Nanocomposites and nanomaterials

Theoretical and experimental study of phonon spectra nano-sized MoS_2 layers and mixed $MoS_2/MoSe_2$ layer crystals

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The spectroscopic study of layer type crystals was conducted during the long period of time beginning from the 1970-s. Investigation was connected with both the electron and the vibration properties of such crystals. During the early period, beginning from the 1970-s, the phonon study of different types of layer crystals: GaSe, GaS, MoS_2, As_2S_3, $MoSe_2$, MoW_2 etc. was made. Moreover, some models explaining observed features, in particular Davydov splitting effect, were proposed. The new period in the study of such crystals begins with the method of Novoselov et al. [1] for graphen that allows preparation of a very thin crystal structure that has 1-10 atomic layers. Layer type crystals MoS_2 and $MoSe_2$ are especially perspective in this field, while they show interesting spectroscopic features if crystal structure consists of only several n=1-6 atomic layers. Electron band structure of such crystals differs from the bulk ones and they demonstrate very intensive luminescence.

In the present work the change of Raman spectrum as a function of the "concentration" layers $(MoS_2)_x/(MoSe_2)_{1-x}$ was considered and the case x=1 was studied for very thin layers. It was shown that even a weak interlayer interaction in crystals can affect intralayer bonding and lattice dynamics. This is similar to Fermi-Davydov resonance in molecular type crystals. If interlayer interaction between some layer states is admitted (like to Fermi resonance in molecule) new states ω_f, and ω_g arise. Two types of Davydov's terms appear in the crystal due to the weak interlayer interaction and exchange excitations between these states: diagonal, D^{ff}, M^{ff}, D^{gg}, M^{gg} and non-diagonal D^{gf}, M^{gf}. The diagonal terms result in the shift of all spectral bands, but non-diagonal give rise to repulsion between the new crystal states. Therefore the shift of high- and low-frequency components of doublet should be in different sides. Similar fact was observed in and in our experiments.

1. *Novoselov K.S., Jang D., Schedin F., Booth T.J., Khotkevich V.V., Morozov S.V., Geim A.K.* Two dimensional atomic crystal. Proc. Nat. Acad. Sci. USA, 2005. **102.** -P. 10451-10453.