# PHYSICAL CHEMISTRY 2004

## *Proceedings*

*of the 7th International Conference on Fundamental and Applied Aspects of Physical Chemistry*

***Volume I and II***

September 21-23, 2004
Belgrade, Serbia and Montenegro

# PHYSICAL CHEMISTRY 2004

## *Proceedings*

*of the 7th International Conference on Fundamental and Applied Aspects of Physical Chemistry*

***Volume I and II***

Editors
A. Antić-Jovanović and S. Anić

| | |
|---|---|
| ISBN | 86-82457-12-x |
| Title: | Physical Chemistry 2004. (Proceedings) |
| Editors | A. Antić-Jovanović and S. Anić |
| Published by: | The Society of Physical Chemists of Serbia, Studentski trg 12-16, P.O.Box 137, 11001 Belgrade, Serbia and Montenegro |
| Publisher: | Society of Physical Chemists of Serbia |
| Printed by: | "Jovan" Printing and Published Comp;<br>300 Copies; Number of Pages: x + 906; Format B5;<br>Printing finished in September 2004. |
| Text and Layout: | Aleksandar Nikolić |

*300 – copy printing*

# THE INFLUENCE OF THE POLARIZABILITY IN SOME BREMSSTRAHLUNG PROCESSES

A. R. Tančić and M. Nikolić*

*The VINČA Institute for Nuclear Sciences, Beograd, Serbia and Montenegro*
**The Faculty of Natural Sciences, Niš, Serbia and Montenegro*

## Abstract

We consider the general results of the theory of the polarizational bremsstrahlung (BrS) and we present the results of recent calculations of the cross sections in the conditions when the radiation of atomic electrons dominates in the total spectrum. For example, we investigated the case when the frequency of the emitted photon is comparable with the energy of the great dipole or plasmon resonance in a cluster (fullerene).

## Introduction

An electron undergoing scattering with some targets absorbs or emits radiations as a result of its acceleration in the target field. A photon is emitted (BrS) or absorbed (inverse BrS). The incident electron gains or loses the corresponding amount of kinetic energy.

In this paper we present recent results of the theory of the polarizational bremsstrahlung PB [1] of clusters and fullerenes. We considered the photon emission in the collisions of electrons with targets under the special conditions. We concentrate our interest on the spectrum of photon emission in the region of frequencies where the polarizability is very large. In this case most of the radiation is formed by the PB. There are two mechanisms of photon radiation during a collision: the ordinary electron BrS (OB) (the photon is emitted by electron decelerating in the static field of the target) and PB (the photon is emitted by the target as a results of its virtual excitations-polarization of target electrons). In the polarizational BrS process the cluster (target) is polarized by a distant collision with the electron. In this case dipole moment is induced in the cluster during the collision process, which is directed along a center-of-mass line of the colliding particles. Since that line rotates in space, the motion of an induced dipole moment is accelerated with a deformed radiating target even it is neutral.

We considered the PB process in collisions of electrons with clusters [1,2] and fullerenes [2,3] because these kind of targets have some features in common with a single atomic system. In the "cluster (fullerene) case" the specific feature of PB process consists in fact that the dominance of the polarization mechanism in the great resonance frequency range is much more pronounced than for atoms. The photon emission spectrum generated in electron-fullerene collisions was described in the main logarithmic approach [1,2]. Recently, experiments of the electron – clusters, and electron-fullerenes [4] have been performed.
We set $\hbar = m_e = c = 1$.

## Results and Discussions

To handle theoretically the metal clusters and fullerenes we can apply the method, which is known for description of atoms [1]. We calculated the PB in the process of the collision of electrons with the clusters (fullerenes). All notations follow those in [2, 3].

The total amplitude of Bs (including OB and PB) radiative mechanisms are [2, 3]:

$$A^{tot} = <\Psi_2 \left| \vec{e}\vec{r} \right| \Psi_1> + \int \frac{d^3 q}{(2\pi)^3} \frac{4\pi}{q^2} <\Psi_2 \left| e^{i\vec{q}\vec{r}} \right| \Psi_1> \vec{e}\vec{q}\, \alpha(\omega, \vec{q}) \quad (1)$$

$\Psi_1, \Psi_2$ are the initial or final wave functions of the electron (respectively), $q$ is the momentum transfer, $\vec{e}$ is the photon polarization vector and $\alpha(\omega, \vec{q})$ is the generalized dynamic polarizability of the target:

$$\vec{e}\,\alpha(\omega, \vec{q}) = i \sum_n 2\omega_{n0} (\omega_{n0}^2 - \omega^2 - i\delta)^{-1} <0 \left| \sum_j \exp(i\vec{q}_j \vec{r}_j) \right| n> D_{n0}(\omega) \quad (2)$$

where $\omega_{n0} = \varepsilon_n - \varepsilon_0$ is the transition energy between the ground and excited sate of the cluster. The delocalized electrons in the cluster are denoted by index j. $D_{n0}$ describes the interaction of the cluster with the radiation field. This interaction we describe in the framework of the Random Phase Approximation with Exchange (RPAE) [1]. Treating the $a/R$ (where $R$ is the radius of the cluster and $a$ characterizes the depth of the surface layer on cluster (or the thickness of the fullerene depth) as a small parameter, we can obtain the expression for $\alpha(\omega, \vec{q})$ which is applicable near a plasmon resonance $\omega_p$. Using the alteration of the electron density of a cluster (fullerene) $\delta\rho(\vec{r})$ under the action of an external field in the RPAE [1, 3], we can obtain the generalized dipole polarizability $\alpha$ for the cluster or fullerene. As an example we calculated the PB spectra for electron-$C_{60}$ collision using the expression [2]:

$$\omega \frac{d\sigma}{d\omega} = \frac{16 e^2 \omega^4}{3 c^3 v^2} \left| \alpha(\omega) \right|^2 [S_1(q_{\min} R) - S_1(q_{\max} R)] \quad (3)$$

where the functions $S_1$ are defined in [2]. In fig. 1 we plotted the PB spectra. Our results are presented as a full curve 1 and correspond to the calculations of $\alpha(\omega)$ in the simplified version of the RPAE [3]. The polarizational mechanism manifests itself in the resonance behavior of the spectrum at $\omega \approx \omega_p$.

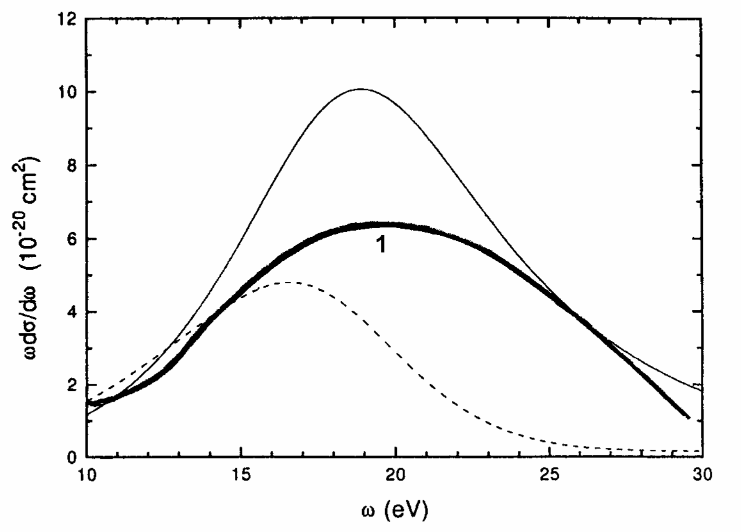


**Fig.1.** PB cross section for $e^- - C_{60}$ collision as a function of emitted photon energy for projectile electron velocities: $v = 3{,}5$ (full curve), $v = 2$ (broken curve) [2], and for $v = 4$ (full curve 1,our result).

## Conclusion

Our results are close to the other calculations [2]. In ref. [2] $\alpha(\omega)$ was partially derived from the empirical data and by applying the dispersion relations. The correct description of PB, in the vicinity of the great plasmon resonance is only possible by accounting the many-electron correlation effects.

## References

[1] M. Ya. Amusia , Tormoznoe izluchenie, Moskow (in Russian), 1990.
M. Ya . Amusia, Atomic Bremsstrahlung, Phys. Rep., 1988, 162, 249.
[2] A. V. Korol and A. Solovy`ov, J. Phys. B., 1997, 30, 1105.
N. Avdonina and R. Pratt, J. Phys. B, 1999, 32, 4261.
[3] A. R. Tancic, NTB, 2001, 1, 149.
[4] V. Kresin, A. Scheidemann and W. Knight, Proc. Int. Symp. on Elec. Collis. with Molec., Clusters and Surfaces, 1993, London
J. Keller and M. Kaplan, Chem. Phys. Lett., 1992, 193, 89.