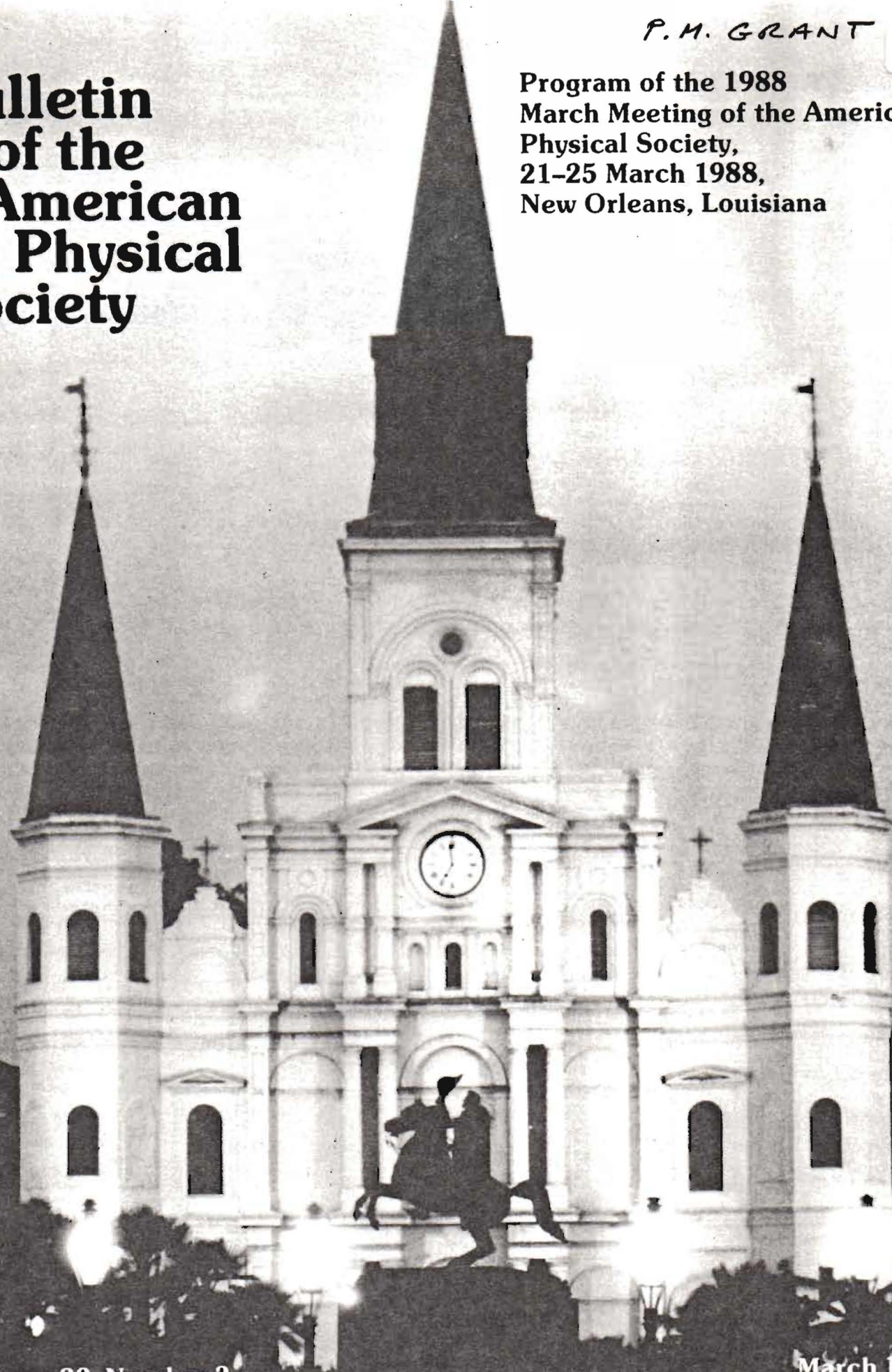


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pseudopotentials and the appropriately prepared atomic gaussian-orbitals basis set. It is shown that the total energy for the antiferromagnetic state is lower than that for the paramagnetic state by 0.1 eV per unit cell in the case of La_2CuO_4 . The resulting stable antiferromagnetic state is found to be an insulator with the energy gap of 0.6 eV, and

the magnetic moment is mainly localized at Cu^{2+} sites with the magnitude of $0.43 \mu_B$. By doping divalent-atoms, holes are created in the lower $\text{Cu } d - \text{O } p$ band. We find that the crossover from the antiferromagnetic to the paramagnetic state occurs at some Sr content x_c .

SESSION M8: HTSC: OXYGEN VARIATION I

Thursday morning, 24 March 1988; Grand Ballroom C, Sheraton Hotel at 8:00; Z. Fisk, presiding.

Invited Paper

8:00

M8 1 J. M. TARASCON, *Bellcore*.

Contributed Paper

8:36

M8 2 Effect of Oxygen Pressure on the Orthorhombic-Tetragonal Transition in the High-Temperature Superconductor $\text{YBa}_2\text{Cu}_3\text{O}_x$.* E. D. SPECHT, C. J. SPARKS, A. G. DHERE, J. BRYNESTAD, O. B. CAVIN, D. M. KROEGER, Oak Ridge National Lab.; H. A. OYE, F.S. Seiler Research Lab.-- In situ X-ray diffraction and thermogravimetric measurements determined the temperature and oxygen content at the structural phase transition. An abrupt, continuous, and reversible transition occurs at a temperature varying from 676°C in 1.0 atm O_2 to 521°C in 0.005 atm. Oxygen content at the transition remains close to $x = 6.6$. In a helium atmosphere, an irreversible transition is observed at 455°C. The c axis contracts at a rate of 1.2% per oxygen atom added.

*Research sponsored by Division of Materials Sciences, U.S. Department of Energy under contract DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

8:48

M8 3 Preparation and Properties of $\text{Y}_1\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$ Samples with Precisely Controlled Oxygen Arrangements. R. BEYERS, E.M. ENGLER, P.M. GRANT, S.S.P. PARKIN, S. LA PLACA, G. LIM, M.L. RAMIREZ, J.E. VAZQUEZ, V.Y. LEE, and R.D. JACOWITZ, *I.B.M.*; B.T. AHN, T.M. GUR, and R.A. HUGGINS, *Stanford U.* — This paper reports on the structures and properties of $\text{Y}_1\text{Ba}_2\text{Cu}_3\text{O}_{7-x}$ samples prepared in controlled oxygen environments using a solid-state ionic technique. The samples were prepared in a sealed chamber that contained a stabilized zirconia solid electrolyte. Passing a known current through the electrolyte allowed precise titration of oxygen into and out of the sample. Measuring the open circuit voltage across the electrolyte enabled the oxygen pressure inside the chamber to be accurately measured. This apparatus also allowed the quenching process to be accurately monitored. Transmission electron microscopy, x-ray diffraction, and neutron diffraction were used to characterize the oxygen ordering for various oxygen contents, quench rates, and annealing temperatures. Resistivity, thermopower, and susceptibility measurements were used to determine corresponding changes in superconducting properties.

9:00

M8 4 Structural Study of $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ as Function of Oxygen Content. H. Jaeger, K. Schulze, G. Kaiser, G. Petzow, *Max-Planck-Institut für Metallforschung, Stuttgart, FRG*; J. Ihlinger, *Universität Tübingen, FRG*. -- Results of a recent structural study of the high- T_c superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ with $0 \leq x \leq 1$ are reported. Bulk $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ samples were prepared with varying oxygen content by a sintering process with subsequent quenching or inert atmosphere treatment. Raman spectroscopy and vacuum hot extraction were used to determine

the oxygen content of the samples. Structure and lattice parameter were derived from x-ray spectra. Samples quenched from 800 and 900°C were found to be of tetragonal structure, quenching from temperatures below 600°C resulted in the orthorhombic structure. It was found that structure, lattice parameters, and oxygen content are strongly correlated. Effects of partial substitution of Cu by Ag on the structure and oxygen content will also be discussed.

9:12

M8 5 The tetragonal phase of $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ -- Does it really exist for $\delta > 0?$ * A. G. MCKALE, H. T. SU, S. S. KAO, W. H. WARNES, J. A. GARDNER, Oregon State University; and J. A. SOMMERS, Teledyne Wah Chang Albany -- Diffraction measurements indicate that the structure of $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ is orthorhombic for $\delta = 1$ and tetragonal for $\delta = 0$. Some x-ray and neutron measurements in oxygen-containing environments have been interpreted as an orthorhombic/tetragonal transition near $\delta = 0.5$ -- approximately 700°C in air or flowing oxygen. Other diffraction measurements have failed to show such a transition. Our perturbed angular correlation measurements on indium tracers substituted at the yttrium site demonstrate clearly that there is no microscopic transition. These measurements, taken in flowing oxygen, indicate orthorhombic phase up to 950°C. We suggest that the transition detected by some diffraction experiments is microstructural, not a true structural transition.
*Supported in part by NSF through grant MSM-8717809

9:24

M8 6 Effect of Oxygen Content and Disorder on the Superconducting Properties of $\text{Y}_1\text{Ba}_2\text{Cu}_3\text{O}_7$ and Its Rare Earth Derivatives. E. M. ENGLER, V. Y. LEE, S. S. P. PARKIN, K. ROCHE, R. JACOWITZ, M. RAMIREZ, P. M. GRANT, R. BEYERS and G. LIM, *IBM Research Division, Almaden Research Center, San Jose, CA 95120-6099*.--A series of samples of $\text{Y}_1\text{Ba}_2\text{Cu}_3\text{O}_x$ have been prepared where oxygen content is varied from $x = 7.00$ to $x = 6.00$. There is a dramatic loss in bulk superconductivity in the region between 6.30 and 6.60 and this behavior has been carefully probed using transport, magnetic and structural measurements. Multiple techniques have been evaluated for precise oxygen content determination. By varying quench rate for samples annealed in Argon, the role of disordering oxygen in the a-b lattice directions can be evaluated. Such disorder effectively leads to a disruption of the 1-dimensional ribbon ordering which appears important for realizing superconductivity in these materials. A similar situation appears to account for the behavior of several rare earth derivatives such as Nd and Lu which have been found to be more difficult to prepare as 90°K plus superconductors. This greater tendency of some of the rare earth derivatives towards disorder may account for the lack of superconductivity in $\text{Pr}_1\text{Ba}_2\text{Cu}_3\text{O}_7$.

9:36

M8 7 Does S Replace O in Orthorhombic $\text{YBa}_2\text{Cu}_3\text{O}_6\text{S}_1$? Q. YIN, C. BLUE, K. ELGAID, D. MCDANIEL, W. HUFF, I. ZITKOVSKY, P. BOOLCHAND,