561st ASRC Seminar

Date: 13:30 ～15:00, 25 July
Location: Meeting room 302, ASRC Building
Speaker: Dr. Pavel Sorokin
(Technological Institute for Superhard and Novel Carbon Materials)
Title: Beyond graphene
－Theoretical studies of new 2D inorganic materials－

The presented talk is devoted to the results of investigation of inorganic two-dimensional materials.

In the first part I will focused on the studies of fabrication of transition metal dichalcogenides (WS_2 and MoS_2). I will report the theoretical analysis of experimental data on unzipping multilayered WS_2 nanotubes by consequent intercalation of lithium atoms and 1-octanethiol molecules The extension of the tube was described in the framework of elastic shell theory with parameters evaluated from the ab initio calculations. Molecular dynamics simulation allowed to directly visualize the unzipping process of WS_2 nanotubes. Also I will discuss the process of cleavage of MoS_2 monolayers where direct TEM and theoretical simulations allow to understand what happens when monolayered 2D films are detached from the bulk surface. *In situ* observations combined with molecular dynamics simulations uncovered that the cleavage processes are reversible, which explained the high quality of the 2D materials by micromechanical cleavage. The perfect correspondence between experimental and theoretical data allowed to understand the mechanism of layer-by-layer cleavage process. It was found that, during the peeling, the MoS_2 atomic layers demonstrate strong layer-dependent mechanical behaviors and transitions of bending mechanisms from homogeneous curving to strain localization and finally to kinking were revealed

The second part is devoted to the theoretical prediction of the new class of 2D inorganic materials based on ionic compounds. Our results based on *ab initio* DFT calculations indicate a general graphitization tendency in ultrathin slabs of the ionic compound including rocksalt and cesium chloride-type structures. We focused on the evaluation of the stability and physical properties of nanometer thickness NaCl layered films and found that the rocksalt films with (111) surface become unstable with thickness below 1 nm and spontaneously split to graphitic like films for reducing the electrostatic energy penalty. The graphitic bulk counterpart is unstable and transforms to another hexagonal wurtzite NaCl phase which locates in the negative pressure region of phase diagram. The electronic band gap of the graphitic NaCl displays unusual nonmonotonic quantum confinement response.

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