# Colossal magnetoelectricity in hexagonal $Ni_3TeO_6$

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Multiferroic and magnetoelectric (ME) materials, with their coexisting magnetic and ferroelectric orders, are of pressing interest for spintronics and information storage technology. Several ways to enhance the magnetoelectric effect were proposed, such as driving the ferroelectric modes to low frequency ("structural softness") by applying strains to thin films [1]. Recent discovery of the colossal magnetoelectric effect at the spin-flop transition in the hexagonal $Ni_3TeO_6$ offered an alternative approach, in which the responses are enhanced due to the soft magnon mode in the vicinity of the magnetic critical point, cf. Fig. 1. This material, showing the largest known to date ME coefficient, has a peculiar second-order spin-flop transition, separating the antiferromagnetic and canted phases. Heisenberg exchange striction couples magnetic ordering to the pyroelectric polarization, giving rise to the polarization

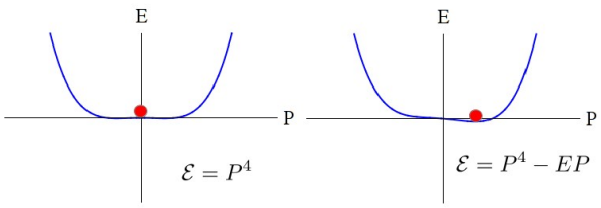


Fig. 1. At the second-order phase transition the flat free energy landscape gives rise to large responses.

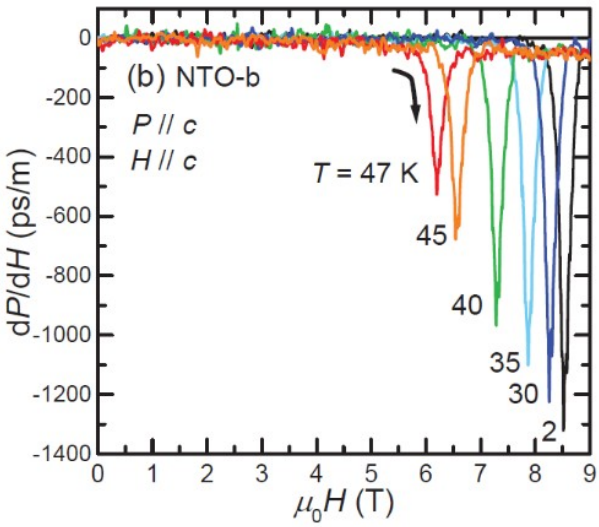


Fig. 2. The experimentally measured linear magnetoelectric coefficient increases as the temperature is decreased, suggesting that the effect is controlled by the quantum critical point.

change across the transition. This enables one to cross the transition boundary by applying magnetic or electric fields, and the linear ME coefficient as large as 1400 ps/m at 2K, to our best knowledge, the largest observed to date [2], cf. Fig. 2. While the phenomenological Landau-type theory describes the essential physics of the ME effect, it does not explain another transition at higher magnetic fields, that was recently discovered. The latter transition at round H=52 T is accompanied by an even larger polarization change, and shows strong dependence on the magnetic field direction, seen in Fig. 4. Using a microscopic Hamiltonian with the parameters determined from DFT calculations, we model the whole phase diagram of this material and obtain the insights into how the competition of exchange interactions and exchange anisotropies gives rise to the rich phase diagram, observed experimentally.


[1] J. C. Wojdel, J. Iniguez, PRL **105**, 037208 (2010).

[2] Y. S. Oh, S. Artyukhin, J. J. Yang, V. Zapf, J. W. Kim, D. Vanderbilt, S.-W. Cheong, Nature Communications **5**, 3201 (2014).


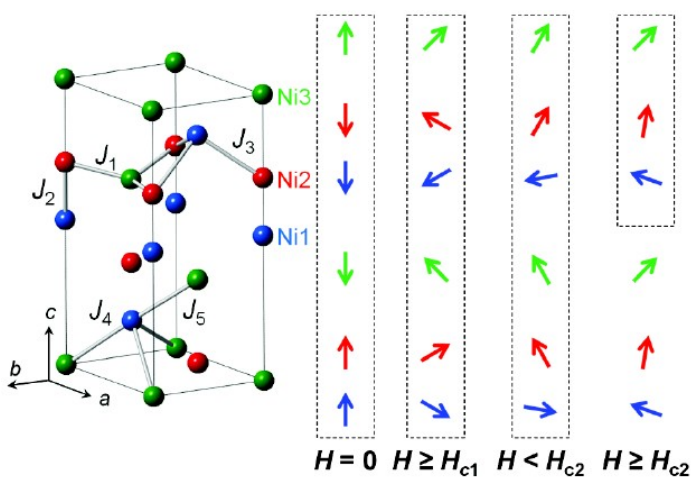


Fig. 3. The nearest-neighbor exchange interactions, included in the model, shown in the hexagonal crystallographic unit cell and various magnetic field-induced spin configurations shown in the rhombohedral magnetic unit cell.

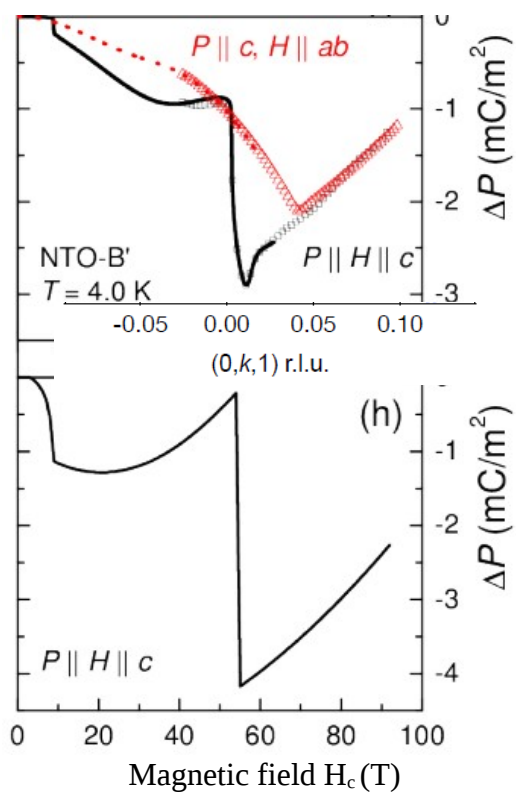


Fig. 4. The polarization dependence on the magnetic field, measured in the experiment (top panel) and calculated from the model with parameters extracted from DFT.