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An SCDFT aspect of renormalized phonon-induced HTSC in doped HTSCD $Mg_{1-x}Al_xB_2$

M.C. SHAH[1], ABDUL GAFFAR LONE, IRSHAD AHMAD MIR, TANVEER AHMAD WANI and TARA PRASAD

Department of Physics UTD, Barkatullah University, Bhopal - 462 026 (India).

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ABSTRACT

The electronic and superconducting state characterization of high phase transition temperature (Tc) superconducting (HTSC) diboride (HTSCD) pure MgB_2 and doped $Mg_{1-x}Al_xB_2$ has been made with renormalization effects in multiband configuration with non-linear, anharmonic E_2g optical phonon induced HTSC by employing the first principles calculations within density functional theory (DFT) for SC (SCDFT) in low temperature lattice dynamics.

Key words: T_C, HTSC, HTSCD, anharmonic, phonon, DFT, SCDFT.

INTRODUCTION

The modern scientific and technological revolution is responsible for increasing interest and impetus in search for high phase transition temperature (Tc) superconductivity (HTSC) in diboride (HTSCD)[1] pure MgB_2 and doped MgB_2 with different cationic dopants so as to be SC at even higher temperature than MgB_2. The amount of nanometer sized precipitates and grain boundaries be found in the doped MgB_2 matrix and a significantly enhanced Tc was reported TcH" 50K on sets of Tc and HTSC in Rb and Cs doped[2] MgB_2. A systematic research for SC in the trivalent, Al^{3+} dopant substitution for Mg^{2+}, without changing valence charge-density distribution, in pure MgB_2 has been carried out with tremendous progress in understanding the SC giving general belief that there is an electron phonon exchange interaction mediated SC with multiple (Two) energy bandgaps and high-frequency optical E_2g phononic modes in strong coupling to electrons in tubular shaped two dimensional (2D) B2Pxy ó bands at Fermi level (E_F) within the strong coupling Migdal-BSC-Eliashbarg's phononic mechanism[3] where coulombic pseudo potential be treated as an adjustable parameter chosen as to reproduce the experimental Tc. In this sense, Migdal-BCS-Eliashberg's phononic theory, inspite of its tremendous success, can be considered as a semi phenomenological theory of SC. The introduction of density functional theory (DFT)[3] in the local density approximation (LDA) to density functional formalism (LDF) by Hohenberg-Kohn-Sham marked a milestone and laying the basis for structural characterization of materials in modern material science. In past, the first principles calculations of electronic structures of HTSCD pure MgB_2 and doped borides have been made at ambient pressures with full potential linearized augmented plane wave (FPLAPW), muffin-tin orbital (FPLMTO) and generalized gradient approximations (FPGGA) methodologies[3,4] employing GGA for e-e exchange correlation energy as implemented m WIEN 97, 2K and ABINIT computer packages with

an emphasis on non-linear, anharmonic, optical E_2g, phononic modes in non-adiabatic effects giving credence to anharmonicity of lattice dynamics and multiphonon interaction in multilayers as controlled by microstrain of B-layers to describe the e-e pairing mechanism of HTSC in pure MgB_2 and doped borides. Recently an extension of DFT to deal with superconducting states, the so called (SCDFT)[4,5] unlike Eliashbarg phononic theory, there are no adjustable parameters and Tc is the result of material specific quantities with three densities-normal and anomalous electronic densities and the diagonal of nuclear density matrix-with a wide range of e-e couplings. The proposal presents a first non-trivial application of strong e-e coupling SCDFT[5,6,7] formalism without any phenononological or adjustable parameter to characterize the electronic structure and SC properties (Tc, energy gap, SC order parameter, e-e pairing phononic modes, etc) of HTSCD. The section II deals with HTSCD, the Section III SCDFT, the section IV elucidates an ab-inito SCDFT aspect of renormalized phonon induced HTSC in $Mg_{1-x}Al_xB_2$ and finally section V concludes predictive power of SCDFT approach with good accuracy for characterizing electronic and SC properties of HTSCD.

HTSCD

The pure MgB_2 possesses the simple hexagonal, omega, C-32, AlB_2 type structure with crystallographic space group P6/mmm. It contains graphite like boron layers which are separated by hexagonal close-packed layers of Mg. The Mg atoms are located at the centre of hexagons formed by boron and donate their electrons to boron similar to graphites. The MgB_2 exhibits a strong structural anisotropy in B-B bond lengths as the distance between the B planes is significantly larger than inplane B-B distance. The TcH"40K of MgB_2 [1] is close or above the theoretical value predicted from Migdal-BCS-Eliashberg's phononic theory and therefore it is considered to be a non-conventional SC but in a strong e-e coupling HTSC. In last five years various dopants- carbon, monovalent alkali, divalent alkaline earths, transition metals trivalent Al, Ge, rare earths, halogens, S, carbohydrates, organic acids in pure MgB_2 imply that structural defects and precipitates of doped matrix with dimensions of nanoparticles doping can modify electronic structures and SC properties such that highly dispersed nanodopant particles act as strong pinning centres responsible for better HTSC performance of doped $Mg_{1-x}A_xB_2$. The MgB_2 could be considered as metallic heterostructure at atomic limits (MEHAL) made up of SC layers interacted by different layers, and there is an evidence that high Tc is due to interband pairing controlled by the electronic structure since the chemical substitution can be one of the most suitable tools to explore how the e-e pairing mechanism in doped MgB_2 [2] depends on the electronic structure. It is found that most successful of a number of cationic substitutional attempts is the Mg substitution with Al^{3+} as investigated by several groups, the Tc is sensitive to boron isotopic substitution while Mg isotopic substitutions does not make a significant change in Tc. The boron isotopic coefficient is only significant and Mg isotopic coefficient á is very small but still non-zero. The reduced á has been assumed as being due to large anharmonicity of optic E_2g phononic modes of B-atom vibrations and thus introduction of Al^{3+} for Mg^{2+} in pure MgB_2 to give the doped $Mg_{1-x}Al_xB_2$ phases with $0.1<x<0.25$ can be understood mainly interms of band filling effects due to electron doping by Al and to the reduced electron-phonon interaction coupling due to change in á and in phonon frequency.

The $Mg_{1-x}Al_xB_2$ is the only known diboride alloy with substitution in the Mg sublattice and rather wide range solubility. The study of $Mg_{1-x}Al_xB_2$ may provide valuable information about genesis of structural anisotropy of electronic states at E_F as orbital relaxation mechanism dominates over the dipolar and Fermi contact mechanism is MgB_2. The SCDFT[4,5] formalism for the calculation of electronic density of states (DOS) at E_F will represent an excellent probe to check not only DOS and its partial components but also characterization of electronic and atomic structural anisotropy.

SCDFT

In the standard SCDFT, one normally defines a Kohn-Sham (KS)[3] system, as a non interacting system chosen such that it has the same ground state density as the interacting one. The KS system consists of non-interacting and SC electrons, and interacting atomic nuclei (ions). The problem of minimizing the Kohn-Sham grand canonical potential can be transformed into a set

of three different equations that have to be solved self consistently one equation for the nuclei, which resembles the familiar nuclear Born-Oppenheimmer (BO) equation and two coupled equations which describes the electronic degrees of freedom and have the algebraic structure of Bogolioubov-de-Geenes equations. With a few physically sound approximations, one finally arrives at the formulation of energy gap equation, formally looking to be that of BCS phononic theory, but with interaction parameters completely ab-initio and desired for normal state DFT calculation. The order parameter is the so called anomalous electronic density and corresponding potential is non local e-e pairing potential interpreted as an external pairing field induced by an adjacent superconductor via the proximity effect. This external field only acts to break the symmetry (gauge symmetry) of SC system and is set to zero at the end of calculations. In order to describe phonon mediated SC, the electron phonon exchange interactions has to be taken into account. In the weak e-e coupling limit, the phonon interaction mediated mechanisms can be added as an additional BCS phonon type interaction. However, in order to treat also the strong electron phonon coupling, the electronic and nuclear degrees of freedom have to be treated on equal footing. In the multicomponent DFT, both the normal and anomalous electronic density and the diagonal of the nuclear density matrix be included with no adjustable parameters.

Ab-initio scdft formalism for HTSCD $Mg_{1-x}Al_x B_2$

In low energy dynamical and strongly anisotropic electronic structure investigations of pure MgB_2 and doped $Mg_{1-x}Al_xB_2$ phases be characterized by the boron quasi 2D $B2P_{xy}$ σ and B2Pz π bands. The first principle calculations of electronic structures of pure MgB_2 and $Mg_{1-x}Al_xB_2$ phases have been made by using the exchange correlation terms in Kohn-Sham equations and full –potential linearized augmented plane wave (FPLAPW), muffin-tin orbitals (FPLMTO) and generalized gradient approximation (FPLGGA) methodologies[3,4] coupling with GGA for e-e exchange correlation energy as implemented in WIEN 97, 2K, LMTART and ABINIT computer packages within DFT at ambient pressures. This reveals that the Fermi surface (FS) of HTSCD has several states with different orbital character– this tubular structure with B2Pxy σ and character are very similar to the E_2g phononic modes, corresponding to B-B bond stretching in B planes. The MgB_2 and $Mg_{1-x}Al_xB_2$ also have 30 bands, to give rise to complicated FS. Without holes in bands, the compound would not be SC. The 3D B2Pxy bands are coupled much less efficiently to phonons, but are near the less crucial to SC. The resoluble feature of the structural characterization in the presence of low energy band gaps on σ and π bands, as clearly demonstrated by several different experiments, thus indicating that calculated electronic DOS at E_F, $N(E_F)$ is sizable and converted probe that on B site relaxation mechanism dominates over the dipolar and Fermi contact interaction mechanism in HTSCD. Thus onset of SC phase transition is much sharper and is more pronounced for Al content x on Tc. The hole like larger FS gradually collapses with Al doping and vanishes far x=5.6 in which an abrupt topological change occurs at x=0.3. The theoretical calculations of electronic energy band structure and FS are in agreement with experimental measurements of de Haas-van Alphas (dHVA) effect in Al doped MgB_2 ($Mg_{1-x}Al_xB_2$) phases.

In this first principle SCDFT[5,6] calculation of HTSCD the four bands are involved. The plots of SC e gap versus temperature T, together with a few recent experimental results are in strong agreement. The value of Tc (34.1K) and the energy gap B σ and B π and T=0K are very close to experimental data, measures the temperature dependent behavior at both band gaps along with their strong non BCS phononic behavior are very well reproduced. If an average of σ and π electron phonon interaction is taken, then the Tc=20K, which clearly shows the importance of multiband (two band) effects in enhancing Tc of HTSCD. Both gaps change sign which is the necessary condition for phonon induced (renormalized E_2g plane modes) SC in presence of repulsive Coulomb interaction. The analysis of gap trends within two band strong e-e coupling Eliashberg phononic mechanism shows that band filling is the main effect of Al doping, although a small increase in interband scattering might be necessary to account for experimental data in single crystals. This yields the detailed understanding of HTSC in doped $Mg_{1-x}Al_xB_2$ in the renormalized anharmonic E_2g optic phonon induced SC using SCDFT.

CONCLUSION

The first non-trivial application of SCDFT to HTSCD pure MgB_2 and Al doped MgB_2 as $Mg_{1-x}Al_xB_2$ phases give electronic structural characterization and SC properties (Tc, energy gap) with normalized, anharmonic, optic E_2g phononic modes induced SC in two band (multiband) with nonlinear anharmonic and non-adiabatic effects in phononic theory.

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