An XAS investigation of nanocomposite HTSCD MgB$_2$

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ABSTRACT

The present proposal focuses on theoretical and experimental on-site electronic and atomic-structural characterization of nano-diamond (nD) and nano SiC doped high phase-transition temperature (T$_c$) superconducting (HTSC) diboride (HTSCD) MgB$_2$ nanocomposite cluster’s single crystal and thin films by using the element specific and local structure sensitive soft resonant MgK/L and BK X-ray absorption edge (XAE) fine structure (XAFS) spectroscopic ideal probe to give potential HTSC properties of nanoparticle carbon embedded in the matrix of nanocomposite borides to drive and to develop high performance doped MgB$_2$ phase with amplified T$_c$.

Key words: T$_c$, HTSC, HTSCD, Nanodiamond (nD), NanoSiC, XAFS, XAS.

INTRODUCTION

The recently discovered binary intermetallic high phase transition-temperature (T$_c$) superconducting (HTSC) diboride (HTSCD) MgB$_2$ in 2001, with T$_c$ ~ 40K$^1$ exceeding by about two times the recorded values of T$_c$ for conventional B1 and A-15 type intermetallic SC, is a promising HTSC for the important large-scale applications for high-field magnets, cryocoolers-cooled magnets, nuclear power control rods, neutron shields, turbine blades, combustion chamber liners, rocket nozzles, ablation shields, etc. The studies of alio/isovalent cationic dopant substitutions in MgB$_2$ for Mg$^{2+}$ and B$^{-1}$ sites, without changing the valence charge density distribution, gives the doped phases with chemical composition for which T$_c$ be maximum with non-stoichiometry requirement with excess of Mg$^{2+}$ or B$^{-1}$. The cationic doping$^2$ turns the electron type (mainly $\pi$ band conduction) non-superconducting boride into the hole-type (mainly $\pi$ band conduction) MgB$_2$ SC. Keeping this strategy in mind, the stretching of lattice c-parameter due to non-stoichiometry induces enhancement of HTSC and T$_c$. The amplified T$_c$ in doped borides is dictated by B2p$_{\sigma}$ $\sigma$ band conduction state in the total electronic density of states (DOS) at Fermi level $E_F$. The high energy part of valence band (VB) of pure MgB$_2$ made up of predominantly of B2p band states forming two distinct sets of bands of B2p$_{\pi\sigma}$ $\sigma$ and B2p$_{\pi}$ $\pi$ types of bands where propagation vector k-dependence differs considerably. These bands are quasi two dimensional (2D) type, form a flat zone in $k_z$ direction Å-A line of Brillouin zone (BZ) and reflect the distribution of pp$\sigma$ band states in B layers. These intricate consequences and interplay of electron-holes interaction and the strong e-e coupling Migdal-BCS-Eliashberg$^3$ phonon exchange interaction coupling in $\sigma$ and $\pi$ bands in two-band model with high frequency anharmonic $E_{2g}$ optic phononic modes in the phase are observed in on-going site-specific and local structure sensitive MgK/L and BK/L x-ray absorption edge (XAE) fine structure (XAFS) spectral features of x-ray absorption spectroscopic (XAS) investigations which suggest that doped borides be the e-e coupling phonon mediated HTSC with enhanced T$_c$. The proposal presents the structural characterization of nD and nano SiC$^{4,5}$ doped HTSCD MgB$_2$ nanocomposite cluster’s single crystals/thin films, by using soft resonant MgK/L and BK XAE XAFS of XAS probe$^6$. The section II deals
with HTSCD, the section III corroborates XAS, the section IV elucidates electronic and atomic structural characterization of nanocomposite Mg\(_{B2-x}\) (nD/SiC)\(_{x/2}\) single crystals/films and finally the section V concludes with potential HTSC properties of nanocomposite borides with amplified high T\(_c\).

**High phase transition–temperature (T\(_c\)) superconducting diborides**

The HTSCD pure Mg\(_B2\) with T\(_c\) ~ 40K and its corresponding alio/isovalent dopant substitutions for B, without changing valence electronic charge-distribution, with nanodiamond (nD)\(^4\), and nano SiC\(^5\) doping on Mg\(_B2\) crystal structure with cosubstitution of boron (B) in nanocomposite form Mg\(_{B2-x}\) (nD/SiC)\(_{x/2}\) with dopant content x ranging from x=0-1.0 doped matrix of nanoparticles C embedded to give different crystals crystallizing in a hexagonal, omega C-32, polytype inequivalent multilayered superlattice phase structural configuration with graphite-like insulating honeycomb B layers of hexagonal B nets separated by hexagonal superconductively active packed Mg layers and with crystallographic space group P6/mmm for Mg\(_B2\) and R3M for nanocomposite HTSCD. The polytype inequivalent multilayered superlattice involves the proximity effects of adjacent and alternate layers interaction between superconductively active Mg\(^{2+}\) and insulating B\(^{1+}\) layers and the Jahn-Teller (JT) polaron orderings in B-planes producing the metal hetrostructures at atomic limits (MEHAL)\(^2\) of periodic lattice distortion (PLD) due to self cationic B/dopant level's charge transfer excitation states mixing, called as polaronic excitations at B/dopant level threshold near T\(_c\) with Peierl's lattice structural instability because of dopant spin-charge degrees of freedom separation and polarization and the T\(_c\) amplification occurring at optimum doping by tunings the chemical potential (~E\(_F\)) at shape resonance of superlattice of quantum wells (Q dots) characterized by dimensional 2D-3D(2DB\(_{2p_y}\) \(\pi\)-3DB\(_{2p_x}\) \(\sigma\)) cross-over of topology of (FS) in MEHAL with size of microscopic units of heterostructures is of the scale of Fermi wavelength \(\lambda_F=0.3\cdot1.5\)nm. The atomic nanolayers provide the thinnest possible metallic slabs (Q-dots) providing periodic potential barrier of electrons in materials. The growth of single crystals/thin films of nanostructured MEHAL SC Mg\(_B2\) with nD and nano SiC doping on Mg\(_B2\) crystal structure with co-substitution of boron yielding nanocomposite form Mg\(_{B2-x}\) (nD/SiC)\(_{x/2}\) with dopant content x=0.0-1.0 will lead to encouraging improvement\(^6\) of HTSC and T\(_c\) in doped matrix of nanoparticles C embedded in matrix and develop high performance of HTSCD.

**X-ray absorption spectroscopy**

The condensed system's XAS involves the incoming x-ray photon complete absorption rendering the photoabsorber's ejected photoelectron transition from the normally occupied photoexcited inner core electronic state (K, L, M), under the fully relaxed static potential of \((N-1)\) passive electrons and screened excited core-hole, to outer unoccupied electronic state with proper symmetry in multielectron configuration interaction states of the N-electron atomic system. The system's atomic photoabsorption coefficient as a function of incident x-ray photon energy displays\(^6\) the complex modulatory oscillations beyond the specific photoabsorption threshold (x-ray absorption edge (XAE)) termed as x-ray absorption fine structure (XAFS) spectral features described\(^6\) respectively as a single electron short range order (SRO), multiple (MS) and MS/single (SS) spherical (SWA) and plane (PWA) wave approximation scattering of photoelectron signal in photoelectron scattering (ES) and electronic energy band structure (EBS) formalisms respectively. The low energy MS-XANES resonance (MSR) and high energy MS/SS EXAFS spectral features of system's XAS spectral curve yields the electronic and atomic structural parameters by using the XAE XAFS data analysis with respective specific computational programmes. The EBS formalism with muffin-tin (MT) potential within local-density approximation (LDA) to density functional formalism (DFT) with linearized methods be valid over entire XAS energy range of MS-XANES and MS-EXAFS spectral features of system's XAS spectral curve yields the electronic and atomic structural parameters by using the XAE XAFS data analysis with respective specific computational programmes. The site-specific and local electronic and atomic structure-sensitive XAS experimental (conventional target tubes and rotating anode generator, and the polarization dependent synchrotron radiation) and theoretical (ES & EBS) probes yield the system's structural parameters.
XAS of nano composite HTSCD MGB$_2$

An impressive number of experimental and theoretical XAS investigations [6] have been made in recent past periods on single crystals and thin films of nanostructured MEHAL SC MGB$_2$ with nanodiamond (nD) and nano SiC doping on MGB$_2$ crystal structure with cosubstitution of boron in nanocomposite form MGB$_{2-x}$ (nD/SiC)$_x$/2 with dopant content $x=0.0-1.0$ to give doped matrix's on-site electronic and atomic structures with nano-particle c embedded.

EXPERIMENTAL

MgK/L XAE XAFS

The MgK/L XAS XAFS$^6$ supports the fact that SC is driven by hole-doping due to nD and nano SiC of covalent B-B $\sigma$ bands. Structurally the doped thin films are textured with columnar nanograins and highly resistive amorphous areas at grain boundaries.

BK XAE XAFS

The BK XAE XAFS$^6$ in single crystals/thin films of nanocomposite MGB$_{2-x}$ (nD/SiC)$_x$/2 borides provides the contribution from B$_2$p$\sigma$ band states in B plane and B$_2$p$\pi$ band states normal to plane for phonon assisted mechanism of HTSC. The high level Si and C codoping act as effective pinning centers or vortices, improving critical current density $j_c$ behavior.

Theoretical XAS

Using the full-potential linearized augmented plane wave (FPLAPW) formalism within LDA to LDF in EBS formalism of XAS spectral evaluation [6] with computer programme WIEN 97, the MS-XANES MSR are calculated for MgK/L and BK XAE XAFS, according to final state rule formulated by Von Barth and Grossman. The B$_2$p partial density of states (PDOS) gives lowering the $\pi$ bands relative to the bonding sp$^2$ $\sigma$ bands causing $\sigma\rightarrow\pi$ charge transfer and $\sigma$-band hole doping, indicating structurally the system with stronger pinning with nanoparticle C embedded in nanocomposite.

CONCLUSION

The MgB$_{2-x}$ (nD/SiC)$_x$/2 with dopant content $x=0.0-1.0$ with nano particles C embedded in doped matrix of nanocomposite borides be investigated experimentally and theoretically with MgK/L and BK XAE XAFS of XAS probe to give strong e-e coupling Migdal–BCS– Eliashberg’s phononic interaction mediated coupling in $\sigma$ and $\pi$ bands in two band model with high frequency anhormonic $E_{2g}$ phononic modes sp$^2$ $\sigma$ bands causing $\sigma\rightarrow\pi$ charge transfer and $\delta$-band hole doping indicates structurally the doped phases be with strong pinning centres with nanoparticles C embedded in nano-composite producing high $j_c$ for high magnetic field applications to give enhanced HTSC and $T_c$.

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