Raman Spectroscopy of Guanajuatite – Natural Topological Insulator

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Topological insulators are a new class of materials which are semiconducting in bulk but conducting on their surface [1]. One of its representatives is bismuth selenide (Bi$_2$Se$_3$), which occurs naturally as a mineral called guanajuatite. Bi$_2$Se$_3$ has a layered structure consisting of quintuples – alternating mono layers of bismuth and selenium atoms in the stoichiometric ratio.

The technique chosen for low-dimensional structure studies is Raman scattering spectroscopy. This is due to the sensitivity of the Raman spectrum to such effects as strain or disorder. We have employed micro-Raman spectroscopy to study the properties of bulk crystal of natural Bi$_2$Se$_3$. Three of four Raman active phonon modes (two A$_{1g}$ and one E$_g$ corresponding to the out-of-plane and in-plane vibrations respectively) are studied in a wide range of temperature (4 - 300 K) with a non-resonant excitation ($\lambda$=632.8 nm).

A linear temperature dependence of active Raman modes, which we applied as a first approximation, enables us to determine the first order temperature coefficients of the phonon energies. Our Results span the range from 1.0 to 1.7 x 10$^{-2}$ cm$^{-1}$/K depending on the mode, which is in reasonable agreement with previously published data on synthetic on Bi$_2$Se$_3$ [2]. It is shown that the widths of the observed Raman peaks in guanajuatite (down to 1.93 cm$^{-1}$) are similar to the corresponding values in the synthesized Bi$_2$Se$_3$ confirming the quality of natural crystals [3]. We also noticed rather unexpected non-monotonic evolution of all the peaks at the lowest temperature. We tentatively relate the observed broadening of the peaks at $T = 4.2$ K to the emergence of otherwise Raman-inactive vibrational modes, activated at low temperature. Possible mechanisms responsible for the effect are discussed.

Fig. (a) Raman spectra of guanajuatite in 4 K and 300 K (b) Energy and peak width for A$_{1g}$ mode in the temperature range of 4 K - 300 K