International Journal of Pure and Applied Physics.
ISSN 0973-1776 Volume 13, Number 2 (2017), pp. 161-166
© Research India Publications
http://www.ripublication.com

Electron Collision Cross Section for Ceramic Coating Molecules SnO_2, TiO_2 and ZrO_2

Jayantilal G. Raiyani
Shree M. M. Science College, Morbi. (Saurashtra)-363642

Abstract

In this paper, we reports on a theoretical study for electron collision with ceramic coating molecules SnO_2, TiO_2 and ZrO_2. The rotational excitation total cross sections (TCS) are calculated in the energy range from 1 to 100 eV. The Born Eikonal Series Approximation method and the hard sphere dipole interaction potential model are employed to present electron-molecule interaction. The results obtained are compared with experiment and theoretical data available in the literature.

1. INTRODUCTION

Nano materials are cornerstones of Nano science and nanotechnology. Nanostructure science and technology is a broad and interdisciplinary area of research and development activity that has been growing explosively worldwide in the past few years. It has the potential for revolutionizing the ways in which materials and products are created and the range and nature of functionalities that can be accessed. It is already having a significant commercial impact, which will assuredly increase in the future. Development of nanostructured ceramic coatings has become an important research area mainly the interesting chemical and physical properties of Nano scaled materials. The controlled formation of functional ceramic coatings promises applications in the area of Nano electronics, gas sensors, photocatalysts and bio-technologies.[1]

In present investigation, the rotational excitation total cross sections (TCS) are calculated for electron scattering by ceramic coating molecules SnO_2, TiO_2 and ZrO_2 at the energy from 1 to 100 eV. The Born Eikonal Series (BES) Approximation method and hard sphere dipole interaction potential model is employed for present

calculations. The hard sphere cut-off parameter "a" is considered as "D/2", where "D" is dipole moment of molecule.[2,3] The present calculated results are compared with theoretical the results of H. S. Desai et-al[4] using FBA using finite dipole model and other theoretical calculated results of M. T. Varellaet-al[5,6] In general the present TCS results forceramic coating molecules SnO_2, TiO_2 and ZrO_2 in the energy range from 1 to 100eV.are found in good agreement with those of compared results.

2. FORMULATION

BORN EIKONAL SERIES METHOD (BES)

In order to take into account somewhat higher terms of Born series, one can use Eikonal approximation. Ashihara[3] et-al (1975) 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 also applied successfully to the low energy electron molecule collisions(Gerjuoy; 1971). In the present investigations an attempt is made to employ Born Eikonal Series method for the cross sectional calculations for the low and intermediate energy electron with ceramic coating molecular collision.

The interaction potential V(r) can be expressed in following form[2],

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

Where $r_>$ and $r_<$ are the larger and the smaller of r and $P_n(\hat{r},\hat{s})$ is the Legendre polynomial of the order n. "a" is the parameter which indicates finiteness of the dipole and related to the dipole moment by the relation D=2aq. Taking n = 1 only one can get the expression for electron finite dipole interaction potential and it is employed in cylindrical polar co-ordinate, one can name a linear dipole model[7].

$$V(\underline{r},\hat{s}) = V(\underline{b},\hat{z}) = o \qquad \text{for } z < a \qquad \text{--- (2)}$$

$$V(\underline{r},\hat{s}) = V(\underline{b},\hat{z}) = -\frac{D}{b^2+z^2} P_1(\underline{r},\hat{s}) \qquad \text{for } z > a \qquad \text{--- (3)}$$

Where, "a"- is the hard sphere parameter (cut-off parameter).

The formula for the Eikonal phase shift function $\chi(b)$ is given by,

$$\chi(b) = -\frac{2D\gamma}{ki} \int_a^\alpha \frac{z\,dz}{(b^2+z^2)^{3/2}} \qquad \text{--- (4)}$$

'γ" is the direction cosine of the dipole axis with respect to the polar axis.

A series expansion of scattering amplitude as give by,

$$f_{E1} = \frac{2D\gamma}{\Delta \exp(a\Delta)} \quad \text{---- (5)}$$

$$f_{E2} = \frac{2iD^2\gamma^2}{ki} k_0(a\Delta) \quad \text{---- (6)}$$

$$f_{E3} = \frac{4}{3}\frac{D^3\gamma^3}{ki}\frac{e^{-a\Delta}}{a} \quad \text{---- (7)}$$

Where $K_0(a\Delta)$ - is a Bessel function, Δ=Iki-kfI is momentum transferred. The differential cross section (DCS) for three terms in Born Eikonal Series Approximation can be expressed as follow,

$$\frac{d\sigma}{d\Omega}(j_0 m_{j_0} \rightarrow j m_j; \theta) = \frac{kf}{ki}\left|f_{E1} + f_{E2} + f_{E3}\right|^2 \quad \text{--- (8)}$$

Summing over $m_j$and averaging over $m_{jo,}$ one gets the DCS for the rotational ransition $j_0 \rightarrow j_o + 1$.

Therefore using the standard formula, one can calculate the expression for the TCS which will be as follows,

$$Q_{j_o, j_o+1} = \frac{2D^2}{ki^2}\left\{\frac{4(j_o+1)}{3(2j_o+1}\right\}\int_{|ki-kf|}^{|ki+kf|}\frac{e^{-2a\Delta}}{\Delta}\,d\Delta$$

$$+\frac{32D^6}{9ki^6a^2}\left\{\frac{6(j_o+2)(j_o+1)j_o}{175(2j_o+5)(2j_o-1)(2j_o+1)}\right.$$

$$+\frac{3(j_o+1)}{25(2j_o+1)}\left\{\left[\frac{\exp\left[-2|ki+kf|a\right]}{4a^2}\left\{-2a(ki+kf)-1\right\}\right.\right.$$

$$\left.\left.-\frac{\exp\left[-2|ki-kf|a\right]}{4a^2}\left\{-2a|ki-kf|-1\right\}\right]\right.$$

$$+\frac{16D^4}{3ki^4a^4}\left\{\frac{j_o+1}{5(2j_o+1)}\right\}\left[\exp\left[-2|ki+kf|a\right]-\exp\left[-2|ki-kf|a\right]\right] \quad \text{--- (9)}$$

3. RESULTS AND DISCUSSION

Aim of the present study is to obtain theoretical the rotational excitation total cross sections (TCS) are calculated for electron scattering by ceramic coating molecules SnO_2, TiO_2 and ZrO_2 from 1 to 100eV.energy range. The Born Eikonal Series (BES) Approximation method and hard sphere dipole interaction potential model is

employed for present calculation. The hard sphere cut-off parameter "a" is considered as D/2, D-is the dipole moment of molecule.

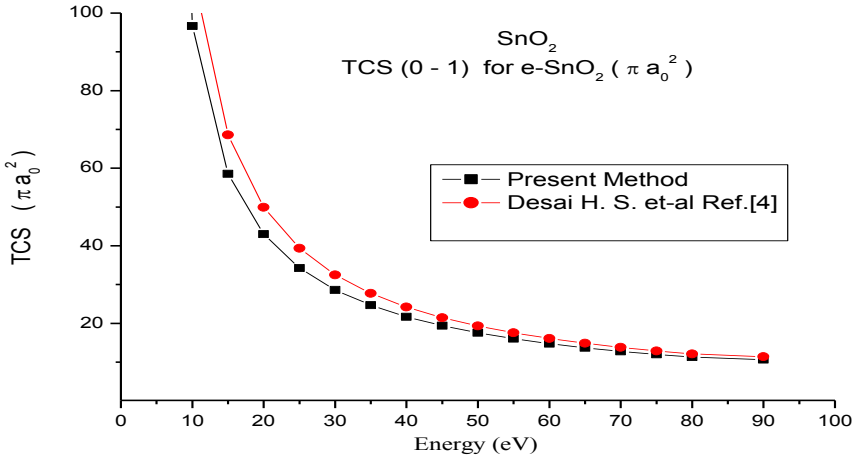

Fig:-1 TCS (0-1) for e-SnO_2 collision

Fig.-1: show the rotational excitation total cross sections (TCS) results for e-SnO_2,in the energy from 1 to 100eV. The present TCS results are compared with the results of H. S.Desai,et-al[4] using FBA method for finite dipole potential model. As shown in fig.-1, it is found that present TCS results decrease sharply at low energy 1 to 25 eV. But at higher energy it decreases slowly. Present results are in good agreement in shape of curves, but differ in magnitude with results of H.S. Desai,et-al.[4] In general the present results are shown in the agreement with the results of H.S. Desai, et-al.[4]

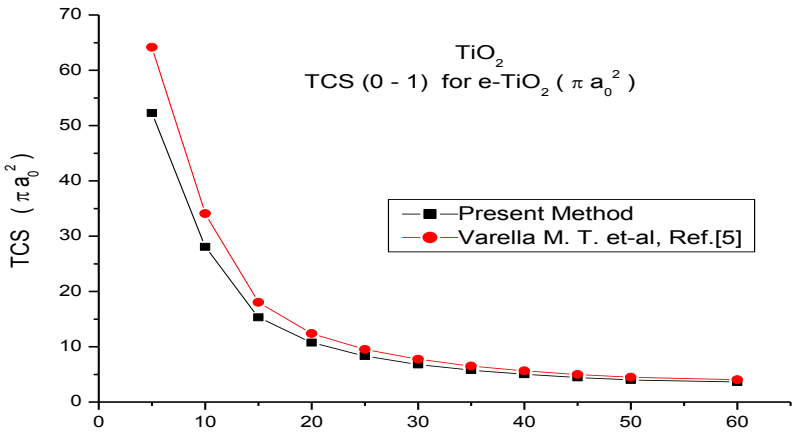

Fig:-2 TCS (0-1) for e-TiO_2 collision

Fig.-2, show the rotational excitation total cross sections (TCS) results for e-TiO_2 in the energy range from 5 to 60eV. The present TCS results are found with sharp decrement at low energy (5 to 25eV) region. At higher energy it decreases slowly. The present TCS results for TiO_2 at energy range from 5 to 60 eV are found better

than results of Varella M.T. et-al[5] In general the present TCS results for ceramic coating molecules TiO_2 at low energy range are found in good agreement with those of compared results.

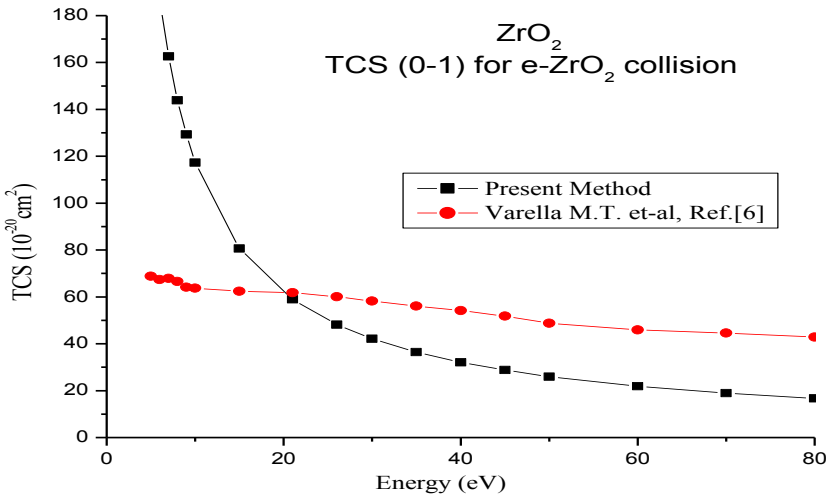

Fig:-3 TCS (0-1) for e-ZrO_2 collision

Fig.-3, show the rotational excitation total cross sections (TCS) results for e-ZrO_2 in the energy range from 5 to 80eV. The present TCS results are found with sharp decrement at low energy (5 to 20eV) region. At higher energy it decreases slowly. The present TCS results for TiO_2 at energy range from 10 to 20eV are found good agreement with results of M. T .Varella, et-al[6] At higher energy from 30 to 80eV, the present TCS results are found lower than as compared with results of M. T. Varella, et-al[6]. In general the present TCS results for ceramic coating molecules ZrO_2 at low energy range are found in good agreement with those of compared results.

4. CONCLUSION

In this work, we have reported a theoretical study of low and intermediate energy of electron collision withceramic coating molecules SnO_2, TiO_2 and ZrO_2 using BES hard sphere dipole potential. The rotational excitation total cross section (TCS) results are presented in comparison with some existing theoretical results.[4,5,6] The present results are in general good agreement with the measured data. This good agreement supports the description of the interaction dynamic considered in the present study and methods used for solving the scattering equations. Hence it will be worthwhile to use hard sphere dipole potential model in Born Eikonal Series (BES) method for better to study of electron-ceramic coating molecules SnO_2, TiO_2 and ZrO_2 collision process in low and intermediate energy region. Calculated data presented in this work, particularly the total cross section will enable completion of a complete set of input data for ceramic coating molecules SnO_2, TiO_2 and ZrO_2. The present results may be improved to consider higher terms in present method.

REFERENCE

[1] S. Mathur et-al, Rev.Adv.Mater.Sci.15, 16-23 (2007)

[2] S. Saha, S. Ray, B. Bhattacharya & A. K. Barua, Phys Rev (USA), 23 (1981), 2926

[3] Ashihara, I.Shimamura and K.Takayanagi, J.Phys. Soc. 38, 1732.(1975)

[4] H. S. Desai and V. M. Chhaya, Ind. J. Pure & Appl. Phys,17,180. (1979)

[5] M. T. Varella, Braz. J. Phys. Vol-.30, 4, 2000.

[6] M. T. Varella, H. F. Bettega, P.Alexandra, Braz. J. Phys. Vol. -30, 1, 2001