

Superconductivity for Electric Systems 2006 Project Summary

PROJECT TITLE:	Phase Relations of High T_c Superconductors
ORGANIZATION:	Ceramics Division, NIST, Gaithersburg, MD 20899
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FY 2006 FUNDING:	\$ 180K

Overall Project Purpose and FY 2006 objectives: Phase diagrams are “blue prints” for successful processing of high T_c superconductor materials. The overall objective of our project is to provide phase relationships of high T_c phases for the second generation wire/tapes (RABiTS and IBAD coated conductor) applications. The phase relationship studies include both bulk and film systems.

Our overall FY 2006 project goal was to continue developing a phase equilibrium database for Ba-R-Cu-O (R=lanthanides) systems. Our emphasis is particularly on the dependence of the $BaO-R_2O_3-CuO_x$ phase relations (under carbonate-free conditions to match the processing conditions of RABiTS/IBAD) on both oxygen partial pressure and on choice of lanthanides. Our phase relationship studies also include phase transformation of selected members of $Ba_2RCu_3O_{6+x}$ at different oxygen partial pressures (with BNL), and modeling of melting events of $Ba_2RCu_3O_{6+x}$ to correlate with the size of R (with BNL and Nanyang University). To understand the interplay of phase equilibria and kinetics in the Ba-Y-Cu-O-OH system during the “*ex-situ* BaF_2 process”, another objective is to understand the phase formation of phases in the Y- and R-containing precursor films using high temperature x-ray diffraction (HTXRD). Low temperature melts are thought to be essential for the growth of high quality $Ba_2YCu_3O_{6+x}$ at temperatures at or below 750 °C during the BaF_2 process, we have continued to include the low temperature melting study as part of our objectives (with ORNL and ANL). In 2006, we have added another objective of studying the phase relationship in films, which are important for coated conductor processing. As an understanding of the interfacial reaction of Y-213 phases with the buffer layers is critical to the control of coated conductor, another objective was to investigate the phase equilibria and kinetics of the interaction of $Ba_2YCu_3O_{6+x}$ with the potential buffer material (with ORNL and LANL). Additionally, by mixing a small lanthanide ion with larger R in R-213 solid solutions, flux-pinning and properties can be tailored and optimized. In collaboration with LANL and the AFRL at Wright-Patterson (AFRL-WP), we continued to characterize the high T_c mixed lanthanide solid solutions for flux pinning applications.

FY 2006 Performance and FY 2007 Plan: We have met our 2006 objectives and have conducted most of our FY 2006 activities to meet the needs of coated conductor development. We have conducted our phase relationships project under the guidance of a ‘phase equilibria advisory team’, and with extensive collaborations with other laboratories. We have successfully applied our experimental procedure and specialized apparatus to construct phase diagrams of the Ba-Ho-Cu-O system under controlled atmosphere conditions in air and in 100% O_2 . To better understand how the phase relationships apply to films processed using the BaF_2 *ex-situ* method, we have focused on film compositions in the vicinity of Y-213 using $SrTiO_3$ as a substrate. We have also prepared films in a combinatorial manner (oxides as starting materials) using the newly procured PLD system and the Bruker D8 x-ray diffractometer which is equipped with a near-microbeam source and an area detector. In collaboration with BNL, the orthorhombic to tetragonal phase transformation temperature of $Ba_2HoCu_3O_{6+x}$ and $Ba_2ErCu_3O_{6+x}$ as a function of p_{O_2} was studied using an ‘oxygen order-disorder transition’ approach. We have also investigated melting for selected members of the $Ba_2RCu_3O_{6+x}$ series. We have completed investigation of the solid solution range of the $Ba_{2-x}(R, Y)_{1+x}Cu_3O_z$ phases at p_{O_2} of 0.1% and 100%, where R=Sm, and Eu. This year we continued to use our vapor furnace thermogravimetric analyzer to investigate the role of $Ba(OH)_2$ -related liquid in low-temperature melting of the Ba-Y-Cu-O-OH system. We have collaborated with ORNL to understand the mechanisms of phase evolution of the BaF_2 films, using films in both Ba-Y-Cu-O and Ba-R-Cu-O systems prepared by e-beam evaporation and TFA methods. We have expanded our study of interfacial reactions to include Y-213 with Gd_3NbO_7 buffer layer and also with CeO_2 , for investigation of the kinetic aspects.

The FY 2007 plan builds upon the FY2006 progress. We will continue our interactions with the ‘phase equilibria advisory team’, and our collaborations with ORNL, ASC, ANL, and BNL on the BaF_2 subproject, with LANL and AFRL-WP on the mixed-lanthanides subproject, and with ORNL and LANL on superconductor/buffer interaction subproject. We will also continue to study phase relations of the Ba-R-Cu-O systems under atmospheric controlled conditions, and complete the phase transformation study of the $BaR_2Cu_3O_{6+z}$ series using modeling (collaboration with BNL and Nanyang University). With our combinatorial PLD capability and our D8 x-ray diffractometer, we will continue to collaborate with ORNL to use the thin-film combinatorial approach for the investigation of the film relationships of systems important for coated conductor applications. For the BaF_2 subproject, emphasis will continue to

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be placed on both modeling and experimental work related to melting equilibria in the multicomponent Ba-Y-Cu-O-F-OH system and pertinent subsystems. In collaboration with ORNL, we will continue to use combined HTXRD and TEM to compare the mechanism of phase evolution of the R-213 superconductor and related films (films will be prepared by both the e-beam evaporation and TFA approaches).

FY 2006 Results:

1. Phase diagrams of the Ba-R-Cu-O (R=Ho systems in 100 % O₂ and purified air) have been constructed and compared with other members of the Ba-R-Cu-O systems.
2. Study of the melting of selected members of Ba₂RCu₃O_{6+x} (R=Sm, Gd, Eu, and Y) shows that one needs to use an anisotropic model to interpret the melting trend of this series as a function of the ionic size of R³⁺.
3. Phase relations and minimum melting for non-binary joints of Ba₂YCu₃O_{6+x} with buffer material, Gd₃NbO₇, have been determined. Neutron studies of selected (La,Y)₃NbO₇ were carried out to understand the structure of this solid solution.
4. A study of the kinetics of the interactions of Ba₂YCu₃O_{6+x} with CeO₂ was completed at three temperatures using x-ray diffraction and TEM. The activation energy of reaction was obtained.
5. A collaboration with BNL to model the phase transition of Ba₂ErCu₃O_{6+x} and Ba₂HoCu₃O_{6+x} as a function of oxygen partial pressure was successfully performed.
6. In collaboration with ORNL, we continue to use the HTXRD technique to compare the mechanism of phase evolution of the Ba₂YCu₃O_{6+z} superconductor and related films using the BaF₂ process on SrTiO₃. We have also prepared PLD combinatorial films on Si and on SrTiO₃ using oxides instead of fluoride for comparison.
7. Phase relationships of films have also been investigated for the selected compositions in the BaO-R₂O₃-CuO systems (R=Nd,Gd,Eu) on SrTiO₃ using the TFA solution approach.
8. The Ba_{2-x}(R, Y)_{1+x}Cu₃O_z systems (R=Sm, Eu) have been characterized in 0.1% O₂ and purified air. The size of the solid solution region varies with the oxygen partial pressure and the size of R (with AFRL and LANL).
9. Decomposition studies of Ba(OH)F show that the reactions can be controlled by varying temperature and gas-phase partial pressure, leading to a potential route for the generation of low temperature liquids during *ex situ* processing.

Research Integration:

To ensure the relevance of our phase equilibrium studies, we work closely with other national laboratories, with universities, and with industry. We continue to interact with the "phase equilibrium advisory team" which includes members from the superconductor industry, government laboratories and universities: ASC, IGC, Oxford Instruments, ANL, ORNL, LANL, BNL, AFRL-WP, and University of Houston. We are currently collaborating on the BaF₂ project with ORNL, ANL, and BNL, and with other scientists of the NIST Ceramics and Metallurgy Divisions and the Center for Neutron Research. We are collaborating with LANL and AFRL-WP on the mixed lanthanide projects, with ORNL and LANL on study of interaction of Y-213 with buffers, with BNL and Nanyang University on phase transformations and on melting of R-213, and with the Ames Laboratory on MgB₂ studies.