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Atomistic structures and transport phenomena at interfaces in lithium battery materials

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ATOMISTIC STRUCTURES AND TRANSPORT PHENOMENA AT INTERFACES IN LITHIUM BATTERY MATERIALS

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Lithium-ion batteries (LIBs) are widely used in mobile devices. Increasingly they are also being scaled up for use as energy-storage devices in hybrid vehicles and fully electric ones. All-solid-state LIBs are expected to be one of the candidates as next generation LIBs because the LIBs can realize higher energy density and safety without liquid electrolytes. In these devices, the solid-solid interfaces, specifically those between electrodes and an electrolyte and grain boundaries within each component, are thought to strongly affect the battery performance. Despite their clear scientific and technical importance, however, so far, few studies have focused on the internal interfaces in battery materials.
In this report, we present investigation combining scanning transmission electron microscope (STEM) observations with atomic resolution and theoretical calculations based on density functional theory (DFT) regarding interfaces in materials of LIBs.
Figure 1 shows a HAADF-STEM image of a twin boundary in $LiCoO_2$, a typical cathode of LIBs[1]. Bright spots correspond to columns of Co atoms. Figure 2 is a HAADF-STEM image of the edge-on atomic structures of a 90° domain boundary along the $[100]_p$ direction in $La_{0.62}Li_{0.16}TiO_3$ samples which is a solid electrolyte of LIBs[2]. Bright spots correspond to columns of La atoms. Both interfaces seem to have smooth contact. However, our DFT calculations reveal that Li ion migration are strongly affected even by these coherent interfaces.

[1] H. Moriwake et al, Adv. Mater, 25 (2012) 618-622
[2] X. Gao et al, *J. Mater. Chem. A*, **2** (2014) 843-852

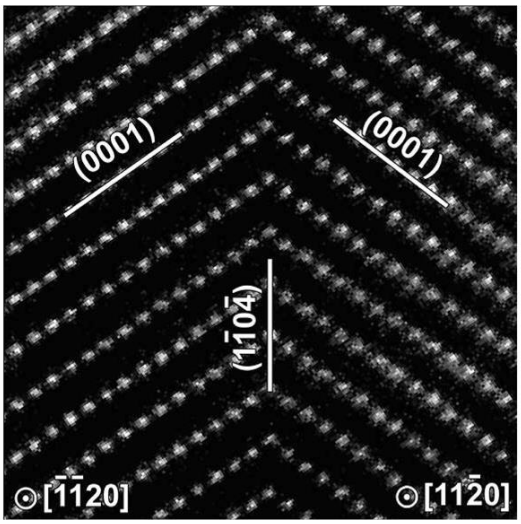

Figure 1 HAADF-STEM image of a twin boundary in $LiCoO_2$ with bright spots corresponding to columns of Co atoms.

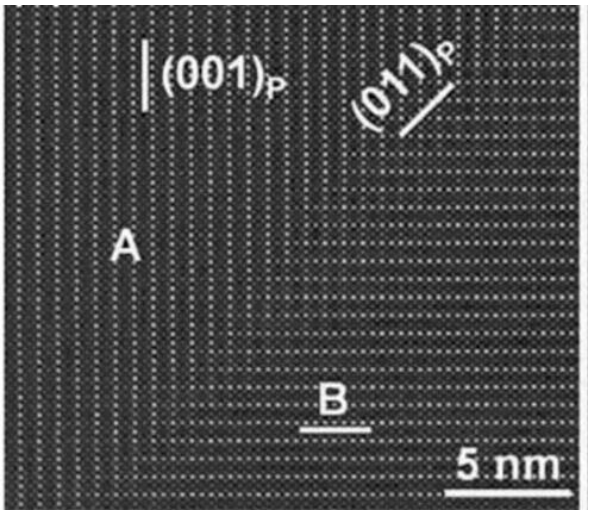

Figure 2 HAADF imagesa of the edge-on atomic structures of 90° DBs along the [100]p direction in $La_{0.62}Li_{0.16}TiO_3$ samples.