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Lattice dynamics and specific heat of antifluorite superionic oxides M_2O (M=Li, Na and K): A comparative study

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Superionic oxides like Li_2O, Na_2O and K_2O are the materials of technological interest, exhibits high ionic conductivity while in solid condition and belongs to the class of fast ion conduction, which allow macroscopic movement of ions through their structure. These superionic conductors find several technological applications. These applications range from miniature light weight high power density lithium ion batteries for heart pacemakers, mobile phones, laptops computers, etc. to high capacity energy storage devices for next generation. Therefore knowledge of the thermal properties of these materials is most significant. Hence in the present study we have studied phonon dispersion relation, phonon density of states and specific heat of Li_2O, Na_2O and K_2O in antifluorite structure by applying lattice dynamical theoretical model. The calculated results are interpreted with existing experimental or theoretical results.

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Influence of neutron flux on temperature dependence of dielectric properties of nano SiO_2

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As a research object it has been taken SiO_2 with 160 m^2/gr specific surface area, 20 nm particle size and 99.5% purity. Nano SiO_2 has been irradiated at full power mode (250 kW) by neutron flux with $2x10^{13}$ n/cm^2s flux density in central channel (channel A1) at TRIGA Mark II light water pool type research reactor in "Reactor Centre" of Jozef Stefan Institute in the Slovenia. It is important to note that the JSI TRIGA reactor has been thoroughly characterized and the computational model used for computational characterization has been thoroughly verified and validated against several experiments. While working at full power mode, the neutron flux has the following composition parts: $5.107x10^{12}$ n/cm^2s (1±0.0008, E_n< 625eV) for thermal neutrons, for epithermal neutrons – as $6.502x10^{12}$ n/cm^2s (1±0.0008, E_n ~ 625eV ÷ 0.1MeV), for fast neutrons - $7.585x10^{12}$ n/cm^2s (1±0.0007, E_n> 0.1 MeV) and finally for all the neutrons in central channel flux density is as $1.920x10^{13}$ n/cm^2sec (1±0.0005). Electric parameters of initial and neutron-irradiated nano SiO_2 have been measured in "Novocontrol Alpha High Resolution Dielectric Analyzer" device at 0,09Hz – 2,3MHz range of frequency and 100K – 400K temperature range in the laboratory of "Condensed Matter Physics F5" of JSI. In the result of the conducted researches it has been revealed that under neutron flux influence extra "charges" are generated inside nano SiO_2 samples. The generated "charges" lead to an increase in polarization in the sample. So it increases the numerical value of real and imaginary parts of dielectric constant in proportion to irradiation. In general tendency specific charges and the ones generated with the influence of neutron flux are polarized more actively under temperature influence. As a result, real and imaginary parts of dielectric constant increase with temperature increase within about 100-300 K range. At about 300-400 K temperature range some "charges" generated under the influence of neutron flux are lost due to temperature effect and polarization reduces. The effects occurred under temperature influence are observed more obviously at low frequencies. Destruction of the charges with different barrier energy existing in the system due to frequency influence, lead to a decrease in numerical value of real and imaginary parts of dielectric constant.

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