Vibrational characteristics of graphene-based materials and hexagonal modification of niobium dichalcogenide: stability, low-dimensional peculiarities and peculiarities of phonon expansion and localization

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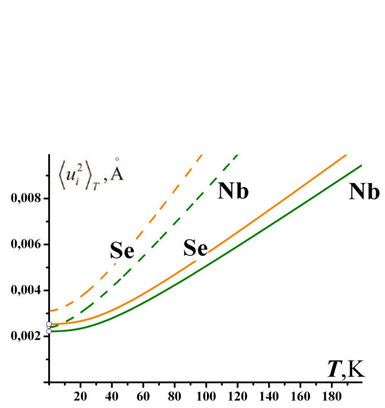
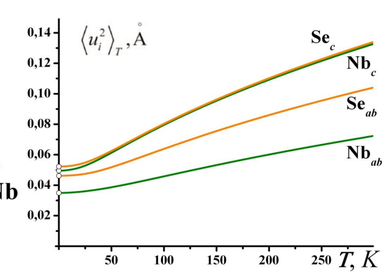
The synthesis of new materials with unique low-temperature properties, characterized by pronounced anisotropy, led to the observation, generally made by neutron-diffraction methods, of completely new features of the electronic and vibrational characteristics of such systems. Recently, "graphene rush" has stimulated numerous experimental and theoretical studies of low-dimensional inorganic conductors. Despite this, the influence of inhomogeneities of crystal structure puts even more questions than answers both in graphene and dichalcogenides of transition metals – their role on the formation of nanofilms and nanotubes as well as on the unique properties of considered nanostructures still remains unclear [1]. Therefore, a detailed analysis of the features of the vibrational and electronic properties of such nanostructures as well as an influence of various types of defects on considered materials is an actual problem. The present work is based on the study and comparative analysis of the behavior of graphene-based and containing defects layered 2H-$NbSe_2$ materials by changing temperature, revealing their general laws and the possibilities of controlling their electronic properties. The main research methods are measurements of elastic and inelastic scattering of X-rays and neutrons in comparison with the results of the original numerical experiment. During the experiment, the intervals of temperature stability were established in layered crystals formed both by monoatomic layers (graphene nanofilms) and multilayered "sandwiches" (dichalcogenides of transition metals) with defects of various types. The influence of defects with broken bonds on the local densities of electronic states (LDOS) of graphene materials was also detected and analyzed.

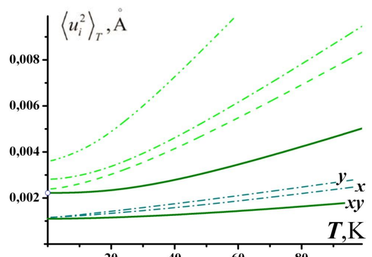
2H-$NbSe_2$

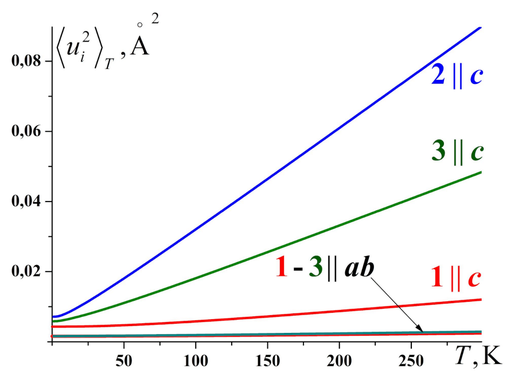
Graphene-based materials

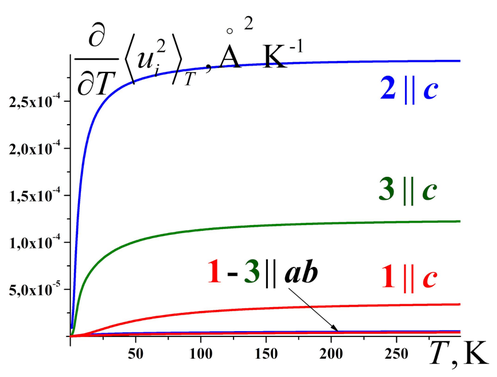
stability



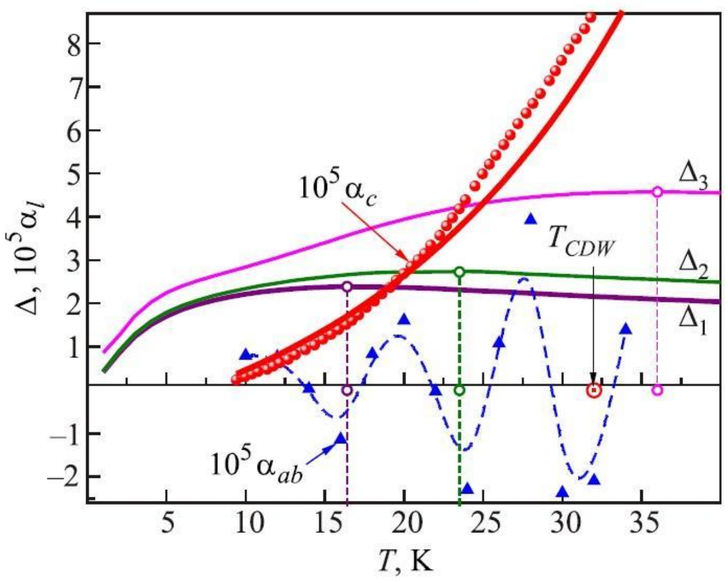






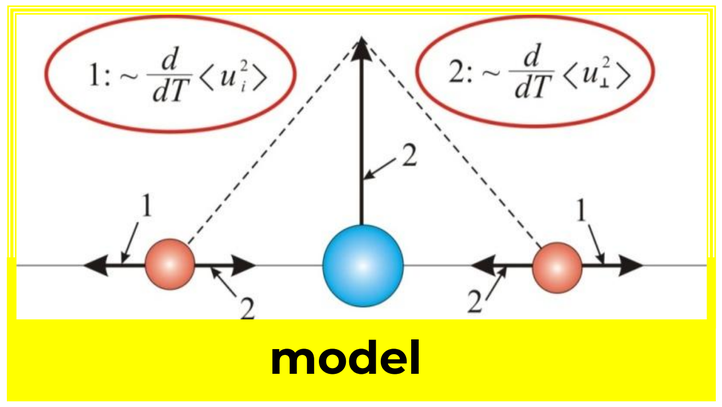


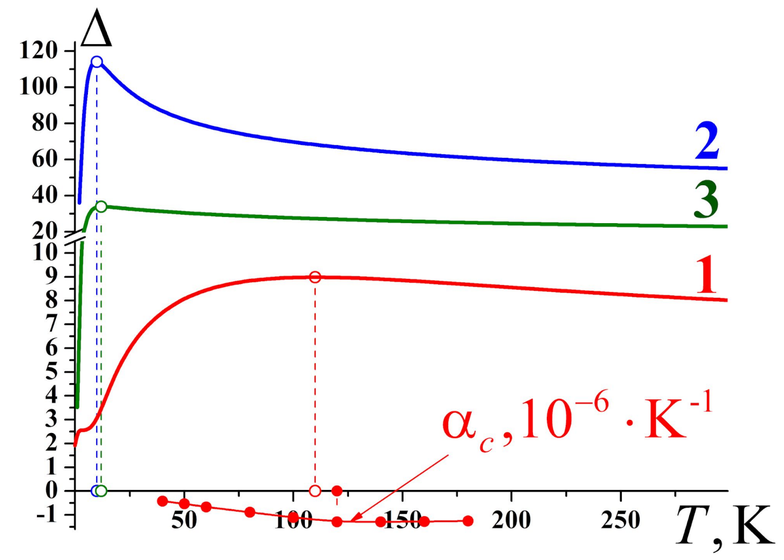
low-dimensional peculiarities



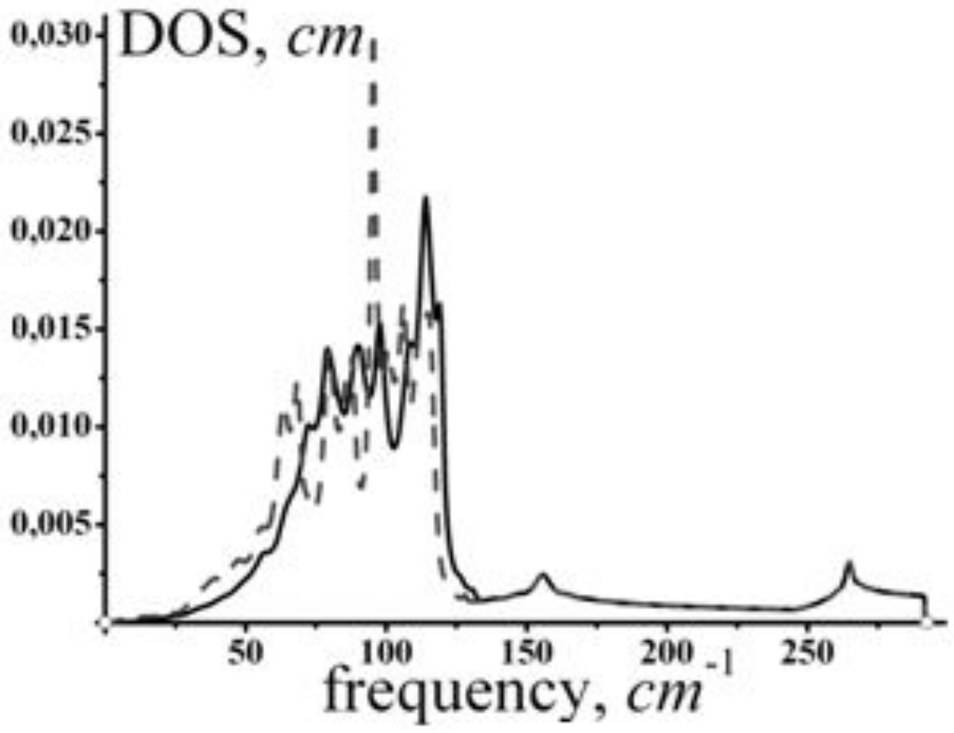
$$\alpha_{\parallel}(T) = A\frac{\partial}{\partial T}\langle u_{\parallel}^2\rangle_T\left[\delta - \Delta(T)\right];$$

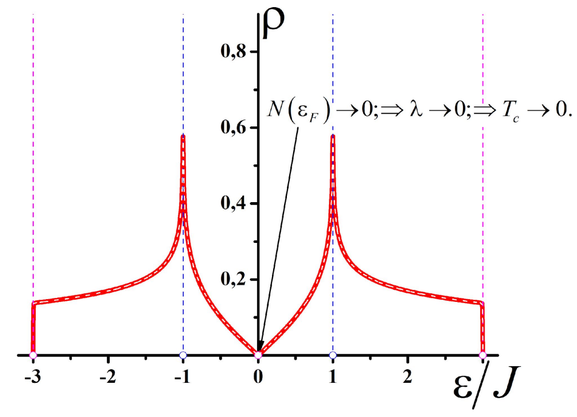
$$\Delta(T) \equiv \frac{\partial}{\partial T}\langle u_z^2\rangle_T \Big/ \frac{\partial}{\partial T}\langle u_{\parallel}^2\rangle_T;$$

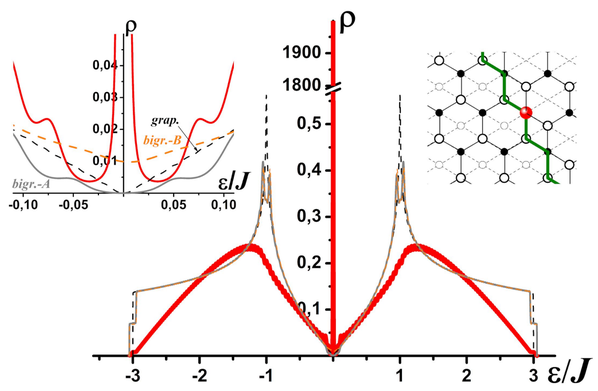


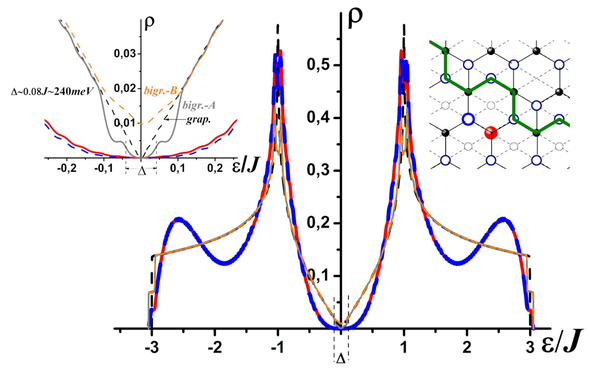


phonon expansion and localization









References

1. V. V. Eremenko, A. F. Sirenko, V. A. Sirenko, A. V. Dolbin, I. A. Gospodarev, E. S. Syrkin, S. B. Feodosyev, I. S. Bondar, and K. A. Minakova, *Low Temp. Phys.* **42**, 99 (2016). (https://doi.org/10.1063/1.4941004).