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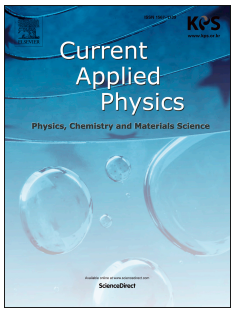

Band structure, electron-phonon interaction and superconductivity of yttrium hypocarbide

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Band structure, electron-phonon interaction and superconductivity of yttrium hypocarbide

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Abstract

Band parameters and superconductivity of yttrium hypocarbide (Y_2C) have been investigated. The computations are performed using first-principles pseudopotential method within a generalized gradient approximation. The equilibrium lattice parameters have been determined and compared with experiment. Moreover, the material of interest is found to be stiffer for strains along the a-axis than those along the c-axis. A band-structure analysis of Y_2C implied that the latter has a metallic character.

The examination of Eliashberg Spectral Function indicates that Y-related phonon modes as well as C-related phonon modes are considerably involved in the progress of scattering of electrons. By integrating this function, the value of the average electron-phonon coupling parameter (λ) is found to be 0.362 suggesting thus that Y_2C is a weak coupling Bardeen-Copper-Schrieffer superconductor. The use of a reasonable value for the effective Coulomb repulsion parameter (μ^*=0.10) yielded a superconducting critical temperature T_c of 0.59 K which is comparable with a previous theoretical value of 0.33 K. Upon compression (at pressure of 10 GPa) λ and T_c are increased to be 0.366 and 0.89 K, respectively, showing thus the pressure effect on the superconductivity in Y_2C.

The spin-polarization calculations showed that the difference in the total energy between the magnetic and non-magnetic Y_2C is weak.