CONTROL OF COMPOSITION OF MINERAL WATERS USING RAMAN SPECTROSCOPY AND ARTIFICIAL NEURAL NETWORKS

I.V. Plastinin[1], A.M. Vervald[1], S.A. Burikov[1,2], E.N. Vervald[1], T.A. Dolenko[1,2], A.O. Efitorov[2], K.A. Laptinskiy[1,2], O.E. Sarmanova[1], and S.A. Dolenko[2]

1. M.V. Lomonosov Moscow State University, Physics Department. Leninskie Gory 1/2, Moscow, Russia, 119991
2. M.V. Lomonosov Moscow State University. D.V. Skobeltsyn Institute of Nuclear Physics, Leninskie Gory 1/2, Moscow, Russia, 119991

At the present time table and mineral waters occupy an increasingly important place among non-alcoholic beverages. Mineral water is used not only for quenching thirst but also for the treatment of various diseases. That is why a control of composition of mineral waters is very urgent problem. Natural mineral water extracted from deep aquifers is a multi-component solution containing ions of inorganic salts, gas molecules and colloidal particles. The composition of natural mineral water is quite complicated and it is determined by the geostructural features of the region where it is extracted. The control of composition and quality of mineral water is the solution of the problem of the identification of dissolved substances (firstly, ions of inorganic salts - sodium (Na^+), calcium (Ca^{2+}), magnesium (Mg^{2+}), chlorine (Cl^-), sulfate (SO_4^{2-}), bicarbonate (HCO_3^-) etc.) and the determination of their concentration.

For determination of the concentration of dissolved in water ions various methods are used: amperometry, potentiometry, voltammetry, chromatography, flow-injection approaches. These methods allow determining the concentration of dissolved ions with high accuracy but they have a lot of drawbacks – they are laborious, time consuming, they require a special preparation of samples. The methods of optical spectroscopy, firstly, Raman spectroscopy (RS), favorably differ from them. These methods do not require a special sample preparation, they are rapid and can be implemented in the remote mode. The principal opportunity of the determination of type and concentration of ions using Raman spectra is caused by two factors. At first, complex ions (for example, sulfate ion) have their own Raman peaks in the spectral region of so-called “finger prints” (500-1600 cm^{-1}). Secondly, presence of ions of inorganic salts in water changes the network of hydrogen bonds in water and it reveals in change of the form of water Raman valence band.

In Figure 1 one can see the Raman spectrum of one of the mineral waters (Novoterskaya Tselebnaya). In the low-frequency region of the spectrum (in the inset) one can observe the peaks of complex ions, a broad structureless band with a maximum near 3400 cm^{-1} is the water Raman valence band.

The problem of determination of the concentration of each of dissolved ions in the presence of the other ions using Raman spectra is multi-parametrical inverse problem of optical spectroscopy. The solution of this problem is complicated by the fact that, firstly, the concentration of ions in the mineral waters are relatively small and, therefore, changes of spectra are also small. Secondly, from the point of view of data processing it is necessary to obtain an information from data of high dimensionality (hundreds of spectral channels). In the case when it is impossible to describe the spectra of studied system analytically, traditional algorithms cannot provide the solution of this problem with acceptable accuracy. Using artificial neural networks (ANN) is effective method of the solution of such multi-parametrical inverse problems.

In this study the problem of determination of the type and concentration of dissolved in water ions was successfully solved by means of ANN for model solutions. The used approach was tested on the large set of mineral waters from different regions of Russia and world (about 150 samples). It was established that the concentration of the most common ions can be determined with sufficiently high accuracy - 10^{-4}-10^{-6} M. It indicates the prospects of using Raman spectroscopy in combination with ANN for the diagnosis of mineral waters.

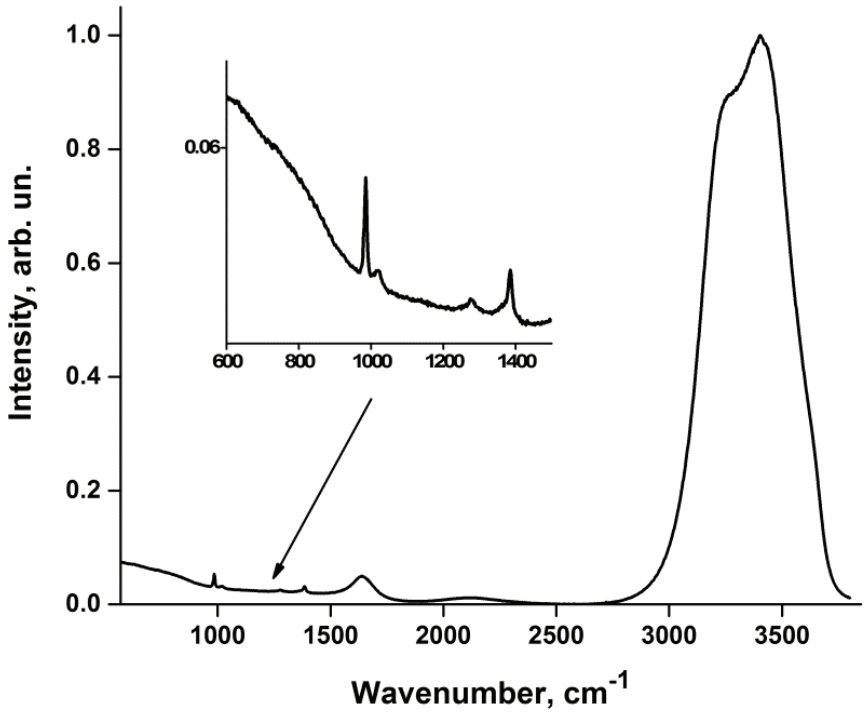

Figure 1 Raman spectrum of mineral water Novoterskaya Tselebnaya.

ACKNOWLEDGEMENT

This study has been performed at the expense of the grant of Russian Science Foundation (project №14-11-00579).