ABM 21P **RAMAN AND INFRARED VIBRATIONAL SPECTRA OF $PbGa_2S_4$ CRYSTAL**

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Raman scattering spectra in different geometries at temperatures 10 - 300 K and infrared vibrational spectra in polarizations E||c and E⊥c for range 50 - 4000 cm^{-1} at 300 K were investigated for $PbGa_2Se$ crystals. Contours of reflection spectra in polarizations E||c and E⊥c were calculated and parameters of phonons and dielectric constants were determined. Temperature dependences of Raman spectra were investigated and soft modes with different temperature dependences in intervals 80 - 150 and 150 - 370 K were discovered. A group of lines attributed to Davydov multiplets was found out and their polarization dependences temperature changes were investigated. Effective ion charges were calculated and a polarizability of ionic charges of Pb, Ga and S in $PbGa_2S_4$ lattice was determined.

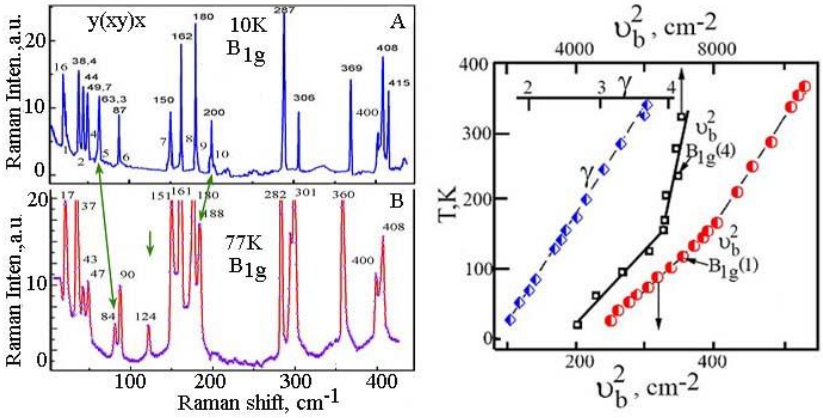

Fig. 1 Raman scattering spectra of $PbGa_2S_4$ crystals measured in y(xy)x geometry at temperatures 10 K (A) and 77 K (B). The temperature dependence of two vibrational modes 23 cm^{-1} (300 K) and 86 cm^{-1} frequency square (300 K) of B_{1g} symmetry (C).

Figure 1 shows Raman scattering spectra in y(xy)x geometry measured at temperatures 77 K and 10 K. A temperature reduction from 77 to 10 K leads to Raman scattering lines narrowing and new lines arising. The vibrational modes 278 cm^{-1} and 369 cm^{-1} shift most strongly on 9 cm^{-1} and 12 cm^{-1}, respectively. Two lines 162 and 179 cm^{-1} are discovered at room temperature in frequencies interval 150 - 240 cm^{-1}. Four lines 151, 161, 180 and 188 cm^{-1} are observed at 77 K, these lines are presented and at temperature 10 K (see Fig. 1). A temperature change from 77 to 10 K has the greatest influence on 188 cm^{-1} vibrational mode it shifts on 12 cm^{-1}. The over three lines practically do not shift. Six vibrational modes are observed in frequencies interval 10 - 100 cm^{-1} (Fig. 1). Low frequency vibration mode B_{1g} (23 cm^{-1} at 300 K and 16 cm^{-1} at 10 K) shifts the most distant at temperature decreasing. Frequencies of vibrational modes at high-frequency increase with temperature decreasing but in low-frequency the situation is opposite. Figure 1, C shows a temperature dependence of frequency square for two vibrational modes $B_{1g}(1)$ and $B_{1g}(4)$. Such change of vibrational mode in $PbGa_2S_4$ crystals indicates about structural instability of this crystal. We suppose that $PbGa_2S_4$ crystal suffers a phase transition at low temperatures. One can speculate that lines 23 and 87 cm^{-1} are soft modes. The temperature dependence of frequency square for both lines is described by relationship $\nu^2 = (\Delta T)^{\gamma/2}$, where γ = 1.1±0.1 for interval 10 - 150 K and γ = 0.7±0.1 in interval 150 - 300 K. At the same time a line 278 cm-1 shifts strongly to high-frequency part with temperature decreasing (Fig. 1). The damping of soft mode (17 and 87 cm^{-1}) isn't found out in investigated temperature interval.