

**Doktorantūras skola**  
**„Funkcionāli materiāli un nanotehnoloģijas”**

**Studiju kurss fizikas maģistrantiem**  
**„Aktuālas materiālu un cietvielu fizikas problēmas”**

**LU Cietvielu fizikas institūta Zinātniskais seminārs**

**Trešdien, 7.decembrī**  
**plkst. 12.30, Ķengaraga ielā 8, konferenču zālē**

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„Initial oxidation of zirconium: oxide – film growth kinetics and mechanisms”

Up to date, the growth kinetics, the microstructural evolution, as well as transport properties of oxide layers grown on metals by thermal oxidation have been investigated mainly at elevated oxidation temperatures (say, at  $T > 500$  K). Contrarily, our knowledge on the low-temperature (of, say, below 500 K) oxidation process is far from complete and still suffers from the lack of reliable quantitative experimental data. The present study addresses the growth kinetics, chemical constitution and microstructural evolution of thin (thickness  $< 10$  nm) zirconium-oxide films, as grown by the dry, thermal oxidation of Zr(0001) and Zr(10 $\bar{1}$ 0) surfaces at low oxidation temperatures ( $T = 300$ -450 K) and at the oxygen partial pressure of  $p_{O_2} = 1 \times 10^{-4}$  Pa.

By monitoring the growth kinetics of thin oxide films on Zr surfaces using real-time in-situ spectroscopic ellipsometry, it was found that the less-densely packed Zr(10 $\bar{1}$ 0) surface oxidizes more readily than the densely packed Zr(0001) surface. The analyses the valence band spectra and local chemical states of Zr and O in thin oxide films (as resolved by XPS) revealed that the oxide films grown at  $T \leq 400$  K are predominantly amorphous, whereas at  $T > 400$  K a tetragonal ZrO<sub>2</sub>-like phase gradually forms. The microstructural development of thin oxide layers was investigated by *in-vacuo* STM. Furthermore, two-stage oxidation experiments using <sup>16</sup>O and <sup>18</sup>O isotopes were performed to reveal the governing atomic transport mechanisms in thin oxide films grown during the initial stages of dry thermal oxidation of pure Zr. To this end, the bare Zr surfaces were oxidized first in <sup>16</sup>O<sub>2</sub>(g) and subsequently in <sup>18</sup>O<sub>2</sub>(g). The <sup>18</sup>O-tracer depth distributions in the oxide films were recorded by ToF-SIMS. It was concluded that the early stage of the oxidation process is governed by oxygen transport to the metal/oxide interface through the lattice and along the grain boundaries of the nano-sized oxide grains, whereas upon continuing oxidation only oxygen lattice transport controls the oxidation process. An oxide-film growth mechanism is proposed.