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An EXAFS analysis of topological HTSC phase transition in iron-oxypnictides

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ABSTRACT

The extended x-ray absorption fine structure (EXAFS) spectroscopic analysis of correlated electronic-structures of high phase transition temperature (T_c) superconducting iron-oxypnictides (HTSCIO) provides the carrier density, coherent metal, spin density wave (SDW) ordering state by tuning the chemical potential or Fermi level (E_F) with alio/isovalent cationic dopants to yield the occurrence of shape resonance in dimensional 2D-3D (Fe3d-As2p (dp) $3z^2r^2$ and x^2y^2 orbitals character bands crossover topology of Fermi surface (F_S) in metal heterostructures at atomic limits (MEHAL) of cationic periodic lattice distortion (PLD) due to quantum wells (Q-dots) in layered structure superlattice.

Key words: EXAFS, T_c, HTSCIO, SDW, Topology, F_S, MEHAL.

INTRODUCTION

The discovery of high phase-transition temperature (T_c) Superconducting (HTSC) iron-oxyprictides (HTSCIO) [1] with T_c >55K and dp conduction band Jahn-Teller (BJT) polaronic structural distortion inducing pseudogap have emergence of HTSC in close proximity to the magnetic phase transition with multi (two) bandgaps and antiferromagnetic long range ordering (AFMLRO) spin density wave (SDW) order instability d-wave symmetry SC order parameter e-e pairing mechanism of HTSC occurring at optimum alio/isovalent cationic dopings by tuning chemical potential (or Fermi energy E_F) at shape resonances of superlattice of quantum wells (Q-dots) occurring near the dimensional 2D-3D (Fe3d-As2p dp bands with $3x^2y^2$, $3z^2r^2$ symmetry character) crossover topology of Fermi surface (F_s) consistent with potential processes of T_c amplification in metal heterostructures at atomic limits (MEHAL) of cationic dopings periodic lattice distortion (PLD) with sensitivity of local electronic structures of Fe_2As_3 SC phases at E_F.

The Competition between HTSC and magnetic SDW interactions in HTSCIO can be accomplished with experimental [2-6] and theoretical [7] investigations of correlated electronic structures and by spectroscopic studies with local lattice instabilities (dp band Jahn-Teller polaronic structural distortion formation) diluted as an upturn of Fe atoms mean square relative displacements (MSRD) for nearest neighbour interatomic distances (Fe-As) in HTSCIO phases so that an intimate correlation between local lattice modes with SC phase transition be revealed in superlattice (stripes) and a sub T_c phase transition as a dopant phase transition flow in network phases (as SC is spinglass (SG) phase coexist at T_c) which is similar to Fs 2D-3D crossover topological phase transition in

FITSCIO as observed in chalcogenides and oxide alloys network glasses.

The present proposal presents the EXAFS analysis of topological HTSC phase transition in HTSCIO. The section II deals with HTSCIO, the section III corroborates achievement of high T_c in HTSCIO, the section IV elucidates experimental and theoretical evidences of correlated electronic structures and finally section V concludes with EXAFS analysis of HTSC topological phase transition in HTSCIO.

HTSC Iron oxypnictides (HTSCIO)

The recently discovered HTSC in iron pnictides (HTSCIO) with maximum T_c in $SmFeAsO_{1-x}F_x$ with x=0.4 and T_c = 56K have square planer sheets of Fe coordinated tetrahedrally by pnictogenes and chalcogenes and the HTSC emerges as the alio/isovalent cationic (anionic doping concentration exceeds about 5% close to antiferromagnetic long range ordering (AMFLRO) spin density wave (SDW) order states in the doped phases and HTSC is achieved by suppressing the SDW states by hole doping with cations or by application of high pressure.

There are four different crystal structures of family of HTSCIO as hole doped RFeAsO with ZrCuSiAs type with R as rare earth's, $A(Fe_{1-x}M_x)As_2$ with M^{2+} as transition metals with $ThCr_2Si_2$ types to FeAs as Cu_2Sb type and α-PbO type superlattice (stripes) with strong crystallographic space group F4 (mmm) and shape phase have cmma shape gap.

The relation between interplay between four different crystal structures can be investigated by phase degree giving rise to the fact that SC and spin glass (SG) phases coexists within small cationic dopings and the core gap structures and gap values exhibit universal features in both Tc_{max} and their plane disordering as measured by EXAFS spectroscopy and reflects in these studies polaronic distortion mediated pseudogap and SC gaps with ordering of nano phases into superlattice (stripes) and the third phase to be below Tc is sub Tc phase transition as a dopant glass flow as spin glass (SG) in network glasses similar to 2D-3D (Fe3d-As2p) Fermi surface crossover topology phase transition as observed in chalcogenides and oxide alloys network glasses.

ACHIVEMENTS OF HTSC IN d-BAND HTSCIO

The parent compound of HTSC iron-oxypncitides (HTSCIO) is LeFeAsO having quasi 2D tetragonal crystalline structure consisting of charged $(LeO)^{\delta+}$ layers alternating with $(FeAs)^{\delta-}$ layers and has a an AFMLRO SDW ordering instability such that the HTSC in doped HTSCIO phases suppressing the AFMLRO SDW ordering magnetic interactions through alio/isovalent cationic dopings traces of impurities or oxygen (holes) introducing hole charge carrier which are transferred charge reserviours to Fe_2As_2 conduction layers so that apparent competition between HTSC and AFMLRO SDW ordering magnetic interactions of Fe^{2+}3d electron spins fluctuation with intervening As2p electrons in d-wave symmetry e-e pairing spins fluctuations gives higher T_c in hole doped HTSCIO.

Correlated electronic structures in htscio

The apparent competition between HTSC and topological phase transition in HTSCIO can be accomplished with correlated electronic structure of Fe_2As_2 conduction layer with local lattice instability (dp BJT polaronic structure distortion formation) detected as an upturn of Fe atoms mean square relative displacements for nearest neighbouring interatomic distance (Fe As) in HTSCIO so that intimate correlation between local lattice (phonon) modes with SC structural phase transition in revealed giving essential in gradients for HTSC e-e pairing microscopic mechanism.

The hole in electron packets as Fermi Surface (F_S) with resting features of wave order k = (ω,π) leading to AFMLRO SDW ordering instability on F_S with correction q = (π,c) as characterized by first principle calculations using local density approach LDA to LDF of density functional theory (DFT), Hartee-Fock random phase approximation (HFRPA) of effective ions and fine 3d electron band model, RRA model extended to two Fe sites unit and having fine orbital symmetry Fe3d, $Fe3d_{x^2y^2}$, $Fe3d_{xy}$, $Fe2d_y$, Fe3yx I the LDA + dynamical mean field theory (DMFT) describes the correlated electronic studies which investigate an explicit multiband (columbic) energy integral μ in DMFT

yielding strong strength of Fe3d spectral weight away from origin and E_F to allow band at binding energies corresponding to U. The strip, they low energy structures (remove below E_F) in $Fe3d_{z^2 x^2}$ and $Fe3d_{x^2 y^2}$ due to d-orbital fluctuations corresponding to CDW charge fluctuations Fe3d degenerate states.

Thus an instability of metallic state due to e-e correlation interaction as the correlated electronic structure typically the low energy electronic near E_F lead to Fermi energy dependent e-e correlational resonance in the dimensional 2D-3D crossover topology of F_s in MEHAL due to quantum dots (wells) in layered superlattice (stripes) HTSCIO.

EXAFS analysis of htsc topological phase transition in htscio

The EXAFS spectral features investigation of the dopant HTSCIO yield the atomic structures with local lattice instabilities (dp BJT polaronic distortion formation) detected as an up turn in Fe atoms MSRD for nearest neighbour interatomic distances (Fe-As) in HTSCIO phases so that an intimate correlation between local lattice modes with SC phase transition be revealed in superlattice (stripes) and a sub T_c phase transition as a dopant phase transition flow in network phases (as SC is spinglass (SG) phase coexist at T_c) which is similar to Fs 2D-3D crossover topological phase transition in FITSCIO as observed in chalcogenides and oxide alloys network glasses.

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