Contribution ID: **38** Type: **Talk**

Theory of Piezoelectricity and Sound Waves in 2D Crystals

Wednesday, 16 September 2015 16:05 (25 minutes)

Piezoelectricity in three-dimensional (3D) materials is a well known physical phenomenon with many applications ranging from medical imaging (ultrasound) to fuel injection in motorcar engines.In earlier work we have investigated by analytical methods piezoelectricity and phonon dispersions in 2D and in multilayer crystals [1];[2].Here we extend this work by taking into account lattice anharmonicities. Starting from a 2D honeycomb ionic crystal structure with D_3h symmetry we use a Hamiltonian which includes anharmonic couplings between in-plane lattice displacements and out-of-plane flexural modes [3].Using methods of statistical mechanics we derive coupled equations for acoustic , optical and flexural dynamic response functions.The resonances of the correlation functions allow us to study temperature dependent phonon lineshifts and dampings.In the limit of long wavelengths and low frequencies we recover macroscopic equations for sound waves,electrical polarization and flexural motion.There the macroscopic quantities such as sound velocities ,piezoelectric coefficients and bending rigidity are expressed in terms of atomistic parameters.Effects due to two-dimensionality are discussed.As specific materials we refer to hexagonal boron nitride and transition metal dichalcogenides.

[1]Theory of elastic and piezoelectric effects in two-dimensional hexagonal boron nitride,K.H.Michel and B.Verberck,Phys.Rev.B 80, 224301 (2009)
[2]Phonon dispersions and piezoelectricity in bulk and in multilayers of hexagonal boron nitride,K.H.Michel and B.Verberck,Phys.Rev.B 83, 115328 (2011);eidem Phys.Status Solidi B 248,2720 (2011)
[3]Theory of anharmonic phonons in two-dimensional crystals, K.H.Michel,S.Costamagna,and F.M.Peeters,Phys.Rev.B 91,134302(2015)

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Session Classification: Two-dimensional systems

Track Classification: DyProSo2015 Main track