Filtering the Energy Band Structure of Free Clusters using Site-Selective Resonant Auger Spectroscopy

***M.Tchaplyguine*[1], *R.Feifel*[1], *M.Gisselbrecht*[2], *R.Marinho*[3], *S.Sorensen*[4], *S.Svensson*[1] *and O.Björneholm*[1]**

[1]*Uppsala University, Department of Physics, Uppsala, SWEDEN*

[2]*MAX-LAB, Lund University, Lund, SWEDEN*

[3]*Institute of Physics, Brasilia University, Brasilia, BRAZIL*

[4]*Department of Synchrotron Radiation, Lund University, Lund, SWEDEN*

Until recently free clusters have been rather difficult to study with synchrotron radiation. Site specific core-level electron spectroscopy that - for example - could provide data for independent cluster size estimation was difficult to perform due to the low "sample" density. Only with the appearance of undulator beam lines it became possible to carry out X-ray photoemission spectroscopy (XPS) and X-ray absorption spectroscopy (XAS) measurements on free clusters [1]. It allowed to separate the core-level transitions for the electrons located on the surface of the clusters and in their bulk. However the challenge of really resonant site- and energy specific selective excitation studies has remained unanswered. Yet the study of free clusters could give information not only about the transition from the separate atoms/molecules to the solid state, but - with the large clusters in question - this study can "purify" our knowledge on the solid state itself - at the nanoscale dimensions. Indeed the unavoidable and often not precisely known influence of the substrate in a standard X-ray solid state experiment is not present in the case of free clusters. Moreover an absolute energy calibration in an XPS, XAS or resonant Auger spectroscopy (RAS) spectrum is simplified for the cluster beam by the presence of the well-established atomic features from the uncondensed atoms.

In the studies reported here the advantages of three experimental foundations - synchrotron radiation of high brilliance and stability, high resolution electron spectroscopy and core-level excitation as a local probe of the electronic and geometric structure - put together have allowed the authors to obtain novel results in the field of cluster physics. Our recently commissioned gas-phase cluster source combined with the soft X-ray beam line I411 at MAX-LAB, Sweden provided high intensity cluster signal in various types of core-level spectra. Argon, krypton and xenon clusters containing from a few tens to more than 3000 atoms were produced in an adiabatic expansion. A Scienta electrostatic energy analyser was used for XPS, XAS, RAS and normal Auger measurements. For argon clusters, studied most extensively, the evolution of the features belonging

to the "bulk" and "surface" secondary electrons emitted as the result of the excitation from the 2p core level to the Rydberg states was possible to follow through the XA spectra. For the first time selective resonant excitation of the electrons from the cluster surface and bulk was performed in a wide range of excitation energies probing the cluster transitions corresponding to the 4s, 3d and higher Rydberg atomic states. Most of the cluster features in these 60meV at 250eV photon energy resolution RA spectra were identified. It has enabled the experiments with the partial secondary electron yield collecting the electrons in the energy windows corresponding either to the definite singly charged final states in atoms, or in cluster surface and bulk. In this series of measurements the cluster features were filtered out from the complex argon cluster XA pattern. The possibilities opened by such site-selective RAS measurements will be further discussed.

[1] O.Björneholm, F.Federmann, F.Fössing, and T.Möller. Phys.Rev.Lett.,v.74, p.3017, 1995.