MAXIMA in X-ray Absorption Near Edge Structure corresponding to one-electron quasi-stationary states (shape resonances) contain various information about objects under investigation. Positions and widths of the maxima depend strongly on arrangements and types of atoms, the presence and nature of defects, the distribution of electric charge, etc. This is why the study of Xanes can be a useful tool for the structure determination, particularly in the case of unordered systems.

A scheme of extracting information from experimental data related to shape resonances was proposed by the author recently [1, 2]. It is based on the S-matrix pole equation within the muffin-tin approach [3]. The system of square-well potentials with depths depending on the orbital quantum number l is used [4].

The scheme has been tested by the determination of geometric parameters of the free molecules N_2, NO_2 and CH_3 NO_2 and the solid compound NaNO_2. It was shown that this scheme enables to determine intermolecular distances up to 1% and valence angles up to 5%.

The method proposed can be applied to investigate parameters of molecules adsorbed on solid surfaces. For example, the adsorption of the O_2 molecule on the Cu(100) surface is studied. By using the oxygen K-spectra the most probable location of the molecule, the molecule-surface distance and the change of the O-O distance caused by the adsorption are found.

The results so far indicate that both structure models present, but do not coexist in the same crystal specimen.

REFERENCES