Strain-dependence of the superconducting critical temperature T_c in Al and Nb from *first principles*

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In the past 20 years, considerable efforts have been devoted to the construction of engineering equations that can predict the critical current density J_c of practical Nb_3Sn superconducting wires for high-energy physics and medical applications. Early studies concentrated on the J_c-dependence on temperature, T, and magnetic field, H. The need to adopt Nb_3Sn wires for higher-field applications has highlighted also a strong dependence of J_c, and possibly T_c, on imposed strain [1]. A few authors have proposed novel scaling laws based on microscopic parameters but, so far, have encountered difficulties in accurately describing the required phonon dispersions and electron-phonon coupling quantities necessary to calculate T_c via the Eliashberg formalism [2,3]. In this work, we present calculations of the T_c-dependence on strain in Al and Nb crystals using the DFT *PWscf* package from the Quantum-ESPRESSO distribution [4]. Comparisons with available experimental data are presented, as well as the challenges that need to be addressed in order to turn first-principles methods into a practical tool for the engineering of superconducting materials. In particular, attention is devoted to the case of Nb and the roles played by Kohn anomalies in this material.

The capability of modelling the T_c-dependence on strain in Nb_3Sn, the compound of higher interest for practical applications, is discussed based on the results and challenges which have emerged from the analyses of pure Al and Nb systems. In this regard, recent advances in the implementation of the Wannier formalism [5,6,7] give access to the sampling of the dense $\boldsymbol{k}$-point grids required to calculate fully-converged electron-phonon coupling quantities. This approach opens the possibility to extend the study of the T_c-dependence on strain to unit cells characterized by a higher number of atoms, e.g. Nb_3Sn. A full *ab-initio* description of the Nb_3Sn T_c-dependence on strain states will be a valuable building block for the most recent scaling equations based on microscopic models.

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