Structural changes in two-dimensional materials under electron beam

H. Komsa[1] E. Sutter[2] Y. Huang[3] M. Ghorbani-Asl[4] V. Vierimaa[1] P. Sutter[2] A. V. Krasheninnikov[1,4]

[1]Department of Applied Physics, Aalto University
[2]Department of Mechanical and Materials Engineering, University of Nebraska-Lincoln
[3]Center for Functional Nanomaterials, Brookhaven National Laboratory
[4]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf

During electron microscope imaging, the beam of electrons with relativistic energies can not only cause unintentional damage, but also lead to possibly useful structural modifications that may further be controlled with nanoscale resolution.

In my talk, I will cover two examples of such modifications from our recent work. First, we have observed structural evolution of layered tin chalcogenides from SnS_2 to SnS, as well the corresponding selenides, upon sputtering of large number of chalcogen atoms [1]. First-principles calculations are used to propose how the transformation proceeds in the atomic level. A dependence of the layer orientation of the resulting SnS is rationalized by a transformation pathway in which vacancies group into ordered S-vacancy lines, which convert via a Sn_2S_3 intermediate to SnS. Absence of a stable Sn_2Se_3 intermediate precludes this pathway for the selenides, hence $SnSe_2$ always transforms into basal plane oriented SnSe.

Second, electron microscopy imaging of monolayer of black phosphorus has proven challenging due to the material's sensitivity to the impacts from the energetic electrons. To aid in understanding the response of this material to the beam and design imaging conditions, we performed computational study of initial damage processes and evaluated the relevant cross sections [2]. We also considered the stability of the sample edges, as well as the vacancy and adatom dynamics.

[1] E. Sutter, Y. Huang, H.-P. Komsa, M. Ghorbani-Asl, A. V. Krasheninnikov, P. Sutter, *Nano Lett.* **16**, 4410 (2016).
[2] V. Vierimaa, A. V. Krasheninnikov, H.-P. Komsa, *Nanoscale* **8**, 7949 (2016).