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Low energy electron collision with polar molecules CO in weakly plasma medium

Abstract

The investigation reported in this paper deals with the theoretical study on polar molecules CO in plasma medium. In the present calculation, the electron- dipole potential is modified and to introduce the screening effects of plasma is characterized by the inverse Debye-shielding length "λ" in a_0^{-1}. The Born Eikonal Series Approximation is used to calculate the differential scattering cross sections (DCS) for low energy the rotational excitation of target molecule CO, using various values of "λ". The results obtained are compared with the theoretical calculated Mohanan S., et al[1] results. It is observed that due to the effect of plasma screening, the DCS increases considerably near the forward direction.

Key Words

Differential scattering cross section; Dipole potential; Debye-shielding length.

INTRODUCTION

In Physics and Chemistry, plasma is typically an ionized gas and is usually considered to be a distinct phase of matter. "Ionized" in this case means that at least one of electron has been dissociated from a proportion of the atoms or molecules. The free electric charges make the plasma electrically conductive, so that it responds strongly to electro-magnetic field. This fourth state of matter was first identified by Sir William Crooks in 1879.

More specifically plasma is an electrically conductive collection of charged particles that responds collectively to electromagnetic forces. Plasma typically takes the form of neutral gas like cloud or charged ion beams, but may also include dust and grain called dusty plasma. They are typically formed by heating and ionizing a gas, stripping electrons away from atoms, thereby enabling the positive and negative charges to move freely[2].

The investigation reported in this paper deals with the study of polar molecules in plasma medium. In the present attempt the electron-molecule dipole potential is modified and to introduce the screening effects of plasma is characterized by the inverse Debye-shielding length "λ" in a_0^{-1}. The Born Eikonal Series Approximation is employed to calculate the differential scattering cross sections (DCS) for the rotational excitation of target molecule like as CO, using various values of "λ". The results obtained are compared with the Mohanan S., et al[1] results. It is observed that due to the effect of plasma screening, the DCS increases considerably near the forward direction.

FORMULATIONS

Ashihara I., et al[3] employed Glauber formulation in Eikonal approximation for electron dipole collisions. They calculated cross section for strongly polar molecules. Although this approximation is originally a high energy approximation, it has been applied successfully to the low energy electron atom collisions[4]. In the present investigations an attempt is made to employ Born Eikonal Series method for the cross sectional calculations for the low energy electron collision with CO molecule in plasma medium.

The interaction potential V(r) can be expressed in following form[7],

$$V(\underline{r}) = -2eq \sum_{n=odd} \frac{r_<^n}{r_>^{n+1}} P_n(\hat{r}, \hat{s}) \quad (1)$$

$$V_{SD} = -\frac{D\cdot\hat{r}}{r^2}e^{-\lambda r} \quad (2)$$

Where

$$\lambda = \left[7430\left\{\frac{K_B T_0}{n}\right\}^{1/2}\right]^{-1} \quad (3)$$

The screening parameter "λ", which is the inverse of the Debye-Huckel length "Λ_D" (in meter), characterizes the plasma medium, "n"-is plasma density in m^{-3} and $K_B T_0$ – is energy in eV., "D" - is dipole moment (in a.u) of the target molecule and "r" is the separation of the projectile electron from the centre of the target molecule[5,6].

Now the plasma screening is applied to the point dipole potential "V_{PD}"- which is asymptotic and holds for r- several times larger than typical target dimensions. Therefore dipole screening potential is a meaningful start, if the Debye-Huckel screening length "Λ_D" is also several time larger than typical target dimension. For water molecule, the electron charge density goes to zero only near r = $2.5a_0^{-1}$[6] and larger bond length in H_2O is about 2.8 a_0^{-1}. Thus in that case we may restrict ourselves to say "Λ_D" > 20 a_0^{-1}, corresponding to which we have restriction $\lambda < 0.05\ a_0^{-1}$. Further the screening factor exp(λr) is obtained under the assumption that for screening electrons,

$$\left|\frac{P.E}{K.E}\right| = \left|\frac{V_{PD}}{K_B T_o}\right| << 1$$

This condition also suggests a large value of "Λ_D". According to eq. (2) and eq. (3) are suitable for weak plasma. However for the coulomb potential, the Debye-Huckel form of shielding is regained even in to hot and dense plasmas[5,6]. In the present case all the same, we can exclude strongly screening plasma for the asymptotic region mentioned here.

The Born Eikonal Series method can be applied to the point dipole potential even at low energies. Initially we attempt same for the first term of Born Eikoanl Series approximation applied to screening dipole potential. The validity of first term of BES for present case is not beyond question; however the plasma screenings slightly alters the range and strength of the dipole potential[7,8].

One of the interesting aspects to be understood is the application of First term of BES method to a thermal and low energy electron molecule collision problem. Consider a molecule in plasma at large distance from the target, the potential due to polar molecule screened by the surrounding plasma may given by eq. (2). Screening dipole potential is used and applied to First term of Born Eikoanl Series approximation to study the differential scattering cross section for polar molecule in plasma medium. The Eikonal Phase shift function X(λ, b) is,

$$\chi(\lambda, b) = -\frac{1}{ki}\int_{-\infty}^{\infty} V_{SD}(\underline{r}, \hat{s})dz \quad (4)$$

Substitute eq.(2) into eq.(4)

$$\chi(\lambda, b) = -\frac{D}{ki}\int_{-\infty}^{\infty}\left\{e^{-\lambda r}/r^2\right\}zdz \quad (5)$$

The n^{th} term of scattering amplitude in Born Eikonal Series method is given by.

$$f_{En} = \frac{iki}{2\pi}\frac{i^n}{n!}\int_0^{\infty} e^{i\Delta b}\left[\chi(\lambda, b)\right]^n d^2b \quad (6)$$

The first term of Born Eikonal Series scattering amplitude is given as follow.

$$f_{E1} = -\frac{ki}{2\pi}\int_0^{\infty} J_0(\Delta, b)\left[\chi(\lambda, b)\right]bdb \quad (7)$$

Assuming the molecule to be rigid rotor point dipole, the first term of BES corresponding to screening point dipole potential calculated for the rotational transition (0→1) is given by

$$\frac{d\sigma}{d\Omega}(\theta, ki, \phi) = \frac{4D^2}{3}\frac{kf}{ki}\left[\frac{1}{\Delta}\left\{1+\frac{\lambda^2}{\Delta^2}\right\}^{1/2}\right]^2 \quad (8)$$

Where Δ = |ki- kf| is the inelastic momentum transfer and ki-is incident momentum of the electron, with the choice of 'λ'=0, the familiar expression for the electron dipole interaction potential is recovered.

RESULTS AND DISCUSSION

Low energy electron collision with polar molecules shown fairly large cross-section, have been considerably investigated in theory as well as in experiments. A detailed account on this subject has been given by Itikawa[9,10]. However, a practical situation of a polar molecule in a plasma medium has not been investigated so far. We examine the effect of the plasma medium on the collision of low energy electron with polar molecules. We have employed the Debye-Huckel screening model for the present problem. We have taken polar molecule like as CO and differential scattering cross section (DCS) are calculated using first term of BES approximation method at incident energies of electron are taken as 0.1 and 0.5 eV. respectively. The specific process studied in rotational excitation transition (0→1).

Itikawa[9,10] had compared DCS results using the close-coupling method and the Born method for e-HCL scattering of (0→1) rotational excitation energy at 1.0 eV. In that case the FBA produced a fairly good agreement with highly accurate close-coupling results for the scattering angle θ < 40°, in which angular region of the DCS are quite large. In present problem we have introduced the plasma screening which can change the picture. The First term of BES results corresponding to various strengths and various incident energy of electron E_i are discussed. Using the formula in eq. (3) and eq. (8), the DCS corresponding to (0→1) transition are calculated for E_i=0.1 and 0.5 eV. respectively. The screening parameter "λ" can be calculated from eq. (3), but we have chosen the representative values $\lambda=0.03a_0^{-1}$ and $\lambda=0.05a_0^{-1}$. Thus $\lambda=0.01a_0^{-1}$ means $\Lambda_D = 100\ a_0^{-1}$.

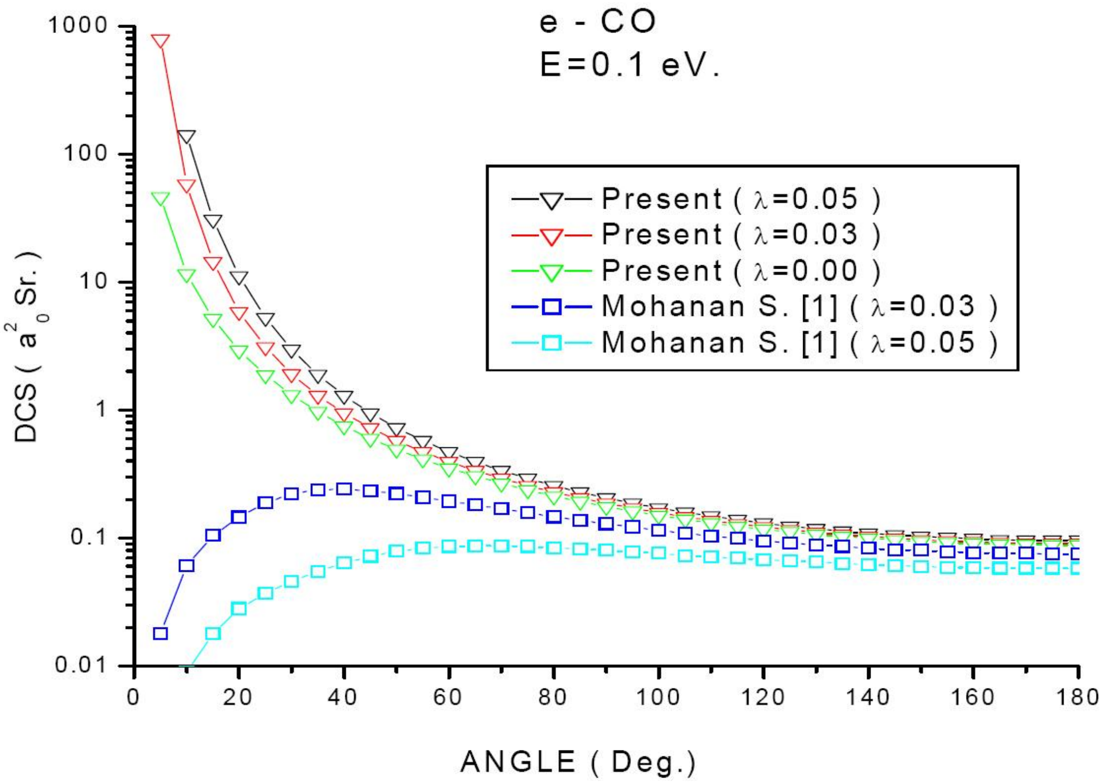

Figure 1 : Differential cross section of e-CO at E=0.1 eV., Triangle line represents present data and square line gives the values from Mohanana S[1].

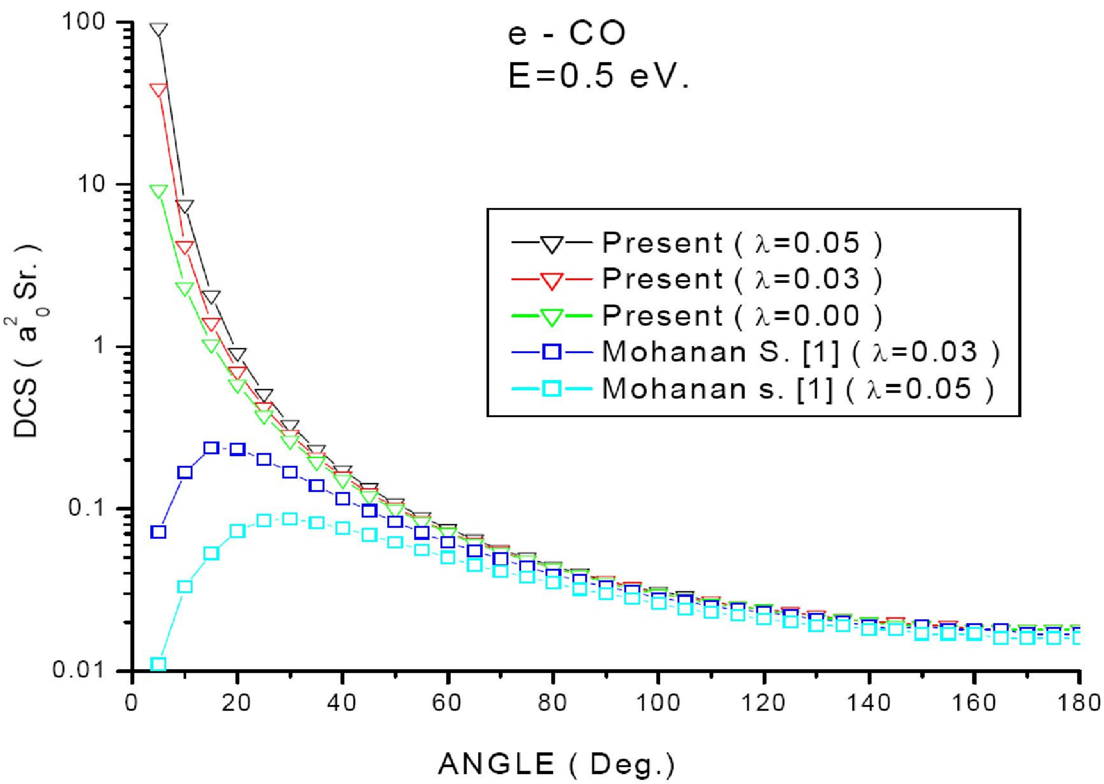

Figure 2 : Differential cross section of e-CO at E=0.5 eV., Triangle line represents present data and square line gives the values from Mohanana S[1].

Figure 1 and 2 show the DCS results of the present calculation for electron scattering by molecule CO in plasma medium at energy 0.1 and 0.5 eV. respectively, using F-BES method with screening parameter $\lambda = 0.03\ a_0^{-1}$, $\lambda = 0.05\ a_0^{-1}$ and without screening ($\lambda = 0$). The present results are compared with the results of Mohanan S. et-al[1] using FBA method at energy 0.1 and 0.5 eV., with screening parameter $\lambda = 0.03\ a_0^{-1}$ and $\lambda = 0.05\ a_0^{-1}$ respectively. It can be seen from the figure 1 to 2 that in the results corresponding to FBA, the plasma screening effect not only reduces the magnitude of the DCS but also alters the angular distribution considerably. But present results corresponding to the F-BES method show that plasma screening increased the magnitude of the DCS considerably and it slightly alters the angular distribution. According to the Mohanan S. et-al[1], the screening factor in eq. (3) reduces the range of the potential so that the small angle scattering is severely affected. Further it can be seen that the DCS at 0.1 eV. more or less isotropic for a weak plasma screening corresponding to $\lambda = 0.01\ a_0^{-1}$, but for strong screening, the forward scattering is eventually wiped out. At higher energies ($E_i > 1.0$ eV.), these effects are confined to small angles (i.e $\theta < 10°$). The present results at angle 80· and above ((i.e $\theta > 80°$), shown good agreement with the results of Mohanan S. et at[1]. So the above result based on FBA and F-BES are expected to be reliable for weakly screen plasma[1].

But in the present case considering the fact that, at the low energy collision, decrement in incident particle energy causes larger DCS. In the case of screening dipole potential, the screening parameter λ - is introduced. Higher value of λ - stands for higher screening as well as it minimizes the target potential by screening. As λ - increases, target potential decreases so larger penetration of incident particle is possible and hence larger interaction time may be given to the collision process. In other words the decrement of potential due to screening is similar to have decrement in incident particle energy. This provides larger interaction time for collision and hence larger DCS compared to unscreened system is obtained. The results of Mohanan S. et-al[1] are not in accordance with this statement. It may be attributed to the mathematical function (arc tan) in their expression of DCS.

It is fact as the energy of incident particle increases, the interaction time for incident particle with target potential is decreasing. In most of cases in literature, it is noticed that DCS decreases as the incident particle energy increases. Similarly DCS increases as the incident particle energy decreases. But the results of Mohanan S. et-al[1] (1990) do not show significant decrement. Hence it will be worthwhile to use screening dipole potential model in Born Eikonal Series (BES) for better to study of low energy electron-molecules collision process in plasma medium.

CONCLUSIONS

The present results obtained by using BES method for very low energy collision under screening are found excellent DCS values as well as angular distribution. The aim of present study is thus fulfilled with low energy results and this present model is a better alternative tool to study the collision in low field plasma with the finite screening. It is fact that as screening increases potential of target decreases, as a result the interaction time between target potential and incident particle increases. It leads to higher DCS values, but in the same case Mahanan S. et al[1] has found decrement in DCS as screening increases. It may be due to arc tan function used in calculations. Lastly in all these discussion the concentration of the polar molecule in the plasma medium is assumed to be small enough, otherwise the change in the energy of the screening electrons, caused by various inelastic processes with the polar molecules would be considerable. The present results may be improved by taking higher term of BES method.

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