PL0002

Pathways for the preparation of functional coatings by simulations at various scales

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The presentation will cover different ways how to support the experimental research in the field of functional coatings by computer simulations. Various levels of theory (ranging from solid-state physics through atomic-scale ab-initio simulations to atomic-scale simulations based on empirical interaction potentials) and various simulation algorithms (ranging from static calculations of properties through searching for a local energy minimum to reproducing the time evolution of growing films) will be considered. The first part [1,2] will deal with a design of multilayered VO_2-based thermochromic coatings. Luminous transmittance and modulation of solar transmittance will be optimized in parallel, instead of a tradeoff between them. The results will be compared with our experiments. The second part [3,4] will deal with the identification of maximum achievable stable N content, [N], in amorphous Si-C-N networks, assuming that it is limited by the formation, presence and loss of N_2 molecules. For example, the difficulties with the preparation of C_3N_4 will be explained by a maximum [N] in CN_x of 42%. Again, the results will be compared with the experiment. The third part [5,6] will deal with reproducing the atom-by-atom growth of crystalline ZrO_2 in a wide range of conditions. Effects of energy distribution function (no only average energy delivered into the films), mass of arriving particles (momentum delivered into the films) and growth temperature will be explained. Extension of the simulation algorithm from films to nanoparticles (from flat to spherical substrates) will be mentioned as well.

[1] J. Houska et al., Sol. Energy Mater. Sol. Cells 191, 365-371 (2019)]
[2] D. Kolenaty, J. Vlcek et al., Sci. Rep. 10, 11107 (2020)]
[3] J. Houska, Acta Mater. 174, 189-194 (2019)]
[4] J. Houska, ACS Appl. Mater. Inter, in print (2020)]
[5] J. Houska, Comp. Mater. Sci. 111, 209 (2016)]
[6] J. Houska, Surf. Coat Technol. 304, 23 (2016)]

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