MS20-P01 | DISCOVERY OF COMPLEX METAL OXIDE MATERIALS BY RAPID PHASE IDENTIFICATION AND STRUCTURE DETERMINATION

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The discovery of new inorganic functional materials is of fundamental importance in synthetic and materials science. In the past, the discovering new materials relied on a slow and serendipitous trial-and-error process, especially in the well-studied oxide systems. Here, we presented a strategy to shorten the period of discovery of new complex metal oxide materials by rapid phase identification and structure determination with 3D electron diffraction (ED) techniques, which do not require pure samples or single crystal growth. With such strategy, three new complex metal oxide materials ($BiTi_{0.855}Fe_{1.145}O_{4.93}$, $BiTi_4FeO_{11}$ and $BiTi_2FeO_7$) were discovered in the simple ternary Bi_2O_3-Fe_2O_3-TiO_2 system. To our best knowledge, it is the first time to discover three new complex metal oxide materials with new structure types in a single study of ternary metal oxide system. The structures of new materials were refined by combining powder X-ray diffraction (PXRD) with powder neutron diffraction (PND). The most striking feature in this system is that $BiTi_{0.855}Fe_{1.145}O_{4.93}$ presents edge-shared five-coordinated iron/titanium polyhedra. In addition, another new phase $BiTi_4GaO_{11}$, which is isostructural with $BiTi_4FeO_{11}$, can be obtained when replacing Fe in $BiTi_4FeO_{11}$ with Ga. This method for developing new materials is available to all fields in chemistry and material chemistry where the limiting factors are impurity, submicrometer-sized crystals, etc.