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A Density-Functional-Perturbation-Theory Study of Superconducting Nb3Sn Under Uniaxial-Strain PETER BYRNE, University of Durham — The effects of strain on superconducting Nb_3Sn are of great interest because they cause significant changes in the performance of these materials during both cool-down and energisation of high field magnets and they give us an insight into the basic superconducting mechanism. There is a lot of experimental data describing these effects because this material is to be used in ITER, but a detailed first-principles understanding is not yet available. In this computational study, a unit cell of Nb_3Sn was subjected to a range of uni-axial strains and allowed to relax fully within a periodic density functional perturbation theory (DFPT) scheme. First order DFPT was then used to calculate the effects of electron-phonon coupling at each strain. The data obtained are compared with experimental measurements on single crystals as well as on wires made using both the "powder in tube" and "bronze route" methods. The calculated values for the strain dependence of the critical temperature (T_C) agree to within 20% with the experimental data and the peak in T_C found under compression may help improve our understanding of the experimental result that T_C of the tetragonal phase is higher than that of the cubic phase.

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