18C/2003P002 Pressure dependence of spin-Peierls transition temperature of (DMe-DCNQI)₂Li

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Introduction

(DMe-DCNQI)₂Li is a one-dimensional 1/4 filled π band system, undergoing the spin-Peierls (SP) transition around $T_{\rm SP} = 65$ K at ambient pressure.[1] Recently Hiraoka et al. have intensively investigated this system by ESR under pressure and suggested that a fractional charge soliton carries the electrical current in the $4k_{\rm F}$ charge density wave state above $T_{\rm SP}$. [1, 2] Furthermore they discussed the pressure dependence of $T_{\rm SP}$ in terms of Cross-Fisher's theory. [3, 4] In the present report, this analysis is confirmed using newly obtained data of the pressure variation of the lattice constant.

Experimental

The X-ray diffraction pattern under pressure was measured using synchrotron radiation at the beam line BL-18C of the Photon Factory, High Energy Accelerator Research Organization (KEK). A diamond anvil cell (DAC) was used for applying pressure. The electronic spin susceptibility χ_e under pressure was obtained by ESR using a clamp type pressure cell.

Results and Discussion

Figure 1 shows the temperature dependences of χ_e under pressure. χ_e decreases exponentially below T_{SP} due to the SP transition. The inset indicates the pressure dependence of $T_{\rm SP} = 0.8 \lambda^2 J^2 / Ka^2$, which was calculated by Cross-Fisher. [3] λ , J, K, and a are the spin-phonon coupling constant, the exchange interaction between the nearest spins, the elastic constant, and the lattice parameter, respectively. The pressure dependence of other parameters than J would not be large under pressure enough to explain the increase of T_{SP} . On the other hand, J is proportional to the square of the transfer energy on the assumption that this system is a Mott-Hubbard insulator. Then J could be enhanced enough as the overlap between wave functions increases under pressure. Following Ref. 4, we can obtain the relation: $T_{\rm SP}(P) \propto J^2(P) \propto \exp(4a_0 \varepsilon P/r_0)$, where a_0 is the lattice constant at ambient pressure, r_0 is the characteristic length of an exponential tail of the wave function, and ε is the one-dimensional compressibility along the c-axis. This relation reproduces well the T_{SP} variation as indicated by the solid line in the inset of Fig. 1.

The X-ray diffraction pattern at ambient pressure is shown in Fig. 2. We focused on (001/2) reflection indicated by the arrow, which corresponds to 2-fold periodicity along *c*-axis: 7.668Å. ε is estimated to be

1%/GPa from the pressure dependence of the (001/2) peak exhibited in the inset. With the observed ε and the parameter deduced from the fitting in the inset of Fig. 1, r_0 is estimated to be $a_0/6$. This result is consistent with the Mott-Hubbard insulator, where the wave function is localized. Thus, $T_{\rm SP}$ is well represented by Cross-Fisher's theory as mentioned in Ref. 4.



Fig. 1 The temperature dependences of χ_e under pressure. Inset: The pressure dependence of T_{SP} .



Fig. 2 X-ray diffraction pattern measured at ambient pressure. Inset: The pressure dependence of the peak indicated by the arrow.

References

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