formalisms based on the Born [1] and Keating [2] models, including Coulomb and retarded interactions, were applied for describing the interactions between atoms. The results obtained in [1] and [2] show the fair sensitivity of FIR-RAS to localized surface phonons.
In this work, we investigate the surface photon-phonon coupling in diamond-type semiconductors, as well as its manifestation in far-infrared reflectance anisotropy spectra. In the investigation, reconstructed (001) surfaces are considered. We apply the adiabatic bond charge model to describe short-range and long-range-Coulomb interactions among ions and bond charges in the bulk and near the surface. Besides, we also include the interaction with the retarded transverse electromagnetic field produced by the vibration of the charged particles. The system of coupled equations for the displacements of ions and bond charges and for the retarded transverse electromagnetic field inside a semi-infinite semiconductor was solved. With this solution, we have calculated spectra of normal incidence reflectivity. Specifically, the theoretical FIR reflectance spectra for Si(001) and Ge(001) surfaces in the (2×1) dimer geometry were studied. Here, the correlation between the resonance structure of the spectra and the excitation of surface-phonon modes was analysed. In addition, we have compared the positions of the reflectivity resonances with the surface-phonon frequencies of Si(001) (2×1) and Ge(001) (2×1) at the $\overline{\Gamma}$ point, which were calculated with the adiabatic bond charge model in [3] and [4], respectively.

Our results show the usefulness of the FIR reflectance anisotropy spectra for measuring surface-phonon frequencies.

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Interface and confined optical phonons in wurtzite ZnO quantum dots

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Quantum dots and nanocrystals made of wide-bandgap wurtzite semiconductors such as ZnO have recently attracted significant attention as promising candidates for many optoelectronic applications. Interpretation of experimental data related to optical response of ZnO quantum dots has been complicated due to the absence of accurate theoretical models for phonon spectrum in such structures.

In this paper we will present our derivation of an integral equation that defines both interface and confined polar-optical phonon modes in nanocrystals with wurtzite crystal structure and arbitrary shapes [1–2]. Based on this equation, we calculated optical phonon modes in spherical wurtzite ZnO quantum dots. Unlike in spherical zinc-blende nanocrystals, the

spectrum of interface and confined optical phonons in wurtzite nanocrystals depends on the z-projection m of the angular momentum l. Moreover, for each pair (l, m) there is one interface optical phonon and $l - |m|$ confined optical phonons ($l - 1$ for $m = 0$). The experimental resonant Raman spectra of spherical ZnO quantum dots exhibit two peaks in the region of polar optical phonons at $393\,\mathrm{cm}^{-1}$ and $588\,\mathrm{cm}^{-1}$ [3]. Taking into account the selection rules for Raman, we show that the observed peaks correspond to the confined TO mode with $l = 4$, $m = 0$ ($\omega = 393.7\,\mathrm{cm}^{-1}$) and the confined LO phonon mode with $l = 2$, $m = 0$ ($\omega = 587.8\,\mathrm{cm}^{-1}$). We also found that the frequencies of the interface optical phonons are very sensitive to the change in the optical dielectric constant of exterior medium while the frequencies of confined optical phonons are much less sensitive. Derived analytical expression and computation procedure can be used for accurate prediction of the interface and confined phonon frequencies in anisotropic nanocrystals.

Preliminary results of micro-Raman spectroscopy investigation of optical phonons in ZnO thin films and nanostructures will also be discussed [4].

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Structural, electronic and dynamical properties of the Ge(001)/Sb(2x1) surface

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The structural, electronic, and vibrational properties of the Ge(001)/Sb(2×1) surface were investigated by using the plane-wave pseudopotential theory and the density functional scheme. The calculated structural parameters for this surface are in good agreement with previous experimental [1] and theoretical results [2]. Lattice dynamical results for this surface are compared with those of the clean Ge(001)(2×1) surface [3, 4] in detail. We have found that the adsorption of Sb results in several characteristic phonon modes below the bulk continuum and in the gap regions, but there are no phonon modes above the bulk continuum. Due to the mass of Sb being heavier than Ge, the surface acoustic phonon energies are generally lower for the Ge(001)/Sb(2×1) surface than for the clean Ge(001)(2×1) surface. Characteristics of surface vibrational modes are determined by examination of atomic displacement patterns. These investigations reveal that the dimer rocking phonon observed for the clean Ge(001)(2×1) surface can be also identified for the Ge(001)/Sb(2×1) surface, but at a much lower energy.