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Theory of anharmonic phonons in graphene SEBASTIAN COSTA-MAGNA, Instituto de Fisica de Rosario (IFIR-CONICET), FRANCOIS M. PEETERS, KARL H. MICHEL, University of Antwerp — Anharmonic effects in an atomic monolayer thin crystal with honeycomb lattice structure are studied by analytical and numerical lattice dynamical methods. Starting from a semi-empirical model for anharmonic couplings of third and fourth order, we study the in-plane and out-of-plane (flexural) mode components of the generalized wave vector dependent Grüneisen parameters, the thermal tension and the thermal expansion coefficients as function of temperature and crystal size. From the resonances of the displacement-displacement correlation functions we study the renormalization and decay rate of in-plane and flexural phonons as function of temperature, wave vector and crystal size. Numerical evaluations are made with graphene as a specific model, The work is complementary to crystalline membrane theory and computational studies of anharmonic effects in two-dimensional crystals.

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