STEM-EDS investigation of grain boundary segregation in oxide materials

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Grain boundary (GB) segregation, a phenomenon that solutes or impurities are enriched at the GB, is one of the perennial topics in materials science, which has been widely studied so far. Thanks to the aberration-corrected scanning transmission electron microscopy (STEM) and energy-dispersive X-ray spectroscopy (EDS), a direct observion of GB segregation phenomenon is possible at atomic resolution, which greatly improved our fundamental understanding towards GB segregation. In this presentation, we will discuss GB segregation in Al_2O_3 and ZrO_2, which represent the cases of impurity and solute GB segregations, respectively.

Al_2O_3 and ZrO_2 model GBs were fabricated by bicrystal methods, of which the GB characters can be well controlled. These GBs were systematically studied using atomic-resolution STEM-EDS. In the case of impurity segregated Al_2O_3 GBs, the dopants only segregated at specific atomic sites, which is highly dependent on the size mismatch between dopants and Al^{3+}. On the other hand, Y^{3+} segregates at ZrO_2 GB with a width of several nanometers, accompanied with the co-segregation of O^{2-} in the case of Y_2O_3 doped ZrO_2. These results suggest that in the case of solute segregation, the GB segregation behavior is dominated by the long-range electric interactions between charged GB core and charged point defects.