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**Lattice dynamics and stability of cubic pseudobinary Fe$_x$Co$_{1-x}$Ti$_{0.50** NICHOLAS LOPEZ, University of Texas at El Paso, Electrical Engineering, BETHUEL KHAMALA, JORGE MUNOZ, University of Texas at El Paso, Physics Department — NiTi is a shape-memory alloy that has a stable cubic structure at temperatures above approximately 340 K. The cubic phase of CoTi is stable above approximately 40 K, whereas the cubic FeTi is stable at all temperatures, so decreasing the number of electrons in the system stabilizes the cubic phase. In this talk we will show phonon dispersions obtained from first-principles electronic structure calculations with displaced atoms for Fe$_x$Co$_{1-x}$Ti$_{0.50}$ with compositions $x = {0.125, 0.0625, 0.0312}$. We also looked at the effect of the Fe atoms occupying Co sites, Ti sites, and their local chemical environment. The composition Fe$_{0.0625}$Co$_{0.4375}$Ti$_{0.50}$ is at the edge of cubic stability at 0 K when the Fe atoms occupy the Co sites and are evenly distributed, but it is unstable when the occupancy is not even or the Fe occupies a Ti site. The effects can be explained using a rigid-band model when the Fe occupies Co sites, changing the number of electronic states at the Fermi level when the number of electrons in the system decreases. The occupation of the Ti sites by the Fe atoms results in more complex changes to the electronic structure, but can also be explained by a combination of decreasing charge and local atomic effects.

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