].

III. RESULTS AND DISCUSSION

A. Angle-integrated cross sections

Figure 1 exhibits results for the angle-integrated elastic and momentum transfer cross section for electron scattering from copper in its $(3d^{10}4s)^2S$ ground state. The overall agreement of the present DBSR34 predictions with results from numerous other calculations is satisfactory, with the biggest differences appearing for energies below ≈1 eV and above ≈20 eV. The results in the low-energy regime are very sensitive to the target description, while coupling to the continuum may additionally affect the results for the higher energies. Without experimental data available for comparison, one can only suspect which calculation most accurately reflects reality. We do emphasize, however, that our structure calculation seems superior to that used in the other calculations. In particular, our optical oscillator strengths agree well with experiment. The CCC calculation, on the other hand, was performed with an optical oscillator strength for the $(3d^{10}4s)^2S \rightarrow (3d^{10}4p)^2P$

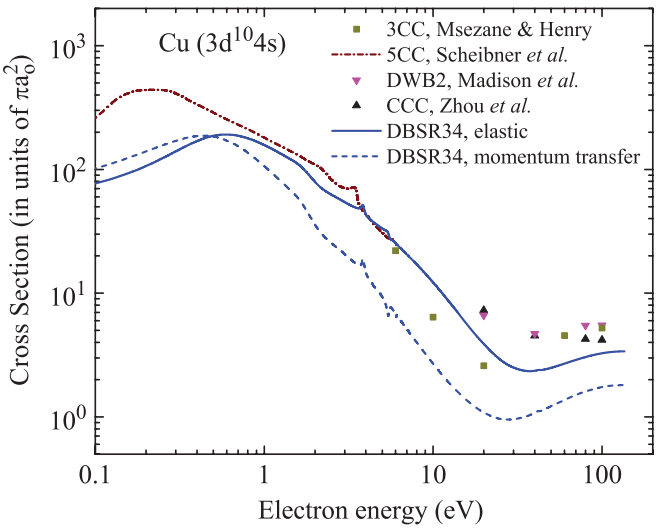

FIG. 1. (Color online) Angle-integrated elastic and momentum-transfer cross section for electron scattering from copper in its $(3d^{10}4s)^2S$ ground state. The results for the elastic cross section from various nonrelativistic calculations, including a second-order distorted-wave (DWB2) model [6] as well as three-state (3CC) [14], five-state (5CC) [15], and CCC [7] models, are compared with the present DBSR34 predictions.

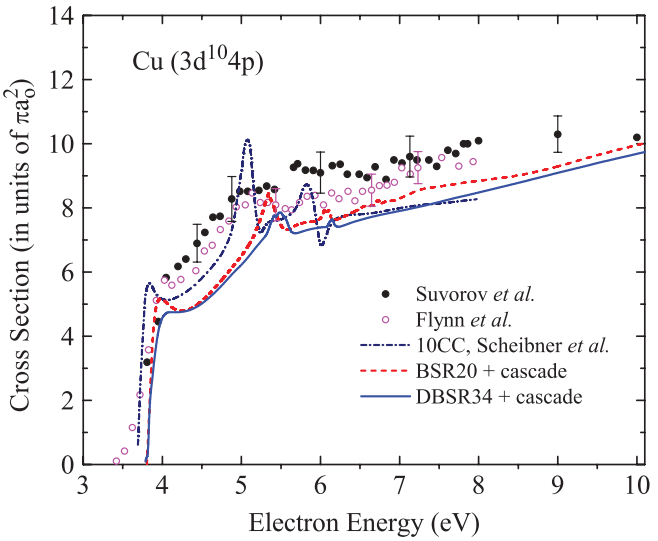

FIG. 2. (Color online) Excitation function of the $(3d^{10}4p)^2P$ state in copper. The experimental data of Flynn *et al.* [17] and Suvorov *et al.* [2] are compared with predictions from a nonrelativistic standard 10-state close-coupling calculation [18], a nonrelativistic 20-state BSR (BSR20) model, and a fully relativistic 34-state (DBSR34) approach. The (D)BSR results include cascade contributions.

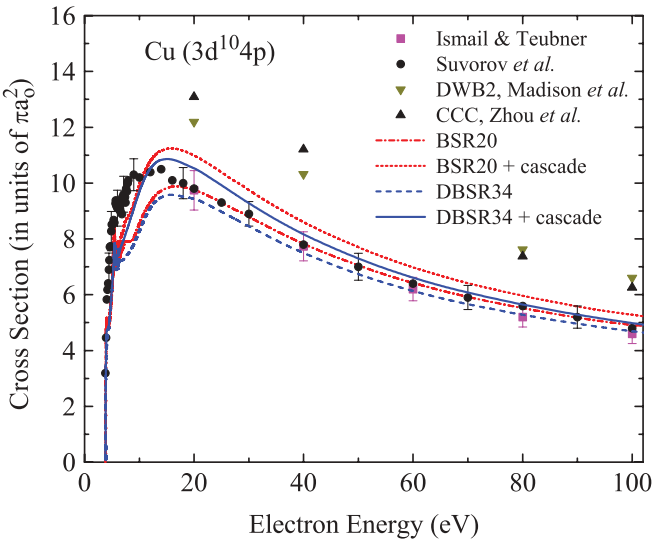

FIG. 3. (Color online) The same as Fig. 2 over an extended range of incident energies. The experimental data of Ismail and Teubner [9] and Suvorov *et al.* [2] are compared with predictions from nonrelativistic DBW2 [6], CCC [7], and BSR20 calculations, as well as the fully relativistic DBSR34 model. The effect of cascading is also illustrated in the (D)BSR curves.

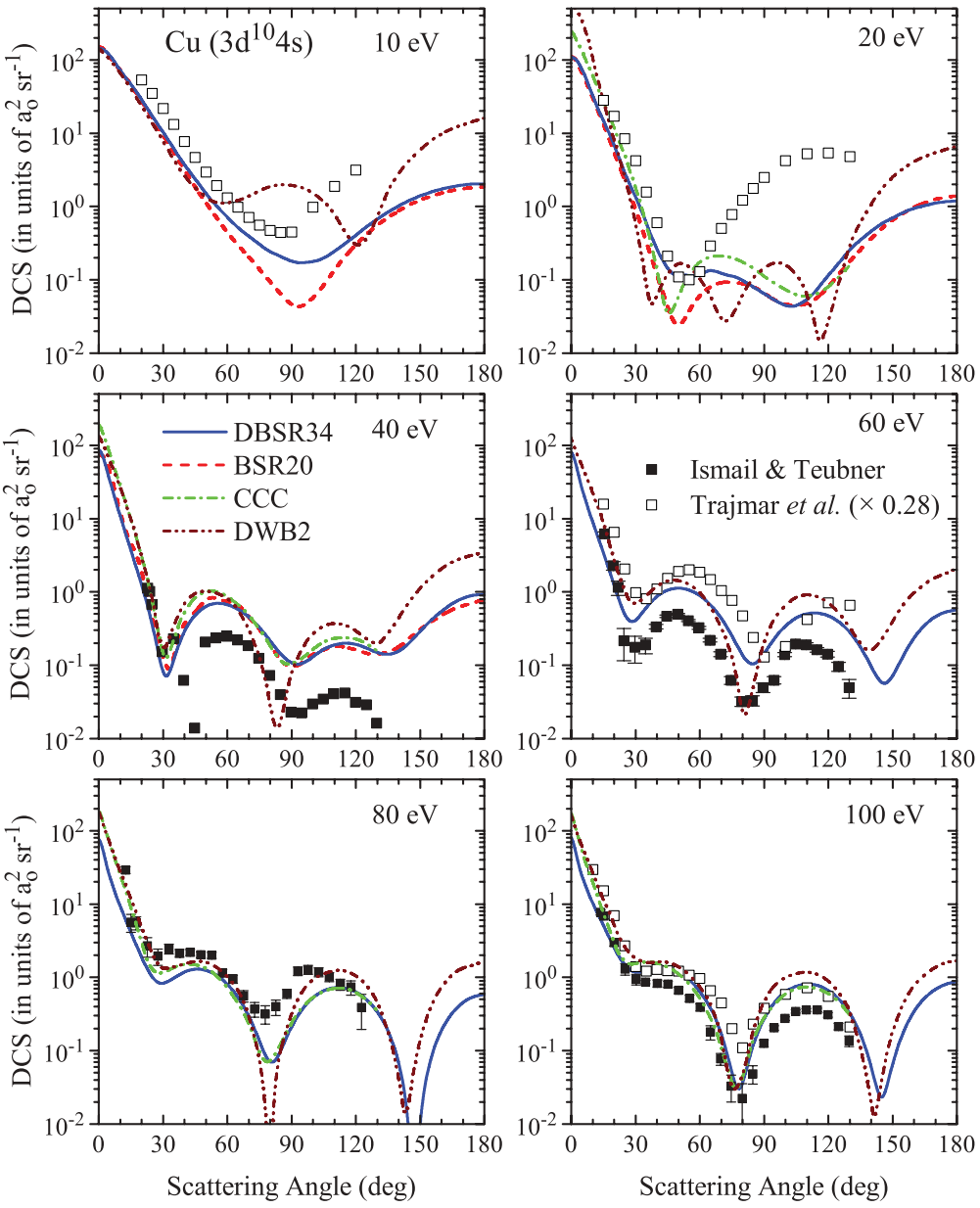

FIG. 4. (Color online) DCS for elastic electron scattering from copper at energies ranging between 10 and 100 eV. The nonrelativistic DWB2 [6], CCC [7], and BSR20 predictions, as well as the fully relativistic DBSR34 results, are compared with the experimental data of Trajmar *et al.* [8] and Ismail and Teubner [9]. The former data were multiplied by a factor of 0.28.

transition that exceeds the experimental value by about 30% [7]. One would expect this problem to appear in the absolute value of the cross sections that are affected by the optical oscillator strength. Furthermore, it should have an impact on the polarizability of the ground state and hence influence the predictions for the elastic cross section.

Our close-coupling expansion yields a ground-state polarizability of $42.4a_0^3$, where $a_0 = 0.529 \times 10^{-10}$ m is the Bohr radius. This result agrees well with those from other available calculations [16] that are in the range $40–46a_0^3$ [16]. Note that about 20% of the ground-state polarizability of Cu originates from excitations out of the $3d^{10}$ core, of which the most important ones are included in the present calculations.

Figures 2 and 3 exhibit the angle-integrated cross section for electron-impact excitation of the $(3d^{10}4s)^2S \rightarrow (3d^{10}4p)^2P$ resonance transition, both in the near-threshold region (Fig. 2) and over an extended range up to an incident energy of 100 eV (Fig. 3). The results have been summed over the unresolved fine-structure levels with total electronic angular momenta $J = 1/2$ and $J = 3/2$, respectively. Except very close to threshold, we found the statistical branching ratio of 2:1 for excitation of the $^2P_{3/2}$ state compared with the $^2P_{1/2}$ state to be a very good approximation, and hence no results for the individual fine-structure levels will be presented in this paper.

The agreement between the current predictions and the experimental data of Flynn *et al.* [17], Suvorov *et al.* [2], and Ismail and Teubner [9] is generally better than 20%, as is

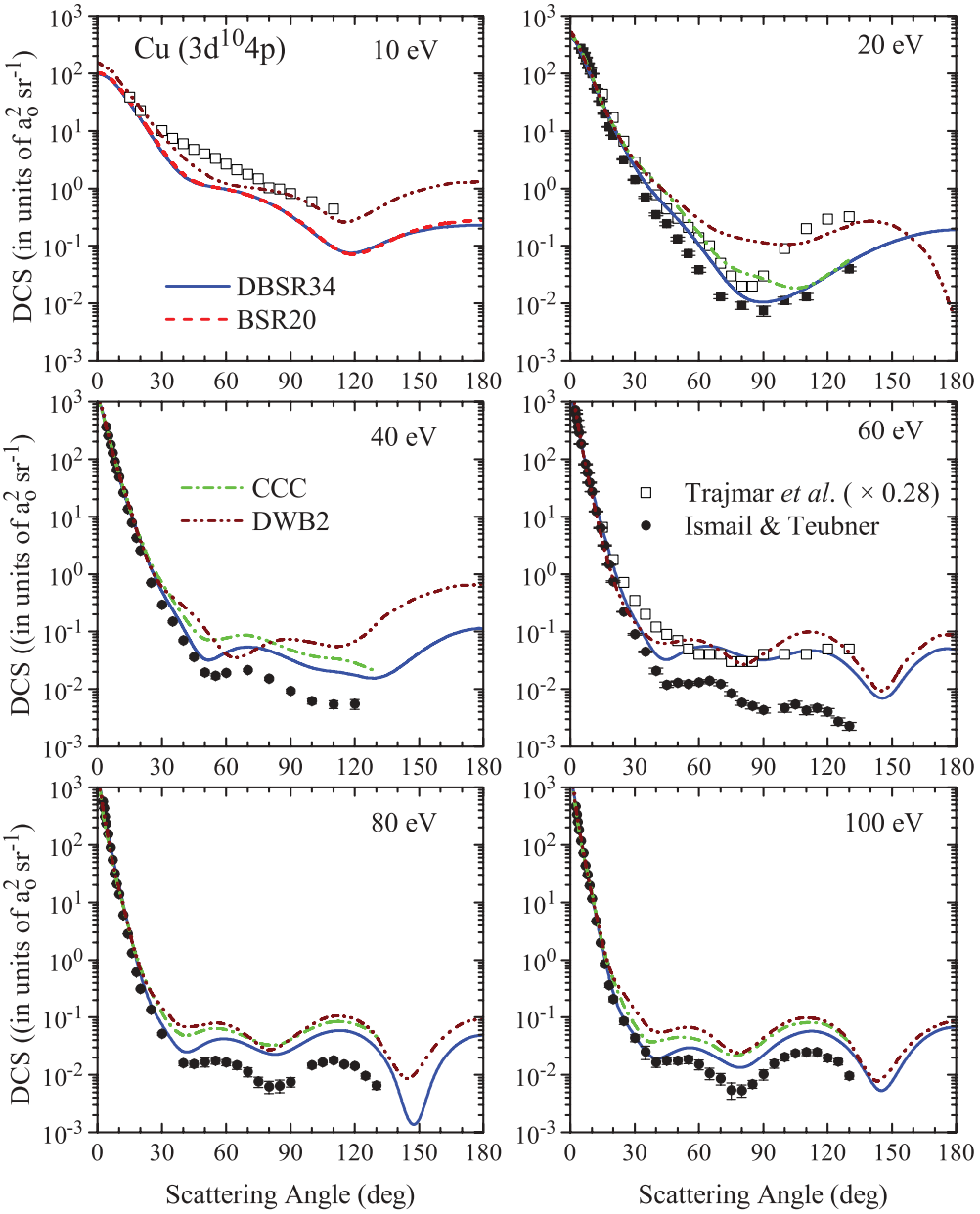

FIG. 5. (Color online) The same as Fig. 4 for electron-impact excitation of the $(3d^{10}4p)^2P$ state in copper.

the agreement with the results from a 10-state nonrelativistic close-coupling calculation (10CC) carried out by Scheibner *et al.* [18]. The differences in the resonance positions found in the various models are most likely due to differences in the structure description. As we mentioned, we expect the latter to be superior in the present BSR and DBSR models compared with the 10CC model shown in Fig. 2 and compared with the DWB2 and CCC calculations shown in Fig. 3. Given that the optical oscillator strength in the CCC model was too large by about 30% [7], it is not surprising that the CCC results are about 30% larger than the BSR20 predictions.

We note that the inclusion of relativistic effects visibly changes the results obtained in our nonrelativistic 20-state BSR20 model. The Breit-Pauli and the fully relativistic results, however, are nearly indistinguishable. Hence the Breit-Pauli predictions are not shown. Also, cascade contributions change the apparent cross sections by 10%–20% and hence should be accounted for if such accuracy is desired.

B. Angle-differential cross sections

Figure 4 shows the DCS for elastic electron scattering for incident electron energies of 10, 20, 40, 60, 80, and 100 eV. The predictions from our nonrelativistic BSR20 and fully relativistic DBSR34 calculations are compared with the experimental data of Trajmar *et al.* [8] and Ismail and Teubner [9]. As suggested in Ref. [9], the former data were multiplied by 0.28 and thus differ from the published results. This factor was motivated by the otherwise serious disagreement for small scattering angles in the DCS for excitation of the $(3d^{10}4p)^2P$ state (see Fig. 5). Even after this correction, the data of Trajmar *et al.* [8] generally lie above the theoretical

predictions, especially at scattering angles beyond about 30°. While our results agree much better with the data obtained by Ismail and Teubner [9], differences between theory and experiment remain in this case as well. Our results agree very well with the CCC predictions [7], as well as the CCO and DWB2 results presented in the latter work. Recall that the experimental data shown in Fig. 1 of Ref. [7] were visually renormalized to the CCC results.

It is worth noting that relativistic effects apparently play a role near the minima in the DCS and particularly at the lower energies of 10 eV and 20 eV, respectively. Generally, the fully relativistic DBSR34 model predicts these minima to be shallower than the nonrelativistic BSR20 calculation. At 40 eV and above, the results from the two models become nearly indistinguishable.

Finally, Fig. 5 exhibits the DCS for electron-impact excitation of the $(3d^{10}4p)^2P$ state. As we mentioned, the experimental data of Trajmar *et al.* [8] were multiplied by 0.28 to obtain good agreement with theory at small scattering angles. The DCS values in this angular range are effectively determined by the generalized oscillator strength. Given that our *ab initio* structure model reproduces the experimental optical oscillator strengths for the two fine-structure levels to better than 5%, we are confident in the magnitude of our theoretical DCS at small angles.

For this inelastic transition, the BSR20 and DBSR34 results are in excellent agreement with each other for all energies considered here. This is not surprising, since Mott scattering from the nucleus does not affect the DCS as directly as it does in elastic collisions. The agreement with experiment is generally satisfactory for scattering angles below 40°. For larger angles, the discrepancies become significant. It should be noted, however, that the DCS values are small at these angles, which makes both the experiment and the calculation increasingly challenging. Even after the renormalization of the Trajmar *et al.* [8] data, the two experimental data sets sometimes differ by an order of magnitude. This corresponds to about a factor of 40 without renormalization.

IV. SUMMARY AND CONCLUSIONS

We have presented results from semirelativistic and fully relativistic B-spline R-matrix (close-coupling) calculations for electron collisions with copper atoms. The results are generally in good agreement with those obtained in previous calculations and with a number of experimental data. Discrepancies with experiment remain for scattering angles larger than about 40°. The present work generally supports the previous DWB2, CCO, and CCC predictions, as well as the absolute experimental data given by Ismail and Teubner [9] at small scattering angles. A data file with angle-integrated elastic, momentum-transfer, and electron-impact excitation cross sections for the $(3d^9 4s^2)^2 D_{5/2,3/2}$ and the $(3d^{10}4p)^2 P_{1/2,3/2}$ states is available from the authors upon request.

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