Subarea POB3.6: Modeling and investigation of physicochemical properties of materials

Title of the presentation: Investigation of morphology, thermal and electron properties of oxide thin films

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Abstract:

The zinc oxide is typically n-type semiconductor with a direct band gap of 3.3 eV at 300 K, that emits light in the near-UV region [1]. ZnO found numerous applications in electronics and optoelectronics as transparent conductive contacts in solar cells, polycrystalline channels in film transistors [2-4]. While doped with Aluminium ZnO is promising material for thermoelectric applications. The thermal conductivity of thin ZnO films is typically two orders of magnitude lower than for bulk crystal and depends on structure and deposition method.

In this work the morphology, thermal and electron properties of oxide thin films were investigated. The ZnO layers were deposited at two substrate temperatures by the Atomic Layer Deposition (ALD) method. Several prominent correlations for the thermal properties as measured by high-resolution Scanning Thermal Microscopy at room temperature were observed. A lower thermal conductivity was revealed in samples grown at 100 °C and these variations were interpreted in terms of changing populations of native donors, affecting the free carrier concentration and, as such, the thermal conductivity. For layers grown at 200 °C a significant change in morphology and the corresponding increase in the thermal conductivity, specifically from 0.28 $Wm^{-1}K^{-1}$ to 2.81 $Wm^{-1}K^{-1}$ was observed. In order to investigate the chemical structure of ZnO layers the X-ray photoemission spectroscopy investigations were conducted. T1 and T2 sets of samples comprise interesting variations in oxygen and zinc sub-lattices for the same sample thicknesses of identical matrixes. Analysis of correlations between morphology with thermal and electron properties allowed to perform a systematic analysis of heat transfer mechanism in polycrystalline thin films based on the phonon transport model, explaining the thermal conductivity in terms of the bulk thermal contributions within the grains and additional thermal resistance introduced by the grain boundaries.

Ref:

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