The Effect of Structural Defects on Magnetic Ground States in Geometrically Frustrated Pyrochlore Systems

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Introduction

Pyrochlore oxide $Yb_2Ti_2O_7$ is a geometrically magnetic frustrated material, in which its subtle magnetic interactions are prone to small perturbations. Due to discrepancies in the reported magnetic ground states, it has become a pressing issue to determine the nature of defects in this system. There have been many reports and publications that presented varied physical properties and inconsistent results with sample-dependence magnetism. The true nature of the defects that affect the material's magnetic ground states has been elusive with no direct evidence yet after more than ten years of research. Our study reports the extended defects that have never been reported before. Our results shed new light onto this geometrically frustrated system that is a quantum spin liquid candidate. It provides a natural explanation on the varied magnetic ground states for this material system.

Experimental

The polycrystalline powder sample that has a white color was synthesized by solid state reaction. The single crystals were grown by the floating zone method. STEM study was carried out on a probe-aberration-corrected, cold-field-emission JEM JEOL-ARM200cF at 200 kV using a JEOL HAADF-STEM detector. The STEM resolution is 0.078 nm, and energy resolution is 0.5 eV at full emission.

Results and Conclusions

Using a direct imaging technique, the structural quality and defects were characterized for the ytterbium titanate pyrochlore at the atomic scale. Besides the previously reported point defects (i.e. such as Yb substitution in Ti B-sites), we frequently observed the extended planar and line defects, which are superdislocations and anti-phase boundary (APB). The lattice strains from these extended defects result in distortions of Yb-tetrahedron. This potentially disrupts long-range structural perfection of the material, which would ultimately disturb the delicate magnetic interactions. This seems to suggest that the broad phase transition reflected in specific heat could be explained by the non-homogeneous distribution of distorted Yb-tetrahedra in a three-dimensional arrangement. These line and planar defects would offer a natural explanation for a non-magnetic, disordered state in stoichiometric single crystals [1].

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References

[1] Shafieizadeh, Z., *et al*., Nature Scientific Reports, **8**, 17202 (2018).

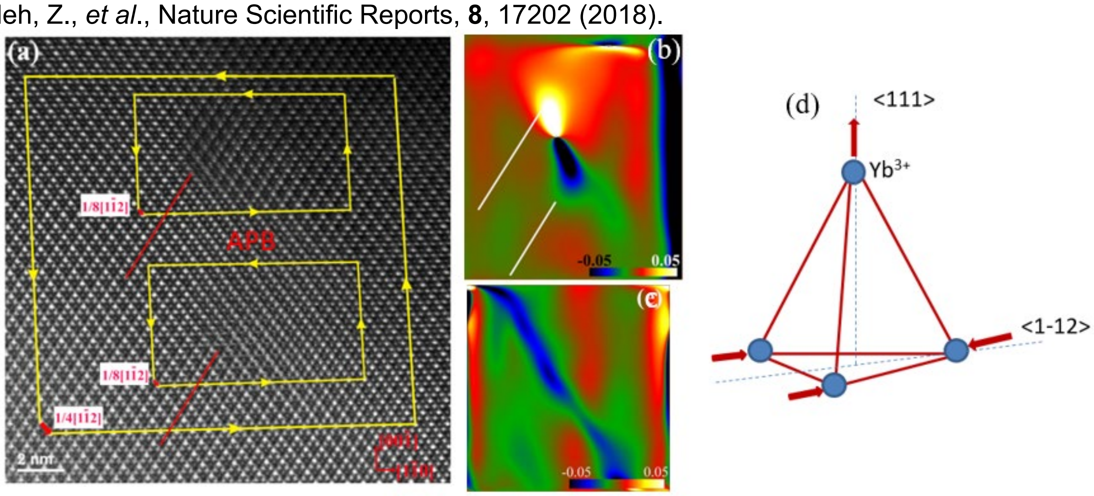

Fig.1 (a) Atomic resolution HAADF-STEM image of a superdislocation; (b) ε_{xx} strain map of the dislocation. (c) strain map of APB. (d) Schematic of Yb^{3+} ions in Yb-tetrahedron displacement away from equilibrium position.