Neutron PDF study of catalysts and battery materials: current status and future opportunities

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Pair distribution function (PDF) analysis has emerged as a powerful tool to study the complex structure of functioning disordered crystalline materials and nanomaterials. The real-space-based PDF analysis utilizes both Bragg scattering and diffuse scattering information, and thus is very sensitive to short-range ordering (SRO) in disordered crystalline materials or intermediate-range/surface structure in nanoscale materials. Particularly, the application of neutron PDF method to investigate catalysts and battery materials have attracted broad interests in recent years. There are several advantages in using neutron diffraction to study these materials: neutron scattering is very sensitive to light elements (Li, C, N and O), which are key ingredients of Li/Na-ion battery materials and varies catalysts. It is also capable of distinguishing adjacent 3d transition metal cations, which are broadly used in battery cathode or low-cost heterogeneous catalysts. The nuclear scattering lengths do not decrease with momentum transfer (Q), making it more accurate in determining the atomic environments of light elements. Moreover, it is highly penetrating and non-destructive, making it an ideal tool to probe structure changes in large devices like Li/Na-ion batteries or gas flowing cell without disturbing the electrochemical/catalytic reactions. Despite these great advantages, neutron PDF characterization of charged and discharged electrode materials or reacted catalysts, has remained somewhat limited. This is in large part due to the difficulty in optimizing the ex-situ sample preparation (for neutron scattering experiments) and the complex sample environment required for in situ neutron diffraction/PDF studies. In this talk, I will discuss the recent progress on the development of in situ/ex situ neutron diffraction/PDF capabilities at NOMAD. Two examples will be presented: one on the in situ neutron total scattering investigation of the structural origin of thermal runaway of high energy density battery cathode materials; the other on quantitative structure study of nano-catalysts using neutron PDF. Perspective on future opportunities will also be discussed.