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Angle dependent phonon spectra and thermal properties of misoriented bilayer graphene[1] MAHESH NEUPANE, Department of Electrical and Computer Engineering, Univ of California - Riverside, PANKAJ RAMNANI, Department of Chemical and Environmental Engineering, Univ of California, Riverside, SUPENG GE, Department of Physics and Astronomy, University of California, Riverside, ASHOK MULCHANDANI, Department of Chemical and Environmental Engineering, Univ of California, Riverside, ROGER LAKE, Department of Electrical and Computer Engineering, Univ of California - Riverside — The Raman spectra of misoriented bilayer graphene (MBG) show angle dependent signatures of the misorientation angle (θ) in the low frequency breathing modes. We investigate these low frequency modes using molecular dynamics including temperature dependent phonon anharmonicity. The calculated vibrational and thermal properties are compared against our experimental data. Our theoretical investigations reveal that the layer breathing mode (LBM) frequencies at 100 ± 10 cm^{-1} for angles $6^\circ \leq \theta \leq 30^\circ$ are consistent with the observed frequencies of ZO modes in the Raman spectrum. For the smaller θ (or larger L), the reduced BZ leads to the zone-folding of the phonon spectrum at the zone center, and leads to broadened optical phonons width in the vibrational density of states. Finally, increasing θ in the MBG leads to a reduction in the lattice specific heat capacity.

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