School of Materials Science and Engineering

Seminar Topic:
Synthesis of Apatite-Type Nanomaterials and their Applications

Associate Professor Dong Zhili

Abstract

Synthetic apatite-type materials have been widely investigated in many fields, such as catalysis, environmental remediation, bone engineering, optical devices, etc, because of their stability in a wide range of chemical compositions and their capability to incorporate different dopants based on the composition design to obtain desired properties. However, it is challenging in some cases to precisely control the compositions to obtain optimized structures with desired properties. In this presentation, we report our work on synthetic apatites with potential applications in bone engineering, photoluminescence and nuclear waste immobilization.

The general formula of the apatite-type compound is $A^{I}_{4}A^{II}_{6}(BO_4)_6X_2$. The A^{I} (Wycoff 4f site) and A^{II} (Wycoff 6h site) positions are two distinct crystallographic sites which accommodate monovalent alkali, divalent alkaline earth, or trivalent/tetravalent rare-earth elements. The B site is occupied by phosphorous, vanadium, silicon, boron, or germanium. X is the anion site for halogens, hydroxyl, or oxygen. Most apatites belong to the space group $P6_3/m$, while some variants belong to the space groups with lower symmetries, e.g. $P6_3$. There are different ways to represent apatite crystal structures, one of which is the polyhedral. In polyhedrals, the $A^{I}O_6$ metaprismatic polyhedra are face-connected to form columns along the c direction, which are linked to the BO_4 tetrahedra. The A^{II} atoms are located in channels surrounded by those columns. Studies indicate that the (0001) projected twist angle of oxygen triangles in the $A^{I}O_6$ polyhedron is a key parameter to probe the structural deviation, and its value can be obtained after the coordinates for each atom are determined from Rietveld refinement. The proposed model of the crystal structure will be explained in this presentation.

Biography

Associate Professor Dong Zhili received his B.Eng. and PhD degrees from Tsinghua University, China. His PhD thesis was completed at Tsinghua University and Osaka University under the Joint PhD Programme of the Ministry of Education of China. He was trained as a materials engineer and scientist during his undergraduate and postgraduate studies, and he subsequently developed his research in the areas of materials engineering, crystal structure/electronic structure – property relationships, and interface structure analysis at Tsinghua University, University of Barcelona, A*STAR and NTU. He has more than 30 years of experience in X-ray diffraction and transmission electron microscopy of materials.

His research interests include:

(a) Processing of metals and alloys
(b) Synthesis of geo-mimetic ceramic materials
(c) Functionalities and applications of geo-mimetic ceramic materials (including apatite-type, perovskite-type, spinel-type, wurtzite-type, anatase-type, olivine-type, and layered-type)
(d) Applications of polyoxometalates
(e) X-ray diffraction and transmission electron microscopy of metals and ceramics
(f) Coating and cross-sectional interface structure analysis by TEM/EELS
(g) Crystal structure/electronic structure – property relationships

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Hosted by: Professor Lee Pooi See

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