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Non-destructive method for measuring the Ca/P ratio in human bone ALEXANDER SLEPKO, ALEXANDER DEMKOV, The University of Texas at Austin — Hydroxyapatite (HA) [$Ca_{10}(PO_4)_6(OH)_2$] is the main mineral constituent in human bone. It crystallizes in hexagonal and monoclinic phase, which are very similar in structure and properties. A critical measure for healthy bones is the Ca/P ratio which in turn affects the dielectric constant of the mineral constituent. The dielectric constant of HA varies between 5 and 20 depending on the Ca/P ratio in the sample [J. Mater. Sci.: Mater. Med. **21**, 399]. We suggest exploiting this large span in the dielectric constant in a non-destructive method to measure the Ca/P ratio in bone by optical spectroscopy. Using density functional theory we calculate the long-range corrected phonon dispersion. We find that only modes around 330 cm^{-1} are strongly affected by the dielectric constant. The shifts in frequency can be up to 20 cm^{-1} as you span the range of the dielectric constant. Thus, by measuring the optical shift and comparing with calibrated samples it is possible to draw conclusions on the Ca/P ratio in the mineral. Importantly, we find the same modes in both the monoclinic and hexagonal phases to be sensitive to changes in the dielectric constant.

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