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Graphene phonons revisited

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We calculated phonon dispersion for graphene with taken into consideration different numbers of nearest neighbors in the Born-von Karman model [1]. Values of force constants were taken from [2-3]. It was shown that quadratic dependence of ZA mode, predicted at [4], depends on set of interatomic force constants and not on number of nearest neighbors, as thought earlier [3]. Our results are in good correspondence with known experimental [5], ab initio [6] and IFC's models [2-3] and could be used for building vibrational thermodynamic model [7] of graphene lattice.

Fig. 1. Graphene phonon dispersion for interatomic force constants taken from [2]. Phonon frequency in cm–1. The locations of the high symmetry points are Γ (0., 0., 0.), M ($\pi/(a\sqrt{3})$, π/a , 0.), K (0., $4\pi/(3a)$, 0.).

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