Designing and guiding the synthesis of C-based tunable nanostructured thin and ultrathin films

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Abstract

By developing the Density Functional Theory (DFT)-based Synthetic Growth Concept (SGC) [1]understood as structural evolution by sequential steps where each one is defined by the previous relaxed state, Fig. 1, we are able address structural evolution and growth of inherently nanostructured tunable thin films for advanced surface engineering.

In addition, the SGC is the theoretical tool behind designing new low-dimensional and graphene-like thin films, by assessing their functionalization (e.g., fluorination and hydrogenation of 2D graphene-like structures [2]) and structural assembly, precursor control and self-organization [3].

Perceiving the Fullerene-like (FL) thin solid films as an entirely new class of C-based thin films, we have employed SGC to understand and control the structural properties and bonding organization of Fullerene-like Carbon Nitride (FL-CNx). FL-CNx is now industrially applied under the trade name of "rubber diamond" exhibiting outstanding hardness and resilience.

By employing SGC, we predicted FL Phospho-carbide (FL-CPx) and successfully guided its deposition by magnetron sputtering. FL-CPx samples characterization by variety of techniques confirmed the SGC predictions for remarkable mechanical properties of FL-CPx (hardness, elasticity, etc.) [4].

The purpose of this presentation is to emphasize, within the context of SGC and its transferability, how modelling can guide the tuning and functionalization of nanostructured thin films. This will be exemplified by the two most recent members of the particular class of FL thin films, namely, the Sulpho Carbide (CSx) [5] and the Carbon Fluoride (CFx) [6].

While the CSx thin films, similarly to what already happened with FL-CNx can find applications as hard and resilient coatings, the very recently synthesized tunable CS_xF_y thin films are especially attractive as protective coatings with outstanding mechanical resilience and with tunable surface properties [7].

Image

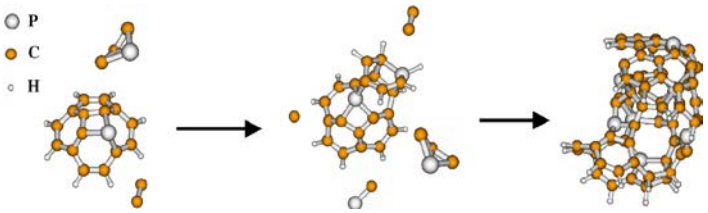


Figure: Synthetic growth with structure evolution by sequential addition of precursors to phospho-carbide (CP_x): from a tetragonal defect to an onion-like conformation.

Recent Publications

1. G. K. Gueorguiev et al, Chem. Phys. Lett. 410 (2005) 228;
2. Renato B. dos Santos et al, J. Phys. Chem. A 116 (2012) 9080;
3. C. Goyenola et. al., J. Phys. Chem. C 118 (2014) 6514;
4. G. K. Gueorguiev et al, Chem. Phys. Lett., 426 (2006) 374;
5. A. Furlan et al, phys. stat. sol. (RRL) 2 (2008) 191;
6. C. Goyenola et al, J. Phys. Chem. C 116 (2012) 21124 ;
7. Chung-Chuan Lai et al., J. Phys.: Condens. Matter 29 (2017) 195701 ;



Biography

Dr. Gueorgui Gueorguiev is currently a Senior University Lecturer at Linköping University, Sweden. He graduated as M. Sc. in Quantum Electronics and Laser Techniques from Faculty of Physics, University of Sofia, Bulgaria in 1993. He was a Fellow of the prestigious Portuguese Instituto Camões at Coimbra University in 1997/1998. In 1998/1999 he worked as a lecturer at University of Trás-os-Montes e Alto Douro, Portugal. In 2003, he completed his PhD degree at Coimbra University, Portugal with the exceptional mark "Cum Laude". In 2003-2005, he was PostDoc Fellow at Department of Physics, Chemistry and Biology, IFM, Linköping University, Sweden. He is currently project manager and research leader of several scientific projects with international participation. His research interests include carbon- and silicon-based nanostructured materials, group III-Nitrides, bismides, thin films, low-dimensional phases, cluster-assembled materials, design/synthesis guidance of nanostructured materials with pre-defined properties, as well as first-principles and effective methods in computational materials science.

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Notes/Comments: