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Anisotropic thermal expansion in wurtzite materials: an ab-initio calculation for ZnO A.H. ROMERO, CINVESTAV-QUERETARO, J. SERRANO, I. MARGIOLAKI, ESRF, M. CARDONA, MPI-FKF — Many opto-electronic devices are based on wurtzite materials, e.g., ZnO, GaN, and SiC. Contrary to cubic structures, scarce experimental data have been reported on the linear thermal expansion coefficients of anisotropic materials. To our knowledge, no first principles calculations have been reported for the anisotropic thermal expansion coefficients. We report here two different approaches for first principles calculations of these coefficients based on the lattice dynamics obtained in the quasiharmonic approximation from the *ab initio* electronic band structure. The first method relies on thermodynamic relations for the entropy and the phonon density of states. The second approach requires the explicit calculation of Grüneisen parameters in the irreducible Brillouin zone. The two methods are applied to wurtzite ZnO and the obtained expansion coefficients are in excellent agreement with those derived from x-ray diffraction data taken with synchrotron radiation at the beamline ID31 of the ESRF. The calculations also provide the so-called zero-point contribution to the lattice parameters, which is also anisotropic and of interest in the analysis of the temperature dependence of electronic gaps.

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