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STRAIN-DEPENDENCE OF THE SUPERCONDUCTING CRITICAL TEMPERATURE T_c IN Al, Nb AND Nb_3Sn CRYSTALS

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ABSTRACT

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. Early studies concentrated on the J_c-dependence on temperature T and magnetic field H. In recent years, the need to adopt Nb_3Sn wires for higher-field applications has highlighted also a strong dependence of J_c on imposed strain [1,2]. Many authors have proposed modified scaling equations that take into account the presence of uni-axial engineering strains and have obtained accurate predictions in the range of small deformations [3]. Mainly, the constituents of these scaling equations are phenomenological models and experimental data fitting. Few authors have proposed novel scaling laws based on microscopic parameters but, so far, have encountered difficulties in accurately describe the required phonon dispersions and electron-phonon coupling quantities [4,5]. Since the mid-90s, Density Functional Theory (DFT) has become a tool capable of describing the dynamical properties of crystals from a full *ab-initio* approach. In this paper, we present calculations of the T_c-dependence of Al and Nb crystals on pressure, uni-axial and shear strains using the DFT *PWscf* code from the Quantum-ESPRESSO distribution [6]. Favourable comparisons with available experimental data have been obtained and will be presented. The agreement with experiments is also paired by our calculations of lattice parameters, elastic constants and phonon dispersion curves. The modelling of the T_c-dependence on strain in Nb_3Sn crystals is complicated by sub-lattice distortions typical of the A15 structures. Consequently, computations on Nb_3Sn crystals require a significant but amenable increase in CPU time.

Recent advances in the code implementation [7] open the possibility to extend the study of the T_c-dependence on strain to unit cells characterized by an higher number of atoms and, therefore, efficiently treat the T_c-dependence on strain for the case of a Nb_3Sn crystal and, possibly, of a non-stoichiometric Nb_3Sn super-cell.

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. Furthermore, the computational study of non-hydrostatic deformations in Nb_3Sn crystals has the potential to elucidate some of the mechanisms behind the strong J_c strain-dependence observed in Nb_3Sn wires under the expected bending and transverse loading modes. DFT shows promise for fundamental predictions of strain effects on LTS superconductors in the near future.

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Calculations in this work have been done using the Quantum-ESPRESSO package.

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