Foreword

Neutron and X-Ray Studies of Advanced Materials VII: Challenges of the Future World

The selection of the manuscripts in the special topic "Neutron and X-ray Studies of Advanced Materials VII: Challenges of the Future World" is based on the material presented during the TMS 2014 Annual Meeting February 16 to 20, 2014, at the San Diego Convention Center in San Diego, California.

The United Nations Education, Science and Culture Organization (UNESCO) declared 2014 the International Year of Crystallography to acknowledge the importance of the first theoretical predictions (M. Laue) and brilliant experimental verification of diffraction phenomena (W. Friedrich and P. Knipping) more than a century ago. During this century the diffraction theory and experimental techniques were immensely developed. Diffraction entered our everyday life including important medical, technological, industrial, and scientific applications. The significance of the diffraction techniques continued to increase in the past 100 years.

The aim of the symposium was to provide a forum for discussion of using state-of-the-art neutron and X-ray scattering techniques to probe advanced materials.

A tutorial on "Sources, Instrumentation And Scattering" was organized during the symposium by Rozaliya Barabash (USA), Klaus-Dieter Liss (Australia), Paolo Scardi and Luca Gelisio (Italy). This two-part tutorial presented a review on neutrons and X-rays, including sources, instrumentation, theories of scattering and diffraction, the concept of reciprocal space, Ewald construction, dynamic and kinematic theory, limit to small crystals, nanocrystals, lattice gradients. The state-of-the-art diffraction analysis of defects was introduced in the tutorial. The tutorial presented some fundamentals of line profile analysis, with basic facts on nanoparticles—their shapes and most typical properties—restricting the attention to the simplest case of metallic systems. How and why nanocrystals produce broad diffraction profiles, and a quick introduction to the Scherrer equation—where it comes from—was also covered. Details of how to build a credible model of a nanocrystal were considered, as well as the importance of using an atomistic point of view to assess, *e.g.*, by Molecular Dynamics simulations, some crystal properties. Examples and possibilities of the new software implementing the Direct Space approach were included in the tutorial. In addition, the differences between the two basic paradigms used to deal with nanocrystalline materials in powder diffraction—in Reciprocal Space (traditional approach) and in Direct Space (according to the Debye scattering equation)—were discussed.

The focused set of papers presented below offers a view of three different aspects of the diffraction and scattering techniques in different laboratories in the world.

The first paper by Poulsen *et al*. from the Technical University of Denmark relates to further development of the X-ray optics. The paper provides a theoretical description of focusing and imaging of synchrotron X-rays by ray transfer matrix analysis. The authors suggest approximate analytical expressions to calculate compound refractive indices of biconcave parabolic lenses. The suggested methodology allows for fast estimation of compound refractive lense characteristics and provides a way for the appropriate design of the advanced optics at synchrotron radiation sources.

The second manuscript, by Okuda *et al*. from Kyoto University of Japan provides an example of the small- and wide-angle scattering techniques. They study diffuse scattering from long-period stacking ordered phases (LPSOs) of $Mg_{97}Y_2Zn_1$ alloy. The authors show that in as-cast polycrystalline state the main LPSO structure is described as 18R. During annealing the 14H structure is growing at the expense of 18R. The authors observe that the in-plane peak position increases with annealing time for isothermal annealing, and at higher temperatures during *in situ* annealing. They interpret it as a peak-overlapping related to different sites. The authors demonstrate that temperature instability during *in situ* annealing agrees within experimental resolution for in-plane ordering in 18R and 14H structures.

The third manuscript by Scardi and Gelisio from the University of Trento (Italy) relates to a new methodology of the powder diffraction study of nanocrystals. Molecular Dynamics simulations of five different FCC clusters of nanomaterials were generated. The authors interpret static and dynamic effects and discuss them using two approaches of diffraction representation: (*) in Reciprocal Space, and (**) in Direct Space. The authors consider the influence of shape on static and dynamic diffraction regularities. The elements chosen by the authors depend on a wide range of parameters such as material stiffness and elastic anisotropy. Therefore, this presents a challenge for the interpretation methodology.

RB is supported by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U.S. Department of Energy.

Guest Editors:
R.I. Barabash, Research Scientist
Materials Science & Technology Division,
Oak Ridge National Laboratory, Oak Ridge, TN 37831-6118
e-mail: barabashr@ornl.gov

G. Kostorz, Professor
Department of Physics, ETH Zurich, 8093, Zurich, Switzerland

B. Fultz, Professor
Materials Science and Applied Physics,
California Institute of Technology, Pasadena, CA 91125

P.K. Liaw, Professor
Materials Science & Engineering,
The University of Tennessee, Knoxville, TN 37996-2200