March 2012

Bond resonance in superconducting rapid cooled alloys: $(Bi_{1.7}Pb_{0.3}Sr_2Ca_{n-1}Cu_nO_{2n+4+\delta})_2$, n=1 to 9 detected by novel local atomic enhanced XRD

K Tyson
San José State University

J Kmiec
San José State University

Juana Acrivos
San José State University

D. Gulamova
Academy of Sciences of Uzbekistan

J Chigvinadze
San Jose State University

Bond resonance in superconducting rapid cooled alloys: $(Bi_{1.7}Pb_{0.3}Sr_2Ca_{n-1}Cu_nO_{2n+4+\delta})_{2,\ n=1\ to\ 9}$ detected by novel local atomic enhanced XRD

K Tyson*, J Kmiec*, JV Acrivos*, DD Gulamova**,and JG Chigvinadze***

San José State UNIVERSITY

*San José State University, San José, CA 95192-0101, USA, ** Physics of Sun (Institute of Materials Science Academy of Science, 700084, Tashkent, Uzbekistan,

*** E. Andronikashvili Institute of Physics, 0177 Tbilisi, Georgia. Work supported by H and C Dreyfus Foundation, US National Lab DOE-SLAC, NSF Ukraine

National ACS Meeting
San Diego CA, March 2012

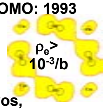
Abstract: We discuss bond resonance in high temperature layer superconducting cuprates, HTLSC alloys: $(Bi_{1.7}Pb_{0.3}Sr_2Ca_{n-1}Cu_nO_{2n+4+\delta})_{2,n=1-9}$ called (2_s:2:n-1:n) prepared in Uzbekistan from melts in concentrated sun flux, followed by rapid cooling, SFQA technology that preserves melt tiling, $T_{c,n}$ measured in Tiblisi, and local atomic enhanced synchrotron X-ray diffraction, XRD near the Cu K-edge at DOE National Laboratory SLAC-SSRL. The SFQA alloys structure indexed in the ideal D^{17}_{4h} Space Group indicates (n-1) units: $(CuO_2)_{1/2}/Ca/(CuO_2)_{1/2}$ are intercalated at each end of the n=1 phase, $[(CuO_2)_{1/2}/SrO/Bi_{1.7}Pb_{0.3}O/Bi_{1.7}Pb_{0.3}O/SrO/(CuO_2)_{1/2}]_2$. Surface effects lead to different n-phase mixing, and periodic lattice distortions, PLD, through bond resonance in crystal axes: $2(r_{Cu^{+2}}+r_{O^{-2}})=4.2Å>a=3.815Å>(CuO_{organic}+(O{=}O\text{-}O)/2^{3/2})=3.2Å$, $c_1=26.4Å$, $c_n-c_1=1.64(n-1)a$, or $\delta c_n/(2a(n-1))\approx-0.2$. Local atomic bonds Cu-Ca, Cu-Sr, Cu-O are detected by local atomic inelastic scattering. $T_{c,n}$ related to bond resonance in the family predicts $T_{c,n}\Rightarrow298K$ as $n\Rightarrow50$, if the superconducting skin depth is within a few μm.

Introduction: Covalent vs ionic materials with grain boundary, GB:

Covalent vs Ionic

1. HRTEM 2212: 1998 WY LIANG et al.

2. Non-bonding Cu_4O_4 HOMO: 1993



JV Acrivos, O Stradella

3. $SrTiO_3\Sigma13$:[015]GB 2001, K vanBenthem

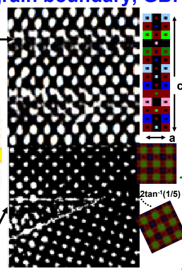


Figure 1: 2212, and ionic $SrTiO_3$ electron density, by high resolution electron microscopy, HRTEM[1] indicate different electron type bonds.

Cartoon of bc plane front:■, a/2 back:▪ ID: Bi, Sr, Cu, Ca, O, vacant = ■,■,■,■,■,■.

$SrTiO_3$[01L] GB are also present in 2:2:n-1:n [1].

K₀ incident XRD, scattered to K_1 at hν resonance , near the Cu K-edge, $Q=K_1-K_0$:
$0|aa_{\neq}Q_{HOMO}>+\varepsilon_0(\exp(i(K_0.R-\omega t))+h\nu\Rightarrow^*|a(-1s)a_{\neq}Q_{HOMO}(Q+q^*)_{LUMO}>+\varepsilon_s\exp(i(K_1.R-\omega t)$ followed in $t\leq10^{-17}$s by core state depletion of elements, $a_{\neq}$ bonded to excited a, by emission/ absorption/ backscattering from Q_{HOMO} and $(Q+q)_{LUMO}$ with ε_0, ε_s in the Q plane, add ΔE to hν, determined by atomic $f_{a,Q}$, neighbor $\chi_{a,l}$ *tensors.*

E levels of possible atomic excitations after t_0, E_0 near Cu K-edge in HTLSC

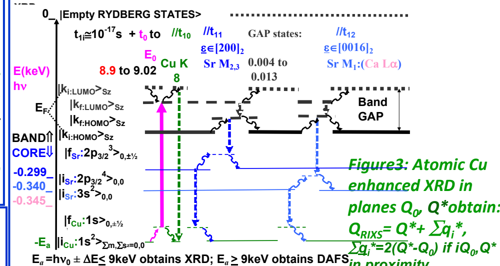
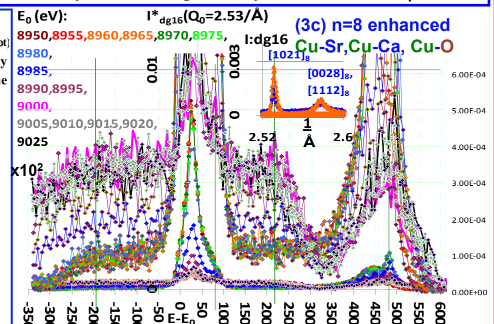


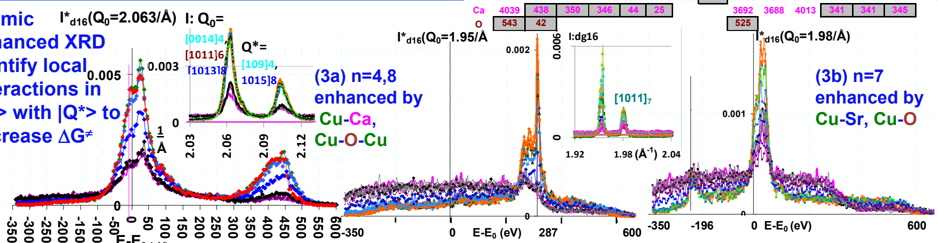
*Figure3: Atomic Cu enhanced XRD in planes Q_0, Q*obtain: $Q_{RIXS}=Q^*+\sum q_i^*$, $\sum q_i^*=2(Q^*-Q_0)$ if iQ_0,Q^* in proximity.*



CORE LEVELS INVOLVED (eV) http://xdb.lbl.gov/Section1/Periodic_Table/X-ray_Elements.html

E_a/F	K 1s	L_1 2s	L_2 $2p_{1/2}$	L_3 $2p_{3/2}$	M_1 3s	M_2 $3p_{1/2}$	M_5 $3d_{5/2}$	N_3 $4p_{3/2}$	$K\alpha_1$	$K\alpha_2$	$K\beta_1$	$L\alpha_1$	$L\alpha_2$	$L\beta_1$	$M\alpha_1$
Cu	8979	1097	952	933	123	77			8048	8028	8905	930	930	950	13
Sr	16105	2216	2007	1940	359	280	134	20	14165	14098	15835.	1807	1805	1872	66
Bi	90524	16388	15711	13419	3999	3696	2580	679	77108	74815	87343	10839	10731	13024	2423
Ca	4039	438	350	346	44	25			3692	3688	4013	341	341	345	
O	543	42							525						

Atomic enhanced XRD identify local interactions in $|Q_0>$ with $|Q^*>$ to decrease ΔG≠



RESULTS:

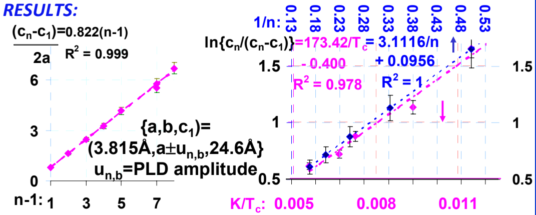


Figure 2: Activity $\ln[c_n/(c_n-c_1)]$ related to $T_{c,n}$ data obtains:

$$-\Delta G^{\neq}_n = k_BT\ln\{c_n/(c_n-c_1)\}= k_BT\{3.112/n+0.096\}$$

$$-\Delta G^{\neq}_n/k_BT =173.42 /T_{c,n} -0.400.$$

Discussion: 1. Resonance is indicated by crystal axes: $4.2Å=2(r_{Cu^{+2}}+r_{O^{-2}})>a=3.82Å>(CuO_{organic}+(O{=}O\text{-}O)/2^{3/2})=3.2Å$ is an average of purely ionic and covalent bonds. **2.** The CuO non bonding Cu_4O_4 HOMO allows [10L] GB formation in rapid cooled sun flux melts. These induce rotation detected by local Cu atomic enhanced XRD of pairs Q_0, Q* of mixed n=4 and n=8 phases formed in melt, indicating strong local Cu-Ca, Cu-Sr, Cu-O bonds. **3.** Interaction between extended electronic states $|Q_0>$, $|Q^*>$ decrease Gibbs free enthalpy of formation, ΔG≠ related to $T_{c,n}$ (fig. 3) that may be due to tiling in melts exposed to sun radiation.

Conclusion: HTLSC, alloys grown by SFQA novel fast cooling, which preserves melt tiling, mix different n phases, and show GB typical of parent $SrTiO_3$ promise useful applications with increased $T_{c,n}\approx$150 to 180K in emerging isolated regions, which appear to be related to Gibbs free enthalpy of formation $\Delta G^{\neq}_n$ by tiling.

ACKNOWLEDGEMENTS: Support for truly interdisciplinary, international work at San José State and DOE National Laboratory SLAC-SSRL, USA; Tiblisi, Georgia and Tashkent, Uzbekistan by the Science and Technology Centre in Ukraine (STCU) #4266 and Georgian National Science Foundation (GNSF) grant 08-477-4-260 and the Camille and Henry Dreyfus Foundation and DOE, and for published and unpublished HRTEM by YW Liang[1] is gratefully acknowledged.

References: [1] (a) W. Zhou, D.A. Jefferson and W.Y. Liang, *"Research Review, High Temperature Superconductivity"* Cambridge University, WY Liang, editor (1998), p.15; (b) W.Y. Liang and Y. Yin unpublished (1998); (c) K van Benthem, RH French, W Sigle, C Elsasser, M. Rühle, *Ultramicroscopy*, 86, 303, (2001); (d) J.V. Acrivos, *Physics and Chemistry of Electrons and Ions in Condensed Matter, J.V. Acrivos, N.F. Mott and A.D* Yoffe, ed, NATO ASI Series C130, 479 (1983); [2] JG Chigvinadze, AA Iashvili, TV Machaidze, *Phys. Letts. A* 300, 524 (2002); [3](a) DD Gulamova, DE Uskenbaev, G Fantozzi, JG Chigvinadze, O.V. Magradze. Zh. Tekhn. Fiz. 79, 98 (2009); (b) T Scopigno et al., *Physica B* 318, 341(2002); (c) JV Acrivos, *Microchemical Journal* 99,239–245(2011)