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FIRST-PRINCIPLES STUDY ON MECHANICAL PROPERTY OF SUPERCONDUCTING MATERIALS

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ABSTRACT

After the discovery of superconducting properties in the early decade of the last century, everyone has been looking for the best materials for the electrical and magnetic applications. Superconducting wires have changed the thought of conventional power transferring mechanisms, so improvement in the other properties like mechanical etc. can establish the materials for better performance. Although high transition temperature (HTC) superconductors show some promising improvements but low transition temperature (LTC) superconductors holding the majority of the markets for their application fields. In this paper, I am reporting mechanical property of low, medium, and high Tc (transition temperature) superconductors by using density functional theory. Nb_3Sn (LTC) with transition temperature 18.3K is the most used superconducting material whereas MgB_2 shows a bit high transition temperature (40K) which helps to categorize this material in the medium transition temperature range. The YBCO /Y123 series of samples show transition temperature (90K) in the HTC range. The bulk modulus (K) is defined as the ratio of the change in the pressure to the resulting relative changes of the volume. The unit cells of all the superconducting materials undergo a slight change in volume due to the press applied to the system. Both the changes in press and volume were calculated with stranded plane wave self-consistency (pwscf) density functional theory codes (Quantum Espresso software package). The results show the lower transition temperature materials show higher bulk modulus in comparison to the high transition temperature superconducting materials. The LTC is more compressible, less rigid than HTC material. The famous YBCO samples are showing better mechanicalproperties.

Keywords: - Superconductor, Mechanical properties, Bulk modulus, Density functional theory