TECHNISCHE UNIVERSITÄT CHEMNITZ

PHYSIKALISCHES KOLLOQUIUM

Mittwoch, den 18.05.2011, um **17:15 Uhr**

Ort: Reichenhainer Str. 90; Neues Hörsaalgebäude, Raum: 2/N013

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Materials Chemistry
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Growth of Oxide Thin Films: Atomic Playground

Molecular dynamics (MD) has been beneficial for unraveling physics of ion-surface processes on the atomic level in many systems. Here, the growth of RuO_2 and Al_2O_3 thin films is studied.

It is our ambition to identify suitable alloying elements for RuO_2 ($P4_2/mnm$), based on quantum mechanically guided design, which improve the transport properties and phase stability. Using *ab initio* calculations, we probe all 4*d* transition metals and identify Nb to be the best choice. Based on this design proposal, Nb alloyed RuO_2 thin films are grown by combinatorial reactive sputtering. Nb is incorporated in the rutile structure. Nanorods are formed and Nb_2O_5 coordination appears at Nb contents ≥ 2.9 at.%. This may be understood based on our *ab initio* MD data. Surface coarsening on the atomic scale occurs due to O crosslinking of two neighboring NbO_6 octahedra. Hence, it is reasonable to assume that NbO_6 octahedra contribute towards the experimentally observed formation of nanorods.

A monoenergetic Al^+ beam generated by a filtered cathodic arc is employed for the deposition of Al_2O_3 films at well defined ion energies. Structural analysis shows that Al^+ energies of 40 eV or larger favor the formation of the thermodynamically stable α-Al_2O_3 phase ($R\bar{3}c$) at the expense of metastable Al_2O_3 ($Fd\bar{3}m$). These Al bombardment induced structural changes in α-Al_2O_3 and γ-Al_2O_3 were studied using *ab initio* MD. Diffusion and irradiation damage occur for both polymorphs in the kinetic energy range from 3.5 to 40 eV. However, for γ-Al_2O_3(001) subplantation of impinging Al causes significantly larger irradiation damage and hence larger mobility as compared to α-Al_2O_3. Consequently, fast diffusion along γ-Al_2O_3(001) gives rise to preferential α-Al_2O_3(0001) growth, which is consistent with our structure evolution experiments.

Alle Zuhörer sind ab 17:00 Uhr zum Kaffee vor dem Hörsaal eingeladen.

Informationen zum Vortrag erteilt Prof. Dr. Frank Richter, Tel. 0371/531-38046