Reg. No: 2016/23/B/ST5/02728; Principal Investigator: dr hab. Izabella Alicja Grzegory

## DESCRIPTION FOR THE GENERAL PUBLIC

Gallium nitride (GaN) is a direct wide bandgap semiconductor of great and still growing technological importance. In particular, Light Emitting Diodes (LEDs) based on GaN induced breakthrough changes in general lighting techniques which was awarded by the Nobel Prize in physics in 2014. Semiconductor devices (including microprocessors (Si), telecommunication lasers (GaAs) and light emitting diodes (GaN)) require single crystalline substrates as basis for epitaxy and processing for a final device. For silicon (Si) or GaAs, the bulk crystals of high quality and large size are being grown by Czochralski or Bridgman methods requiring stoichiometric melts to be cooled down for single crystal growth. For GaN such stoichiometric melt cannot be obtained due to presence of nitrogen in the GaN crystal which leads to decomposition of GaN at high temperatures and formation of N<sub>2</sub> gas and liquid gallium. To make GaN thermodynamically stable, sufficiently high pressure of N<sub>2</sub> gas is necessary. For example, at 1500°C, the equilibrium pressure of N<sub>2</sub> should be as high as 1.0 GPa (10 000 atm.!). The temperature of  $1500^{\circ}$ C seems nominally high, however it is still significantly lower than the one expected for melting of GaN. A direct confirmation of a high melting temperature is extremely low solubility of nitrogen in gallium. For example, at  $1500^{\circ}$ C (and corresponding N<sub>2</sub> pressure of 1.0 GPa) this solubility is not higher than 0.5 at.% [3]. Even though such challenging conditions are required, the first high quality GaN crystals that could be used for epitaxy and device processing were obtained at the Institute of High Pressure Physics about 20 years ago.

**Diamond** – Typical for growing of bulk diamond crystals are Fe (Ni, Co, Cr) – C systems at the conditions of high pressure (of about 5-8.0 GPa) necessary for thermodynamic stability of diamond and temperatures of  $1400 - 1600^{\circ}$ C. The concentration of carbon in the liquid iron is at the level of **15 at.%** and which the optimum one for stable and efficient growth of diamond crystals from the solution.

**Nitrogen in "diamond metals"** – The interaction of transition metals, especially Fe, Ni an Cr, with nitrogen was intensively studied because of significant influence of N on the properties of construction steels but also because these metals and nitrogen (as well as silicon and oxygen) are the most important geophysical components. Due to this, geophysicists have performed a large amount of research of Fe(Ni)-N systems at high pressure and high temperature conditions that are natural for the Earth mantle. The available data indicate that solubility of nitrogen in the liquid transition metals (at high temperatures!) attains very interesting, high values even for relatively low pressure of N<sub>2</sub> gas . For instance, at  $p_{N2}$ = 10MPa (app. 100 atm.) and 1600°C, the N solubility in Fe-35%Cr solution is as high as 10at.%, what is significantly above N-solubility in liquid gallium at the typical conditions of high pressure solution growth of GaN ( $p_{N2}$  = 1.0GPa, T=1500°C). Therefore, for pressures required for GaN stability at T>1400°C (much higher than 100 atm.!) one can expect N solubility in Fe and its mixtures with Co and Cr on the level of 10-20wt% which is extremely promising for growth of GaN from liquid solution.

Justification of the proposed research - Both diamond and GaN require high pressure conditions to be grown in the lab. However, the physical reasons behind this requirement are different. For diamond, the pressure is necessary to prevent stability of its crystal structure against graphite whereas for GaN, the pressure is necessary to prevent its stability against the system of its constituents: liquid gallium and molecular nitrogen. So far, the best large artificial diamond crystals were grown by crystallization from carbon solution in metals by HPHT technique. This technique involves carbon source, metallic solvent (Fe, Ni, Co) and diamond seed that are subjected to temperature gradient and high pressure. Adopting this technique and having in mind the fact that N solubility in Fe and its mixtures with some other metals is exceptionally high at HPHT conditions, we are proposing the following idea of the research: to replace the carbon source by the GaN crystalline or polycrystalline ingot and the diamond seed by the GaN single crystalline seed while ensuring the conditions just the same as in case of synthetic diamond growth. The technical feasibility of this idea is justified by accessible resources of participating institutions and the expertise and achievements of involved institutions in HPHT experiments. There is a direct access to high pressure gas systems of high volume (2.0GPa, 1600°C, 1-5 dcm<sup>3</sup>) used previously for crystal growth of GaN at the Institute of High Pressure Physics PAS and to the toroid and multi-anvil high pressure (8.0GPa, 2500°C) systems for bulk growth of diamond at the Institute of Superhard Materials in Kyiv. Both mentioned institutions have very well established collaboration in the field related to the topic discussed in this proposal. All things considered above give an unique opportunity to use competencies and technical possibilities from both "GaN" and "diamond" sides to solve a very interesting and challenging scientific problem.