Absolute cross sections for silver clusters (Ag_n, n=1-4) by electron impact

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Synopsis The modified addidtivity formula [1] for homonuclear cluster is employed to calculate the elastic, total and ionization cross section of silver cluster form ionization threshold to 20 keV and is compared with available experimental data [2,3]. The absorption, polarization, exchange and correlation effects are introduced in an optical potential through SCOP formalism [4]. The elastic and total cross sections are reported for the first time.

The ionization of particles by electron impact is one of the basic processes in mass spectrometry. Besides, this interaction plays an important role in many practical applications, e.g. gas discharges, plasmas, radiation chemistry, planetary upper atmospheres etc. Hence, a large number of theoretical and experimental studies have been done for decades, to calculate/measure electron induced ionization cross section in gas phase for atoms and molecules. However, the cross section data for clusters, especially for metal clusters, is lacking.

The present study gives theoretical insight into evaluation of elastic, total and ionization cross section for silver clusters (Ag_n, n=1-4) by the impact of electron from ionization threshold to 10 keV. The spherical complex optical potential (SCOP) [4] method is used to calculate absolute elastic and total cross sections and then ionization contribution procedure [4] is employed to derive the contribution of ionization from the inelastic cross section. The energy of low ling excited state [5] is considered as threshold value for the present calculations. The modified additivity formula [1] employed presently for the clusters is,

$$\sigma_e(X_n) = n^a \sigma_e(X) \qquad (1)$$

This modified rule is based on geometrical concept for homonuclear cluster. Where $\sigma_e(X)$ denotes the cross section for atoms X, n represents the cluster size and a is the hard sphere packing fraction.

Table 1: Ratio of ionization cross section of neutral silver atoms to its clusters for 46 eV.

Cluster	Present	Franzerb [2]	D.Koch [3]
Ag	1	1	1
Ag2	1.58	1.53±20%	1.3±10%
Ag3	3.74		3.8±10%
Ag4	2.52		2.2±10%

In general, present calculations shows good agreement within the reported uncertainty of Franzreb *et al*. [2] throughout their energy range and that of D. Koch *et al*. [3] for a=2/3 till about 20 eV. The overestimation of the present calculation is expected, since the modified additivity formula is designed to calculate total cross section and experiments were done for partial cross section only.

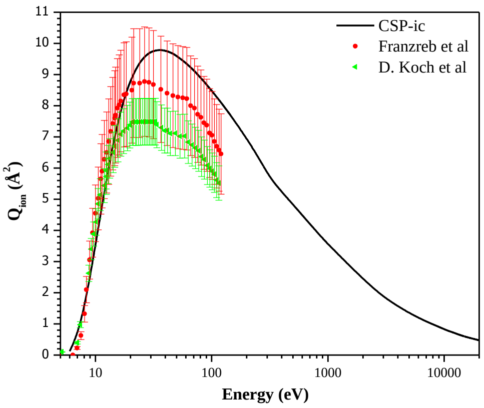

Figure 1. Ionization cross section (Q_{ion}) for silver dimer.

Fig.1. displays the Q_{ion} for silver dimer (n=2) up to 20 keV with reported experimental results. The present calculation shows higher value of cross section around the peak. The present calculation gives qualitatively good agreement within experimental error of previous data.

References

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