STRUCTURAL PHASE TRANSFORMATIONS AND HIGH- T_c SUPERCONDUCTIVITY

J.D. Axe, H. You, D. Hohlwein, D.E. Cox

Department of Physics

*National Synchrotron Light Source

Brookhaven National Laboratory

Upton, New York 11973

BNL--40048

S.C. Moss and K. Forster

Department of Physics

University of Houston

Houston, TX 77004

DE87 013308

P. Hor, R.L. Meng and C.W. Chu

Department of Physics

Space Vacuum Epitaxy Center

University of Houston

Houston, TX 77004

There is an intimate if imprecisely understood connection between high T_c superconductivity and crystal structure instability. Most of the highest T_c superconductors ($T_c \approx 20K$) discovered in the past 20 years have the so called A15-type structure, which is marginally stable in the sense that many of the A15 compounds spontaneously distort at low temperatures into a lower symmetry structure. These distortions are driven by unstable low frequency phonon modes. It is believed that these "soft" phonon modes enhance the attractive interaction between electrons and thus tend to increase T_c . On the other hand (the argument goes) phase transformations which lower the symmetry introduce structural gaps at the Fermi surface of metals which compete with superconductivity and tend to decrease T_c .

The recent discoveries of $T_c \approx 40K$ (much higher T_c 's are rumored) in the $LaCuO_4$ -type systems raise questions concerning the importance of lattice instabilities to superconductivity in these systems. We have

performed high resolution synchrotron x-ray powder diffraction measurements on the superconductor $\text{La}_{1.8}\text{Ba}_{0.2}\text{CuO}_4$ which show unusual temperature dependent broadening of certain Bragg peaks, as shown in Fig. 1. This pattern of peak broadening can be consistently explained as an unresolved splitting due to a spontaneous reduction of the tetragonal symmetry of the high temperature structure to a lower monoclinic (or possibly triclinic) form.

In order to confirm this interpretation of the powder diffraction data, we were also able to carefully reduce the size of the highly collimated synchrotron x-ray beam and to isolate and study individual $\approx 70\mu\text{m}$ single crystals within the powder aggregate. Fig. 2a shows more clearly than the powder data the splitting of the reflections upon cooling. Fig. 2b shows a greatly enlarged image of the diffracted beam from the same microcrystalline reflection shown in Fig. 2a, using a novel high resolution Weissenberg camera that we have developed. Again the splitting is clearly evident.

The relationship of the structural transformation we have discovered to the superconductivity which occurs at lower temperature ($T_c \approx 36\text{K}$) is unclear. But in view of the interplay between superconductivity and structural transformations noted above, further structural studies with larger single crystals should prove rewarding. It must be pointed out that the degree of monoclinic distortion that we have found is very small, and that the brightness of a synchrotron x-ray source was essential for high resolution powder and single crystal diffraction experiments presented here.

FIGURE CAPTIONS

Fig. 1a Comparison of the width of powder diffraction peaks in the high- T_c superconductor $\text{La}_{1.8}\text{Ba}_{0.2}\text{CuO}_4$ at 300K and 10K. Many peaks show an unusual broadening as the temperature is lowered. The triangles represent instrumental resolution.

Fig. 1b The temperature dependence of the width of two peaks shown above. The onset of the broadening indicates a phase transformation at $T \approx 130\text{--}150\text{K}$.

Fig. 2a Splitting of the (110) rocking curve of a small ($70\mu\text{m}$) single crystal of $\text{La}_{1.8}\text{Ba}_{0.2}\text{CuO}_4$ at low temperature.

Fig. 2b Magnification of direct image of diffracted beam from crystal studied in Fig. 2a. The horizontal splitting is direct evidence of two slightly different (110) lattice plane spacings at low temperature.

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency, contractor or subcontractor thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency, contractor or subcontractor thereof.