Elastic cross sections of electron scattering with Zn and Cd atoms below 4 eV

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(Received 26 March 1991)

Theoretical elastic cross sections of electron scattering with Zn and Cd atoms are provided with a static-exchange plus correlation-polarization potential formalism. A *p*-wave shape resonance state is predicted for Zn as well as Cd atom. Elastic total cross sections and differential cross sections at an angle of 90° are given at the energies between 0.01 and 4 eV.

PACS number(s): 34.80.Bm

Only a few investigations have been made for the scattering processes of very slow electrons with Zn and Cd atoms. According to Hortop and Lineberger [1], stable negative ions of Zn and Cd do not exist; the main features of the scattering parameters would be the low-lying shape resonances with very high and sharp peaks of total cross sections at the resonance energies. Primary experimental results for the positions of *p*-wave shape resonance states of Zn and Cd below 0.5 eV were given by Burrow, Michejda, and Comer [2] using an electron transmission method. Relative differential cross sections (DCS) at an angle of 90° were measured by Kazakov [3] at very low energies. The only *ab initio* calculation was performed by Sin Fai Lam [4] using a relativistic static-exchange plus polarization potential method, but the theoretical prediction was given only for the positions of the *p*-wave shape resonance states without any results for cross sections. In this paper, our earlier calculations for alkaline-earth atoms [5–7] are extended to the elastic scattering of very slow electrons with Zn and Cd atoms while paying attention to the low-lying *p*-wave shape resonance states. The purposes of the present calculations are to give a theoretical explanation of the experimental curves of Kazakov for DCS and to make up for the lack of cross sections in both theory and experiment. The first inelastic thresholds of Zn and Cd are near 4 eV. Below this point the inelastic channels and effects of relevant configurations are not significant, and one particle model is powerful with suitable effective potential to describe the elastic scattering. Therefore, first theoretical results are given for the elastic cross sections below 4 eV.

The details of the theoretical method are given in our previous papers [5,6]; here only the results are provided. The total cross sections are plotted in Fig. 1. It is clear that a sharp peak is produced for each atom in the total cross section below 0.5 eV, which is associated with the *p*-wave shape resonance state. The correlation potential is used both with and without (parameter-free) a scaling factor (=0.8) in the present calculation (see details in Ref. [4]) and the corresponding results provide two limitations of the present data. The shape resonance states occur at very low energies, so that the background of the *p*-wave phase shifts are expected to be very small and the contributions of *s* and *d* waves to the total cross sections are relatively small compared with the resonance partial wave. This implies that the resonance energies can be approximated by the maximum points of the cross sections. Then, the present calculations predict a *p*-wave shape resonance state for Zn near 0.22 eV with unscaled, and near 0.31 eV with scaled, correlation potential and a *p*-wave shape resonance state for Cd near 0.1 with unscaled, and near 0.18 eV with scaled, correlation potential. The positions of the *p*-wave resonance states are qualitatively in agreement with the measured values of Ref. [2] and the theoretical data of Sin Fai Lam [4]. Because other results of cross sections are not available, comparisons cannot be made for the total cross sections. The total cross sections

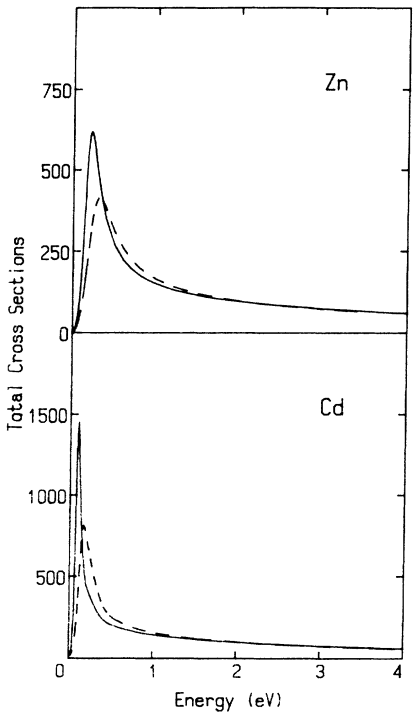

FIG. 1. Total cross sections (in 10^{-16} cm^2). The solid lines represent the results of unscaled correlation potential; the broken lines represent the results of scaled correlation potential. The two sets of data agree well above 1 eV.

below 0.5 eV are predominated by p resonance partial wave, and the energy dependence of the total cross sections in the energy region is much different from our earlier results of heavier alkaline-earth atoms [7], for which stable negative ions exist with a p-wave electron absorbed and where very sharp and high peaks are not observed. observed.

The energy dependence of DCS is plotted in Fig. 2. The relative DCS at an angle of 90° was measured by Kazakov [3]. In his experiment a very deep minimum structure was observed in the energy dependence curve of DCS for Zn at 0.35 eV as well as for Cd at 0.25 eV and it was attributed to a p-wave shape resonance state. But in the present results, the correspondence curves have minimum points below 0.01 eV and the minimum structures are caused by the zero points of s-wave partial cross sections very close to the zero energy rather than by p-wave shape resonance states at the resonance energies. There is no minimum structure in the present DCS curves at the p-wave resonance energy for Zn as well as Cd. In our previous calculations [6,7] for alkaline-earth atoms the DCS has a minimum point near 0.1 eV. The causes of the minimum structure are similar for Zn, Cd, and alkaline-earth atoms except that in the present case the minimum point occurs at a smaller energy. The discrepancy in the minimum point position between the measurement of Kazakov and ours might be understood if one noted a later similar measurement of Kazakov and Khristoforov [8] for the Ca atom. In their later paper the authors pointed out that the minimum point of DCS was shifted to a higher energy (by 0.4 eV) by the large width of the instrument function for the primary beam. Therefore, if the minimum point position of Zn and Cd in the experiment of Kazakov was also shifted to higher energy as in their measurement for the Ca atom, the actual position of the minimum point should be very close to zero as indicated in the present calculation.

The main sources of error in the present calculation are the local correlation-polarization potential and the neglect of the relativistic effects. The position of the low-lying p-wave shape resonance states or the resonant part of the p-wave phase shifts and the magnitude of the resonance peaks are quite sensitive to the strength of the local potential. While the phase shifts of s, d, and other higher partial waves and the background part of the p-wave phase shift are not sensitive to the strength of the correlation potential even at 0.1 eV, and as shown in our calculations for rare gas atoms [9], the present method can give quite good quantitative data for these quantities at such low energies. Therefore, we expected that the present results of total cross sections are quantitatively reliable at the energies above 1 eV, where the effect of the p-wave shape resonance at a very low energy is expected to be small, and that the reliability of the DCS at an angle of 90°, which is mainly determined by the contributions of s and d waves, is fair even at the energies below 1 eV. It can be seen in Figs. 2 and 3 that the potential strength insensitive quantities of unscaled and scaled

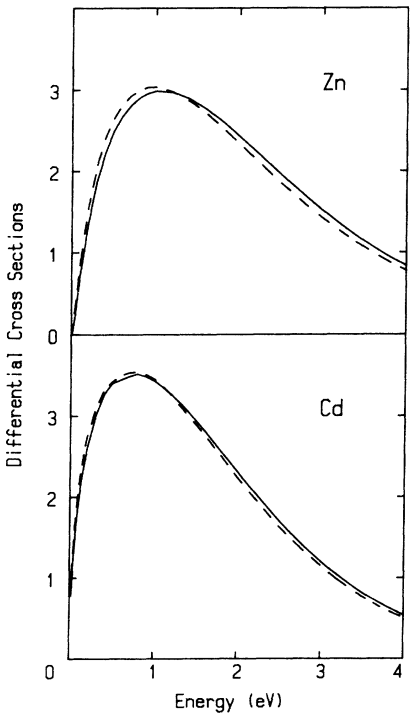

FIG. 2. Differential cross sections (DCS) (in 10^{-16} cm^2) at an angle of 90°, the same as in Fig. 1. The DCS at 90° is not very sensitive to the strength of correlation potential and the two sets of data coincide well in the whole range of plotted energy.

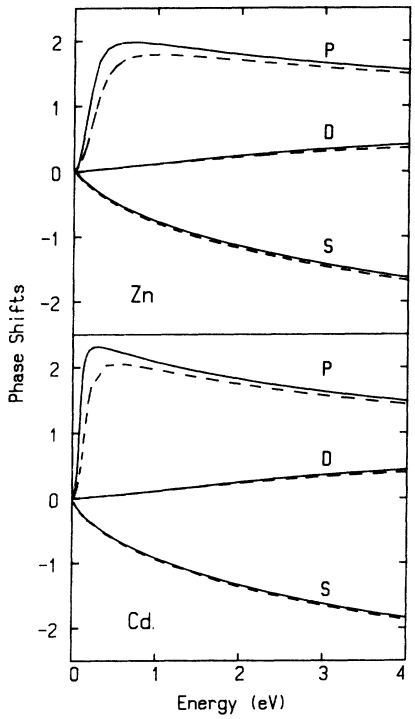

FIG. 3. Energy dependence of the phase shifts of s, p, and d waves, as in Fig. 1. The phase shifts of s and d waves are not very sensitive to the strength of the correlation potential. The two sets of data of s and d waves agree well in the whole energy region; the two sets of p-wave data agree well above 1 eV, where the shape resonance part of the phase shift is small.

correlation potentials coincide well in the plotted energy region. We have given two limitations of the results with unscaled and scaled correlation potential. Although the present results of the p-wave shape resonance states below 1 eV are only qualitative, the above conclusions about the characteristics of the structures will not be changed by the approximation. The relativistic effects on the total cross sections are generally small except in the shape resonance region. To make quantitative comparison, more reliable and complete experimental data and more complicated calculations are needed.

This work was supported by National Natural Science Foundation of China, Grant No. 9189012-06.

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