Metastable states of matter: a path towards new 2D and 1D materials

Igor ABRIKOSOV (Linköping University, Sweden)

Abstract

Materials are at the heart of modern scientific and technological development. To participate in and to contribute to the solution of existing and future global challenges, we must explore novel design concepts. In this respect, exploration of metastable states of matter greatly enhances opportunities to design new advanced materials. Combining theoretical simulations with experiment and broadly varying external parameters, pressure, temperature and composition allows one to discover phases which could not be synthesized otherwise. In this talk, we pay special attention to one of the major challenges of the high-pressure synthesis in terms of applications: the need to recover the synthesized materials at ambient conditions. We demonstrate feasibility of using high pressure in a search for materials with reduced dimensionality. Starting with 2D materials, we discuss a discovery of a new Dirac material, layered van der Waals bonded BeN_4 polymorph [1], followed by a realization of an ideal Cairo tessellation in NiN_2, which is a pentagonal 2D material [2].

Next, we turn out attention to 1D materials, which attract great attention since the pioneering works of Peierls. Still, the synthesis of truly monoatomic chains remains elusive. We have explored a novel path of experimental synthesis of monoatomic one-dimensional chains by their chemical stabilization in ionic compounds. We have demonstrated that in synthesized at high pressure sodium halides Na_4X_5 (X = I, Br, Cl) with *hP*18 Ga_4Ti_5-type structures, transfer of valence electrons from cations to anions has led to the formation of halogen chains connected with other atoms only by ionic interaction and having one-dimensional electronic structure. The Peierls physics in the systems is confirmed by theoretical calculations, newly synthesized incommensurately modulated *i-hP*18-Na_4X_5 (X = I, Br, Cl) compounds, as well as by the discovered *hP*36 phases of Na_4Cl_5 and Na_4Br_5 [3].

[1] M. Bykov, T. Fedotenko, S. Chariton, D. Laniel, K. Glazyrin, M. Hanfland, J. S. Smith, V. B. Prakapenka, M. F. Mahmood, A. F. Goncharov, A. V. Ponomareva, F. Tasnádi, A. I. Abrikosov, T. Bin Masood, I. Hotz, A. N. Rudenko, M. I. Katsnelson, N. Dubrovinskaia, L. Dubrovinsky, I. A. Abrikosov*,* Phys. Rev. Lett. **126**, 175501 (2021).

[2] M. Bykov, E. Bykova, A. V. Ponomareva, F. Tasnádi, S. Chariton, V. B. Prakapenka, K. Glazyrin, J. S. Smith, M. F. Mahmood, I. A. Abrikosov, and A. F. Goncharov*,* ACS Nano **15**, 13539 (2021).

[3] Y. Yin, N. Jena, F. Knoop, G. Garbarino, F. Tasnádi, F. Trybel, S. I. Simak, M. I. Katsnelson, A. Aslandukova, A. Aslandukov, X. Li, A. Antunes, F. Iasmin Akbar, K. Glazyrin, H. Fang, J. A. D. Ball, N. Dubrovinskaia, L. Dubrovinsky, I. A. Abrikosov *et al.,* arXiv:2512.08349.