Computer simulation of elastic constants of hydroxyapatite and fluorapatite

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Hydroxyapatite (HAP) and fluorapatite (FAP) are essential components of dental enamel and bone. In this paper, we report a computational study of the elastic properties of HAP and FAP using ab initio and force field techniques. We have obtained the HAP and FAP elastic stiffness constants in hexagonal symmetry by fitting the Hooke law for both the energy-strain and stress-strain relations. Our ab initio HAP stiffness constants differ from the results of previous calculations, but follow similar trends. The HAP and FAP stiffness constants calculated with the ab initio method are very similar, although FAP is slightly stiffer than HAP in the hexagonal plane, and more compliant along the hexagonal axis. The pseudo-single-crystal HAP experimental stiffness constants in current use are critically reviewed. Combining the data from the ab initio simulations with the experimental FAP stiffness constants, several alternative sets of HAP stiffness constants are proposed. The mismatch in propertie