Complex structure and composition metal-oxides

through solution processing

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**Abstract.** Solution based processing routes have gained much interest for the preparation of complex nano-structured materials. Benefits are found in the simple processing routes to complex composition and structure materials, allowing for large-scale, low cost technological exploitation. The molecular approach of solution processing provides unique possibilities to create atom-scale tailored materials even in large scale from metal-organic molecular building blocks, which can be crystallised for purification.

 However, although the solution chemical routes have seen a rapid development during the recent decades proving to achieve unique materials of various shapes and complexities there is still need for further development, in particular regarding reproducibility and crystal quality. Here, the complex often multi-step processes, including kinetically controlled reaction chains makes it hard to gain a fundamental understanding allowing for highly controlled processing of high quality, complex composition metal-oxides, not the least when considering the important doped oxide semi-conductors.

 This talk gives a short, general description of solution based processing using hetero-metallic alkoxide precursors and inorganic salts complexed with organic groups, and the thermal processing taking the precursor molecules into the ceramic target materials. Advantages and challenges with the two precursor systems are discussed.

 Examples of processes yielding complex, nano-structured functional metal-oxides as nano-particle, nano-phase sponges and thin- and ultra-thin films are given. A particular focus is put on the relationship between the choice of precursor and processing parameters, and the final metal-oxide microstructure, atomic structure and properties. This includes the dopant atom oxidation-state, coordination and distribution, which strongly determines the optical and magnetic properties of a given doped oxide. These are important structural details often missing also for other chemical and physical materials preparation techniques which leads to slow progress in important fields such as fossil-free energy conversion, e.g. solar fuel catalysis and magnetic oxide semi-conductors. Metal-oxide systems discussed include Co- Al- and Ln-doped ZnO, CoFe2O4 (CFO) – (Sr,La)MnO3 (LSMO) multilayer films.

…..The phase-development taking place upon heating of gels, powders or liquid precursor concentrates to yield the target oxides were studied in detail with a wide range of analytical techniques including: TG-DSC, XRD, XPS, IR-spectroscopy, EXAFS, SEM-EDS, and S/HRTEM-ED/EDS/HAADF/EELS and ePDF. In some cases, DFT calculations were employed to derive plausible complex dopant structures supported by the above experimental techniques.

 The examples are chosen to give a general discussion about how the choice of precursors and processing parameters can be used to obtain high quality complex oxides of various micro-structures, as well as target materials with potential for use in sensors, catalysis, solar-cells and fuel generation, photo-active self-cleaning surfaces, optically active materials, and electro- and magnetic thin films.