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3D Atom Dynamics in Pt-NiO Nanocrystals

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The Pt has been used as an efficient catalyst in photocatalysis process for water splitting and oxygen reduction reaction (ORR) during fuel cells operation. However, it is being proposed to substitute platinum as a catalyst since it is expensive and inhomogeneously distributed in the world. A good alternative to replace pure Pt nanoparticles is Ni@Pt core-shell nanoparticles to enhance the kinetics. Control on the chemical composition of the core has led to production of NiO nanoparticles. Nevertheless their physical properties and catalytic behavior are not yet completely understood. Additionally their atomic distribution is only assumed due to the lack of information from localized characterization techniques such as transmission electron microscopy (TEM). Here, we present an analytical approach to extract the spatiotemporal dynamics of Pt-NiO encoded into TEM exit wave functions in order to account for electron beam-induced alterations [1].

Three-dimensional (3D) atom structure in nano-scale objects can be revealed from exit wave function [2, 3]. The three time snapshots of phase image of a Pt-NiO nanoparticle are shown in Fig. 1. The corresponding exit wave functions are reconstructed from focal image series acquired by bright-field transmission electron microscopy (TEM) operated at low electron dose-rates (56, 92 and 185 $e^{-}Å^{-2}s^{-1}$), respectively, to induce only weak object excitations and facilitate object relaxations between successively delivered electrons. It is interesting to see that there are two types of valleys, namely, type A and type B. The type A valley marked as green crosses shows larger/ darker contrast and type B marked as red crosses shows smaller/ lighter contrast. This contrast difference mainly arises from presence of one Pt atom in the type A valley which is displaced due to magnetic spin interaction. It worth noting that these two types of valley forms super-ordering in Fig. 1(a) while the ordering degrades in Fig. 1(b) and (c) as a result of more electron dose. The 3D tomograms (Fig. 2) associated with these three exit wave were reconstructed with the methods published in [1, 3]. This method involves determination of the z-height of the surface atoms via maximum propagation intensity and the number of atoms in columns via Argand plot analysis. The Fig. 2 shows that the Pt-NiO nanoparticle is a truncated cube, and some of the edge columns is completely removed in different time snapshot due to accumulation of the electron dose. Thus, as a perspective, our approach uncovers a correlation between electron dose and chemical evolution of the nanocrystal edges and the degradation of internal super-structure.

The detail structural dynamics will be discussed in detail in the presentation.

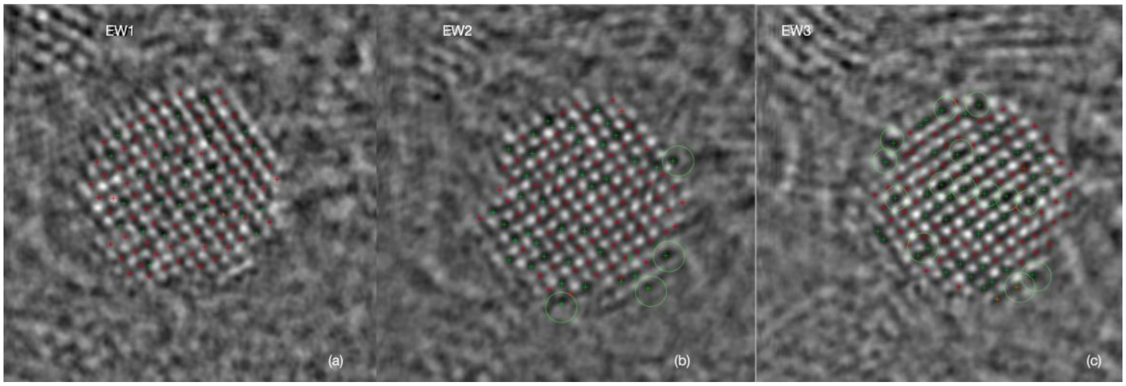

Figure 1. Three phase images of reconstructed exit wave function of a Pt-NiO nanoparticle. The green and red crosses show two different types of channels (valleys). The type A valley marked as green crosses shows larger/ darker contrast and type B marked as red crosses shows smaller/ lighter contrast.

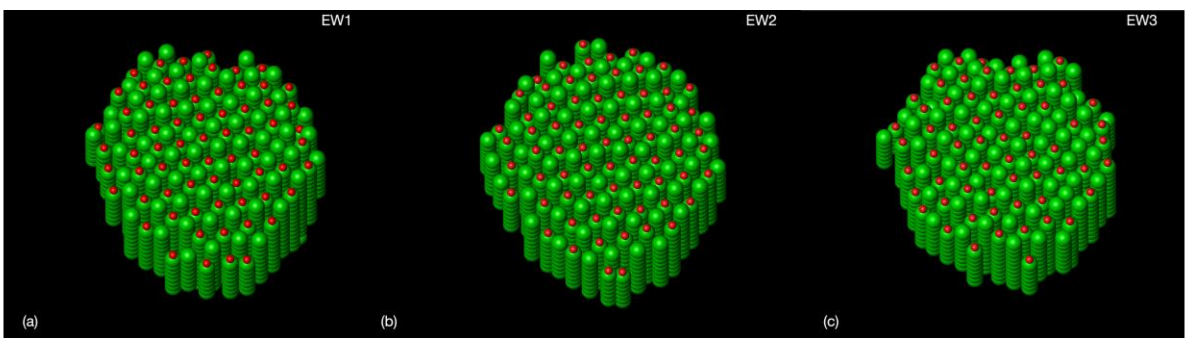

Figure 2. 3D atom dynamics of reconstructed NiO nanocrystal. As we can see that some of the edge columns completely removed due to accumulation of electron dose. The red dot represents surface oxygen and the green dot presents the Ni atom. The oxygen in side the NiO nanoparticle is not shown here.

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