Friday 1st November 2019
9.05-9.55am
2150 Torgersen Hall

LAYERED ATOMIC ARRANGEMENTS IN COMPLEX CRYSTALLINE SOLIDS

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Abstract

In this presentation, I will introduce a novel atomic layer stacking model to describe the crystal structures of numerous complex materials. The layer stacking sequences involve pseudo close-packed layers, which I refer to as triangular atom nets or hexanets. The interesting features of the model involve atom patterns that are to be found within these hexanet layers. For instance, in fluorite-structured compounds, with an ideal, 2:1 ratio of O:M ions, the atomic patterns reside within the mixed cation layers. In oxygen deficient fluorites, there are holes (interstices) in some or all of the oxygen hexanets. If the cations in the cation hexanets or anion holes in the anion hexanets are randomly arranged, then the structure becomes indistinguishable from fluorite. In the case of anion holes, the holes are actually oxygen vacancies, incorporated in the lattice to charge compensate for aliovalent cations. To illustrate the layer stacking concept, I will consider a sequence of MxOy oxide compounds in which the metal cations progress in oxidation state from monovalent (M^{1+}) to octavalent (M^{8+}). I will use concepts relating to geometric subdivisions of a triangular atom net to describe the layered atom patterns in these compounds (concepts originally proposed by Shuichi Iida[§]). I will demonstrate that as a function of increasing oxidation state (from M^{1+} to M^{4+}), the layer stacking motifs used to generate each successive structure (specifically, motifs along a 3 symmetry axis, such as the kagome, woven basket pattern), progress through the following sequence: MOM, MO, mO, oMo, OMO (where M and O represent fully-dense triangular atom nets, while m and o represent partially-filled triangular atom nets). I will also show how the layered atom concepts apply to complex intermetallic phases. Specifically, I will discuss the aluminum-rich compound, $Al_{20}Mn_2Ce$.

[§] *S. Iida, "Layer Structures of Magnetic Oxides," J. Phys. Soc. Japan 12 (3) (1957) 222-233.*

Bio-sketch

Kurt Sickafus is Professor in the Department of Materials Science and Engineering (MSE) at The University of Tennessee (UT). Kurt served as the Head of the UT-MSE department from 2011 - 2015. Kurt graduated from Ohio Wesleyan University in 1978 and received his Ph.D. degree from Cornell University in 1985 (Materials Science & Engineering). Kurt also worked as a postdoctoral researcher in the Cavendish Laboratory, University of Cambridge (1985-1987) and as a staff member at I.B.M. (1987-88) and at Los Alamos National Laboratory (1989-2011). Kurt's primary expertise is in the area of radiation damage effects in ceramics, especially the radiation damage behavior of complex oxides. Kurt is a Fellow of both Los Alamos National Laboratory and the American Ceramic Society.