Processes Stimulated in Organic Samples by Cluster Projectile Bombardment

M. Kański¹ and <u>Z. Postawa¹</u>

¹ Jagiellonian University, Faculty of Physics, Astronomy and Applied Computer Science, Smoluchowski Institute of Physics, Łojasiewicza 11, 30-348 Kraków, Poland

zbigniew.postawa@uj.edu.pl

Energetic ion beams have numerous applications in various fields of science and technology. Applications of particle bombardment include surface cleaning, surface smoothing, implantation of dopants in semiconductors, focused ion beam milling for integrated circuit repair and TEM sample preparation, reactive ion etching, and cancer treatment.

Particularly interesting applications of ion beams are the analytical techniques of Secondary Ion Mass Spectrometry and Secondary Neutral Mass Spectrometry (SIMS/SNMS), especially when applied to 3D chemical imaging of organic and biological samples. Several conditions should be achieved in these approaches to allow for the chemical analysis of organic materials. For example, the primary kinetic energy transferred to the sample should be low enough to avoid substantial collision-induced fragmentation. On the other hand, this energy must be sufficient to initiate molecular desorption and ionization.

The fundamental challenge is to find conditions that fulfill all of these demands. Various projectiles have been tested, and it has been found that cluster projectiles are an especially interesting choice. A variety of cluster projectiles have been utilized, starting with "standard" ones like Au_n , Bi_n , C_{60} , or Ar_n gas clusters and progressing to more sophisticated configurations like $(CO_2)_n$ or $(H_2O)_n$. The impacts of these projectiles lead to new energy deposition pathways and ejection processes. Another interesting direction for developing SIMS/SNMS techniques is the application of new substrates like graphene or water.

Recent progress in the implementation of these new concepts will be presented. The processes involved in molecular emission in these novel analytical configurations will be discussed based on the results of the Molecular Dynamics computer simulations.

The work has been supported by Polish National Science Center Grant no. 2019/33/B/ST4/01778. Computer simulations were performed on the PLGrid Supercomputer infrastructure.