Center for Nanostructured Graphene - Highlights in 2020

Irradiation engineering for the controlled generation of quantum emitters in hexagonal boron nitride

Quantum emitters are a key technological platform to enable applications such as quantum information processing, quantum sensing and metrology. The recent discovery of quantum emitters in 2D materials such as hexagonal boron nitride (hBN) has triggered a large amount of theoretical and experimental research. Quantum emitters in hBN operate even at room temperature and thus could open the door to quantum applications without the use of expensive cryogenic cooling systems. The main challenge in this new field is that the generation mechanism as well as the microscopic nature of these quantum emitters remain elusive. In 2020, we demonstrated a new method to generate quantum emitters in high-quality hBN by oxygen irradiation and subsequent thermal annealing. We showed that increasing the fluence of the oxygen atoms (defined as the number of atoms per unit area) enhances the density of luminescent centres by ten. Our colleagues at the Helmholtz Zentrum in Dresden-Rossendorf used molecular dynamics simulations to model the oxygen irradiation of hBN at conditions comparable to our experiments. These simulations clarified the generation mechanism of luminescent centres in hBN. With the generation mechanism at hand, we could also find the most likely defects formed during our process, namely V_NC_B and V_B^- (see Figure 1b). *Ab initio* calculations of the optical properties of these two defects showed excellent agreement with our experiments and thereby shed light on the microscopic nature of quantum emitters in hBN. Our new methodology relies on inexpensive and widely used equipment and could enable low-cost and large scale generation of room-temperature quantum emitters. Furthermore the method can be adapted to other semiconducting 2D materials for generating known or even novel quantum emitters.

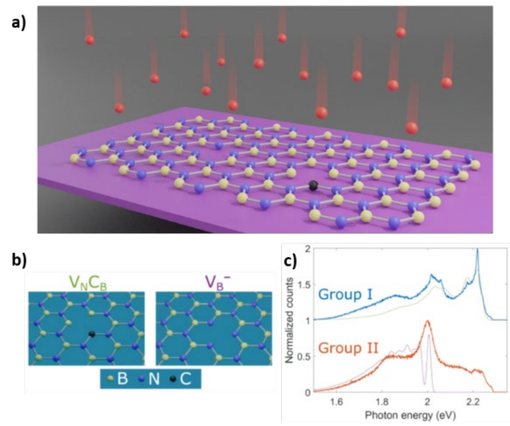

Figure 1. a) High-quality flakes of hexagonal boron nitride are irradiated with oxygen atoms and subsequently annealed at high temperature. b) Molecular dynamic simulations help to identify the most-likely defects formed by our process, namely V_NC_B and V_B^-. c) Ab initio calculations of the photoluminescence spectrum for V_NC_B (green) and V_B^- (purple) show excellent agreement with the experimental spectra for group I (blue) and group II (red), respectively.

M. Fischer, J. M. Caridad, A. Sajid, S. Ghaderzadeh, M. Ghorbani-Asl, L. Gammelgaard, P. Bøggild, K. S. Thygesen, A. V. Krasheninnikov, S. Xiao, M. Wubs, N. Stenger (2021): "Controlled generation of luminescent centers in hexagonal boron nitride by irradiation engineering", Sci. Adv. **7**, eabe7138, doi:10.1126/sciadv.abe/8138

Terahertz spectroscopy is a new measurement standard for CVD graphene

Assessment of electronic properties has been a major cornerstone for graphene science and technology ever since the beginning in 2004. With the introduction of large-scale graphene, the conventional strategy of fabricating electric devices to this end is impractical, destructive and expensive. Over the past decade, researchers at CNG have worked intensively on development of new, fast, non-destructive methods based on graphene's absorption of terahertz radiation, and in understanding how information on the intricate structure of graphene films can be read out from terahertz spectra. This effort has resulted in numerous international collaborations and 20 peer reviewed journal publications since 2012. We have recently published an overview of the key methods and the many results gained through collaborations in 2D Materials, becoming one of the most read papers in 2021. In 2020, the method was accepted as a new measurement standard for graphene, one of the first official standards in the field of graphene worldwide. This work, embodied in the paper and the measurement standard, has been internationally recognised as a milestone towards establishing a viable graphene industry. This is an example on how fundamental research in method development can be lead to industrial impact to the benefit of society.

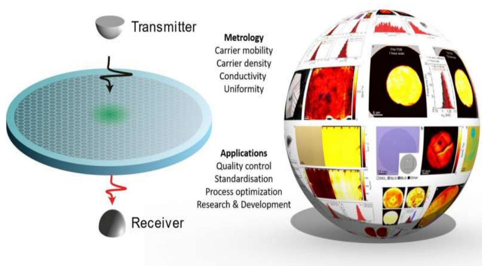

Figure 2. The conductivity, carrier mobility, carrier density and uniformity can be measured from the absorption of terahertz pulses across graphene-coated Si wafers or roll-2-roll graphene, generating a firm base for understanding how defects influence the electronic characteristics, as well as R&D and quality control in industrial settings.

P. R Whelan et al, (2021): "Case studies of electrical characterisation of graphene by terahertz time-domain spectroscopy ", 2D Materials, 8, 2; P. U. Jepsen et al, IEC TS 62607-6-10: Nanomanufacturing - Key control characteristics - Part 6-10: Graphene-based material - Sheet resistance: Terahertz time-domain spectroscopy (Accepted in 2020, will be officially published in 2021), doi.org/10.1088/2053-1583/abdbcb