Ab Initio Phonons in Tantalum Under Pressure

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We have calculated phonon spectra for tantalum, from ambient to very high pressures, using the plane−wave pseudopotential formalism and taking into account spin−orbit coupling. The comparison with available all−electron results and with experiment is fair. The P = 0 distinctive features of group VB (V, Nb, Ta) are well reproduced but tend to disappear upon increasing pressure, leading to a conventional bcc metal behavior. An effective Gruneisen coefficient has been extracted from our data, and is compared to values used in effective EOS (equation−of−state) tables.