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$La_{0.625}Ca_{0.375}MnO_3$에 대한 고분해능 중성자 산란 실험과 탄성계수, 저항 측정에 대한 연구

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High resolution neutron powder diffraction, and resistivity and elastic constant measurements of $La_{0.625}Ca_{0.375}MnO_3$ at high temperatures

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1. INTRODUCTION

We have investigated the high temperature phase transition occurring in a CMR material, $La_{0.625}Ca_{0.375}MnO_3$. Although recent attention was paid mostly to low-temperature magnetic transitions in CMR materials, it is known that there occurs a structural phase transition at high temperatures. The transition is from a rhombohedral phase to an orthorhombic one, as temperature decreases. In order to uncover detailed features of this transition, we carried out high resolution powder diffraction from room temperature to 1000 K. We also measured resistivity and elastic constant as a function of temperature in the transition region. From the resistivity and elastic measurements, and the Rietveld refinement analysis of the powder diffraction data, we were able to conclude that this transition is first order and two possible phases coexist in the intermediate transition region between 740 K and 770 K.

2. EXPERIMENTS

The high resolution neutron powder diffraction (HRPD) was made with the HANARO reactor in KAERI. Neutron was monochromatized by Ge(311) and its wavelength 0.184 nm. The mass of the sample is 1.40 g. Structure parameters were refined by the Rietveld analysis software Fullprof. The background was fitted to fifth order polynomial. The pseudo-Voigt function was used to model the peak shape. Young's modulus and elastic dissipation were measured by three point bending (TPB) method using TMA/SS (Thermo-mechanical analyzer/strain-stress, Seiko). The specimen, which was prepared to the shape of thin plate, was laid on two wedges of the support. The quartz rod applies the 0.01 Hz sinusoidal mechanical force to the midspan of specimen. The specimen gets bent to the parabolic curve according to the force. The deflection of the specimen center from the horizontal level gives the information of elastical properties; the Young's modulus is derived from the magnitude of the deflection and the elastic dissipation from the phase difference.

3. RESULTS AND DISCUSSION

The Young's modulus and elastic dissipation for 0.01 Hz is plotted in Fig. 1. When temperature is raised across the structural transition temperature, the Young's modulus decreases rapidly by about 50 %, accompanied by a large elastic dissipation. The dip of Young's modulus is also discovered. It implies that any phonon modes are softened around T_s.

When temperature is raised, the orthorhombic (Pnma) phase is transformed into the rhombohedral (R-3c) phase through the intermediate region where the Young's modulus decreases abnormally and the elastic dissipation increases greatly. To make clear the characters of this transition, we carried out the measurements of resistivity shown in Fig. 2, converting the temperature scanning direction. The temperature where resistivity changes most abruptly, is shifted in the heating measurement by about 4 K relative to the cooling one. This thermal hysteresis is the principal character of first order transition.

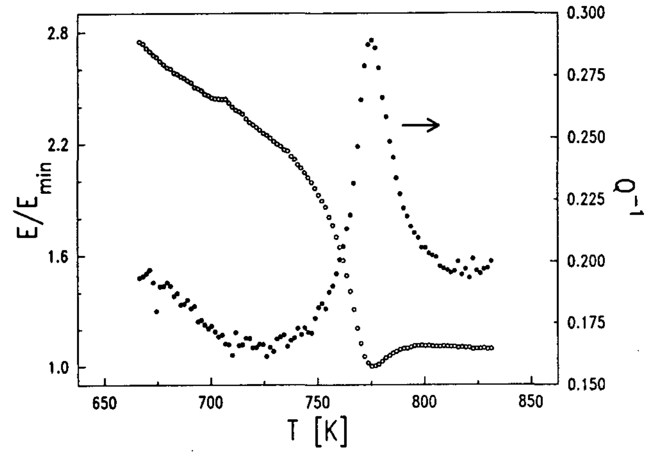

Fig. 1. The Young's modulus and the elastic dissipation.

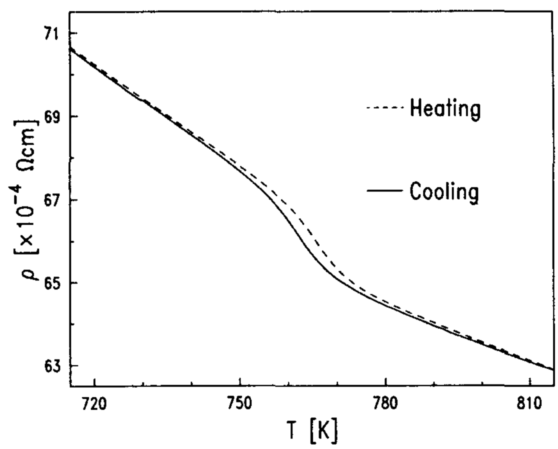

Fig. 2. The resistivity. The thermal hysteresis is discovered.

The fact that the elastic constant and the resistivity are continuously varied regardless of first order transition makes us inspect that two phases may coexist in the intermediate temperature. From the HRPD measurement in the temperature range 730-770 K, the phase separation picture could be verified. The profiles for the Bragg reflection $(1\ 1\ 1)_c$ are shown in Fig. 3 to present clearly the evidence for the phase separation. The phase separation can explain the continuous softening of Young's modulus in the intermediate range of temperatures. Although this structural transition is first order, the continuous variation of Young's modulus is possible owing to the mixture of the elastically hard Pnma phase and soft R-3c phase with an appropriate mixing rate depending on temperature. The large elastic dissipation also seems to be based on this phase separation. The externally induced time-varying bending deformation in TPB method brings about the instability of the domain distribution. The domain boundaries fluctuate to follow new equilibrium positions by phase flip. Irreversible processes are induced in the course of this fluctuation.

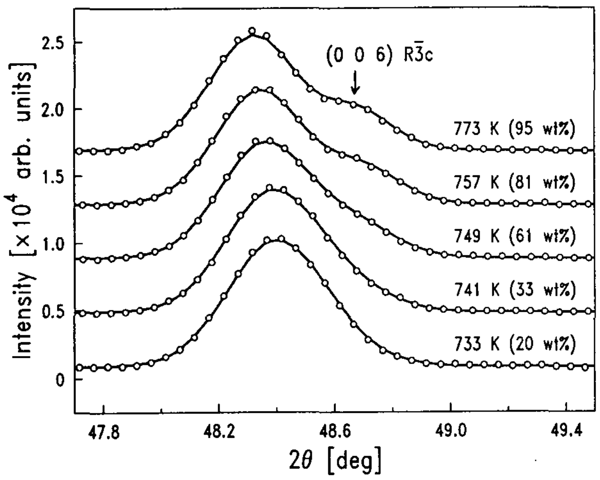

Fig. 3. The profiles of $(1\ 1\ 1)_c$ Bragg reflection.

4. CONCLUSIONS

The thermal hysteresis in the resistivity measurements shows this transition is first order. We could verify two structural phases are mixed between 740 K and 770 K, from the attentive HRPD measurements for the transition region. In this phase separated region, the Young's modulus is softened gradually, accompanied by the drastic increase of the elastic dissipation.