MS.81.5

Acta Cryst. (2011) A**67,** C180

Control of thermal expansion behavior by zn deficiency in $Mn_3Zn_{1-x}N$

Qingzhen Huang,[a] Cong Wang,[b] Lihua Chu,[b] Qingrong Yao,[a,c] M.M.Wu,[a,d] Ying Sun,[b] J. W. Lynn,[a] D. A. Neumann,[a] *[a]NIST Center for Neutron Research, Gaithersburg, MD 20899, (USA). [b]Center for Condensed Matter and Materials Physics, Dept. of Physics, Beihang University, 100191 Beijing, (China). [c]School of Material Science and Engineering, Guilin University of Electronic Technology, Guilin 541004, (China). [d]Department of Nuclear Physics, China Institute of Atomic Energy, Beijing, 102413, (China).*

We report the controllable zero thermal expansion (ZTE) behavior with a larger temperature range in the antiperovskite $Mn_3Zn_{1-x}N$ (x=0-0.07) system. The system has a cubic lattice and two magnetic order states. One magnetic order occurs at 185 K where the paramagnetic state (PM) at high temperature transforms to a non-collinear antiferromagnetic state (M1), accompanying with ~0.5% of the cubic lattice increasing in M1 state. Another non-collinear antiferromagnetic order (M2) occurs at low temperature (below 180 K). The M2 has no magnetic lattice affect compared to the PM phase and its magnetic ordering temperature depends on the vacancy x at Zn site. The M1 phase has ZTE behavior and the ZTE temperature can be adjusted by the vacancy x at the Zn site. The coefficient of thermal expansion (CTE) was achieved to $5.83x10^{-7}$ K^{-1} in the wide temperature range from 5 K to 180 K in $Mn_3Zn_{0.93}N$. The quantitative analysis of neutron diffraction data gives a quantitative description about the "spin – lattice" correlation that the change of the magnetic moment, due to the spin re-arrangement induces the lattice contraction, and coincidentally counteracts the normal positive thermal expansion, which is the origin to introduce near zero thermal expansion effect. It is suggested that the zero thermal expansion can be designed by adjusting the spin moment and its changing process with temperature.

Keywords: antiperovskite, magnetostriction, zero thermal expansion

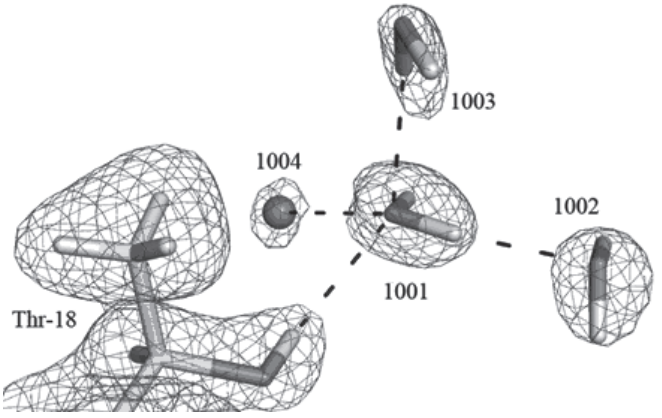
MS.82.1

Acta Cryst. (2011) A**67,** C180

Neutron structure of type-III antifreeze protein leads to ice interface model

Alberto Podjarny,[a] Matthew P. Blakeley,[b] Isabelle Petit-Haertlein,[b,c] Michael Haertlein,[b,c] Alexandra Cousido-Siah,[a] Tatiana Petrova,[d] Eduardo I. Howard,[e] *[a]IGBMC, Illkirch, (France). [b]ILL,Grenoble, (France). [c]PSB, Grenoble, (France). [d]IMPB, Pushchino Russia, [e]IFLYSIB, La Plata, (Argentina).* E-mail: podjarny@igbmc.fr

Antifreeze proteins (AFPs) inhibit ice growth at sub-zero temperatures. The prototypical type-III AFPs have been extensively studied, notably by X-ray crystallography, solid-state and solution NMR, and mutagenesis, leading to the identification of a compound ice-binding surface (IBS) composed of two adjacent ice-binding sections, each which binds to particular lattice planes of ice crystals, poisoning their growth. This surface, including many hydrophobic and some hydrophilic residues, has been extensively used to model the interaction of AFP with ice. Experimentally observed water molecules facing the IBS have been used in an attempt to validate these models. However, these trials have been hindered by the limited capability of X-ray crystallography to reliably identify all water molecules of the hydration layer. Due to the strong diffraction signal from both the oxygen and deuterium atoms, neutron diffraction provides a more effective way to determine the water molecule positions (as D_2O). Here we report the successful structure determination at 293K of fully perdeuterated type-III AFP by joint X-ray and neutron diffraction providing a very detailed description of the protein and its solvent structure. X-ray data were collected to a resolution of 1.05 Å, and neutron Laue data to a resolution of 1.85 Å with a "radically small" crystal volume of 0.13 mm^3. The identification of a tetrahedral water cluster in nuclear scattering density maps (see figure) has allowed the reconstruction of the IBS-bound ice crystal primary prismatic face. Analysis of the interactions between the IBS and the bound ice crystal primary prismatic face indicates the role of the hydrophobic residues, which are found to bind inside the holes of the ice surface, thus explaining the specificity of AFPs for ice versus water.



Keywords: neutron diffraction, antifreeze protein, protein crystallography

MS.82.2

Acta Cryst. (2011) A**67,** C180-C181

Neutron scattering reveals human pyruvate dehydrogenase complex organisation

Olwyn Byron,[a] Gordon Lindsay,[a] Swetha Vijayakrishnan,[a] Sharon Kelly,[a] David Bhella,[a] Donna McGow,[a] Margaret Nutley,[b] Alan Cooper,[b] Peter Kropholler,[b] Philip Callow,[c] Trevor Forsyth,[c] Robert Gilbert,[d] David Gilbert,[e] *Colleges of [a]Medical, Veterinary and Life Sciences, [b]Science and Engineering, University of Glasgow, Glasgow G12 8QQ (UK). [c]Institut Laue Langevin, 38042 Grenoble, Cedex 9 (France). [d]Wellcome Trust Centre for Human Genetics, University of Oxford, Oxford OX3 7BN (UK). [e]School of Information Systems, Computing and Mathematics, Brunel University, UB8 3PH (UK).* E-mail: olwyn.byron@glasgow.ac.uk

Mammalian pyruvate dehydrogenase complex (PDC), a key multi-enzyme assembly responsible for glucose homeostasis maintenance and conversion of pyruvate to acetyl CoA, comprises a central pentagonal dodecahedral core consisting of two subunit types (E2 and E3BP) to which peripheral enzymes (E1 and E3) bind tightly but non-covalently. Neutron scattering, deuteration and a range of molecular-biological, protein-chemical and biophysical techniques were used to resolve a conflict between two extant models of PDC core organisation (the 'addition' (60+12) and 'substitution' (48+12) models) and to demonstrate clear differences in subunit content and organisation between a recombinant hPDC core (40E2+20E3BP), generated under defined conditions where E3BP is produced in excess, and its native bovine (48E2+12E3BP) counterpart.

The first ever low-resolution structures of human recombinant full-length (rE2/E3BP), truncated (tE2/E3BP) and native bovine heart (bE2/E3BP) PDC cores obtained by SAXS and SANS will be presented. These structures, corroborated by negative stain- and cryo-EM data, clearly reveal open pentagonal core faces, favouring the