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First principles study of the spin-orbit coupling effect on the Tl-Pb superconducting alloy[1] OMAR DE LA PEÑA-SEAMAN, Institute of Physics (IFUAP), Benemerita Universidad Autonoma de Puebla (BUAP), ROLF HEID, KLAUS-PETER BOHNEN, Institute of Solid State Physics (IFP), Karlsruher Institute of Technology (KIT) — We have studied the influence of spin-orbit coupling (SOC) on the phonon dispersion, the electron-phonon (e-ph) coupling and on the superconducting properties for the Pb-Tl alloy in the stable fcc-phase doping regime. This system have been studied within the framework of density functional perturbation theory, using a mixed-basis pseudopotential method and the virtual crystal approximation (VCA) for modeling the alloy. The Eliashberg spectral function ($\alpha^2F(\omega)$) and the electron-phonon coupling parameter (λ) have been calculated with and without SOC. The observed effects of SOC in the full phonon dispersion and $\alpha^2F(\omega)$ consist in a softening of the phonon frequencies and an increase of the e-ph coupling matrix elements, which become weaker on the Tl-rich side. SOC enhances λ by as much as 48% in some cases and improves its overall behavior as a function of the concentration for the alloy, leading to a very nice agreement with experimental data from tunneling measurements.

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