

## DS 4: Thin Film Properties I

Time: Monday 15:30–17:00

Location: SCH A 316

DS 4.1 Mon 15:30 SCH A 316

**Ultrafast laser induced structural motion in crystalline and amorphous gold** — ●OTHMANE BENHAYOUN<sup>1</sup>, EMILIANO PRINCIPPI<sup>3</sup>, BERND BAUERHENNE<sup>1</sup>, DMITRY S. IVANOV<sup>2</sup>, and MARTIN E. GARCIA<sup>1</sup> — <sup>1</sup>University of Kassel, Theoretical physics II, Kassel, Germany — <sup>2</sup>Moscow, Russia — <sup>3</sup>Elettra-Sincrotrone Trieste S.C.p.A., Trieste, Italy

A recent Ultrafast Electron Diffraction (UED) experiment showed a time-dependent nonuniform compression and expansion of a monocrystalline gold foil. This led to the time modulation of the Au Bragg peaks in both height and width. The same effect is however not observed in polycrystalline gold. We thus perform Molecular Dynamics - Two Temperature Model (MD-TTM) simulations aiming to understand the results of the experiment. In our simulations, we obtain similar peak oscillations and determine the major mechanisms that lead to such lattice dynamics.

DS 4.2 Mon 15:45 SCH A 316

**Co-electrodeposition of compositionally complex Co-Cr-Fe-Mo-Ni alloy thin films** — ●HONGSHUAI LI, MARTIN PETERLECHNER, and GERHARD WILDE — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

A compositionally complex Co-Cr-Fe-Mo-Ni alloy with a face-centered cubic structure was successfully obtained by electrochemical deposition using a constant current density. An aqueous electrolyte with several additives was developed to accomplish the electrodeposition of films onto Cu substrates. The characterization reveals that the deposited films are metallic with a face-centered cubic structure, including impurities incorporated during deposition. In addition, mechanical tests were performed to study adhesion and hardness by nano-scratch tests and nanoindentation. Mechanical tests show a high hardness and nonetheless microscopically ductile behavior. The electrolytes developed in this study may be a promising approach for the electrodeposition of Co-Cr-Fe-Mo-Ni compositionally complex alloy coatings.

DS 4.3 Mon 16:00 SCH A 316

**Thermally controlling the length of transition and alkali metal squarate wires** — ●EGZONA ISUFI NEZIRI<sup>1,2</sup>, KARL-HEINZ ERNST<sup>1,2</sup>, and CHRISTIAN WÄCKERLIN<sup>3,4</sup> — <sup>1</sup>Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland — <sup>2</sup>University of Zürich, 8006 Zürich, Switzerland — <sup>3</sup>Paul Scherrer Institute, 5232 Villigen, Switzerland — <sup>4</sup>EPFL, Swiss Federal Institute of Technology Lausanne, 1015 Lausanne, Switzerland

Low-dimensional metal-organic nanomaterials on surfaces can be engineered to yield promising, novel and highly customizable chemical/physical properties such as magnetism, electronic structure and catalytic properties. A variety of metal elements, including alkali, transition and even lanthanide metals have been used to direct the metal-organic assembly.

Here metal-organic structures obtained from squaric acid (H<sub>2</sub>C<sub>4</sub>O<sub>4</sub>) molecules, co-deposited with K and Ni atoms on a hot Au(111) surface, are studied by XPS and STM. We find that both K and Ni lead to the formation of condensed arrays of wires, composed of M-squarate (C<sub>4</sub>O<sub>4</sub>(2-)). Controlling the length of these wires is possible by a thermally activated process: Ni-squarate wires tend to get longer at higher temperatures while K-squarate wires get shorter.

DS 4.4 Mon 16:15 SCH A 316

**Deep learning-supported in-situ HRTEM experiments on single-layer carbon** — ●CHRISTOPHER LEIST<sup>1</sup>, HAUYUAN QI<sup>1,2</sup>, and UTE KAISER<sup>1</sup> — <sup>1</sup>Central Facility Materials Science Electron Microscopy, Ulm University, 89081 Ulm, Germany — <sup>2</sup>Faculty of Chemistry and Food Chemistry Dresden, Technische Universität Dresden, 01062 Dresden, Germany.

We perform in-situ experiments on single-layer carbon using the Cc/Cs-corrected low-voltage transmission electron microscope SALVE, resolving structure and dynamics down to the level of the single atom. These types of experiments create large amounts of data both in terms of numbers of individual images acquired and the amount of information per image. Conventional image analysis methods, e.g., hand-crafted filter kernels, often require heavy user supervision and tremendous time cost, posing strong limitations on the data volume making them inconvenient for use in these experiments. Deep learning in the form of convolutional neural networks offers a reliable and effective way to handle large amounts of complex image data. Using simulated data we train a modified U-Net like neural network to identify atom positions and their structure i.e. polygons while at the same time removing contaminated areas from the evaluation in real micrographs. Thus, gaining the ability for both largescale statistical evaluation and mapping atomically-resolved the material's transformation.

DS 4.5 Mon 16:30 SCH A 316

**Microstructure and mechanical properties of Ta-Al-B coatings** — ●CHUN HU<sup>1</sup>, SHUYAO LIN<sup>1</sup>, MAXIMILIAN PODSEDNIK<sup>2</sup>, ANDREAS LIMBECK<sup>2</sup>, NIKOLA KOUTNÁ<sup>1</sup>, and PAUL H. MAYRHOFER<sup>1</sup> — <sup>1</sup>Institute of Materials Science and Technology, TU Wien, Getreidemarkt 9, Vienna, A-1060, Austria — <sup>2</sup>Institute of Chemical Technologies and Analytics, TU Wien, A-1060 Wien, Austria

Alloying is a simple yet powerful tool to tune properties of hard coatings. Here we report stoichiometry, microstructure and hardness evolution of Al-alloyed TaB<sub>2</sub>-z coatings. Sputtering a stoichiometric TaB<sub>2</sub> target results in sub-stoichiometric TaB<sub>1.23</sub> with a mixed hexagonal-TaB<sub>2</sub> (α-AlB<sub>2</sub>-type) and orthorhombic TaB structure. Co-sputtering an AlB<sub>2</sub> target\* with half the sputtering power density\* increases the B content and strongly promotes the α-phase, while only little Al is incorporated (Ta<sub>0.997</sub>Al<sub>0.003</sub>B<sub>1.64</sub>). The coating shows a small grain size and the overall highest hardness. Further increasing the AlB<sub>2</sub>/TaB<sub>2</sub> sputter ratio allows for B/Metal ratios of 1.97 and 2.29 with Al metal-fractions up to 48 at%. These coatings are single-α-phased with a smooth surface but gradually decreased hardness due to the increased AlB<sub>2</sub>-fraction. The structural evolutions are underpinned by ab initio calculations.

DS 4.6 Mon 16:45 SCH A 316

**X-ray characterization of an above-RT bi-stable sublimable molecular spin-crossover Fe(II)-complex** — ●YAHYA SHUBBAK<sup>1</sup>, MIGUEL GAVARA EDO<sup>2</sup>, ARNO EHRESMANN<sup>1</sup>, and EUGENIO CORONADO MIRALES<sup>2</sup> — <sup>1</sup>Institute of Physics & Center for Interdisciplinary Nanostructure Science and Technology (CINSA<sup>T</sup>), University of Kassel, D-34132 Kassel — <sup>2</sup>Institute of Molecular Science (ICMol), University of València, S-46980 Paterna

Spin crossover (SCO) molecules are a promising type of material that can undergo reversible switching between low-spin (LS)- and high-spin (HS)-states upon external stimuli (heat, light, pressure, etc.) [1], making them useful for information technology, data storage, and optoelectronics [2]. However, most SCO molecules need to be cooled significantly for this transition to be observable. We have investigated the hitherto unknown electronic structure of the complex molecule bis[hydrotris(1,2,4-triazol-1-yl)borate]iron(II) ([Fe(HB(tz)<sub>3</sub>)<sub>2</sub>]) [3] capable of above-RT transition by XPS and XAS measurements, since the distinct electronic structure in both spin-states unmistakably prove the transition between them. [1]P. Gütllich and H. A. Goodwin. Spin Crossover in Transition Metal Compounds I. Springer Berlin Heidelberg, May 2004. 356 pp. [2]E. P. Geest et al., Contactless Spin Switch Sensing by Chemo-Electric Gating of graphene. In: *Advanced Materials* (2020), p. 1903575. [3]S. Rat et al., Solvatomorphism and structural-spin crossover property relationship in bis[hydrotris(1,2,4-triazol-1-yl)borate]iron(ii). In: *CrystEngComm* 19.24 (2017).