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Mechanical and thermodynamic properties of solid Zirconium using a tight-binding approach ILAN SCHNELL, MATTHEW JONES, SVEN RUDIN, ROBERT ALBERS — We use a tight-binding model that is fit to ab-initio DFT-GGA electronic-structure calculations for Zirconium. We will address difficulties involved with the fitting procedure and give zero-temperature results for elastic constants, force constants, and phonons. It turns out that the force constants obtained from our model are rather long-ranged. Within the quasi-harmonic approximation, we calculate phonon spectra for different crystal structures and at different pressures, allowing us to evaluate the Gibbs free energy as a function of pressure and temperature. We calculate parts of the phase diagram and other material properties, such as specific heat, and compare these to experimental data.

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