

## MM 22: Interface Controlled Properties, Nanomaterials and Microstructure Design III

Time: Tuesday 10:15–11:30

Location: C 230

MM 22.1 Tue 10:15 C 230

**Strain engineering for CMOS microelectronics** — ●COSTANZA MANGANELLI<sup>1</sup>, IGNATHI ZAITSEV<sup>1</sup>, AGNIESZKA ANNA CORLEY-WICIAK<sup>1</sup>, CEDRIC CORLEY-WICIAK<sup>2</sup>, MARVIN HARTWIG ZOELLNER<sup>1</sup>, CARSTEN RICHTER<sup>3</sup>, EDOARDO ZATTERIN<sup>2</sup>, MICHELE VIRGLIO<sup>4</sup>, BEATRIZ MARTIN-GARCIA<sup>5</sup>, and DAVIDE SPIRITO<sup>1</sup> — <sup>1</sup>IHP Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — <sup>2</sup>ESRF -European Synchrotron Radiation Facility, Grenoble, France — <sup>3</sup>IKZ -Leibniz -Institut für Kristallzüchtung, Berlin, Germany — <sup>4</sup>Università di Pisa, Pisa, Italy — <sup>5</sup>CIC nanoGUNE BRTA & IKER-BASQUE, Basque Country, Spain

The significance of strain engineering in CMOS microelectronics extends across diverse applications, encompassing opto-electronics, sensing, and quantum technologies, and a variety of materials from SiGeSn semiconductors to 2D materials (MoS<sub>2</sub>, hBN and perovskites). Experimental analyses (Photoluminescence, Raman, X-Ray Spectroscopy) and simulation platforms enable the prediction and optimization of material processes and device design. We present a systematic study elucidating how the temperature-dependent distribution of strain can impact the optical and transport performance of semiconductor devices. Our investigation focuses on strained Ge microdisks, crucial components for developing guidelines for integrated light emitters. We also explore the role of metal electrodes in quantum confinement buses within CMOS-compatible devices. This research provides valuable insights into strain effects on semiconductor devices, laying a foundation for developing and optimizing future microelectronic devices.

MM 22.2 Tue 10:30 C 230

**A theoretical analysis on the bulk photovoltaic effect in strained microstructures** — ●IGNATHI ZAITSEV<sup>1</sup>, DAVIDE SPIRITO<sup>1</sup>, JACOPO FRIGERIO<sup>2</sup>, CARLOS ALVARADO CHAVARIN<sup>1</sup>, MICHELE VIRGLIO<sup>3</sup>, ANKE LÜDGE<sup>4</sup>, WOLFGANG LÜDGE<sup>4</sup>, RAFFAELE GIANI<sup>2</sup>, and COSTANZA LUCIA MANGANELLI<sup>1</sup> — <sup>1</sup>IHP - Leibniz-Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — <sup>2</sup>L-NESS, Dipartimento di Fisica del Politecnico di Milano, Polo Di Como, Italy — <sup>3</sup>Università di Pisa, Pisa, Italy — <sup>4</sup>LPCon GmbH, Berlin, Germany

Strain engineering in microstructures is a powerful tool for optimization of electronic and optical properties in semiconductor devices. We propose a proof of concept for the development of a cost-effective, compact, fast, and non-destructive approach to probe non-uniform strain fields in semiconductors, exploiting the bulk photovoltage effect. We show a benchmark case represented by an array of silicon nitride stripes deposited at different pressure conditions on a germanium substrate. First, we verify their surface deformations by means of Raman spectroscopy; secondly, we reproduce that in a finite element method simulation platform by combining mechanical simulations with deformation potential theory to then estimate the band edge energy landscape. Finally, we discuss theoretical behavior of the photovoltage signal based on the semiconductor sample characteristics such as defects and doping as well as deformation.

MM 22.3 Tue 10:45 C 230

**Influence of Trench Geometry on the Directed Capillary Self-Assembly of Anisotropic Gold Nanoparticles** — ●STEFAN M. SCHUPP<sup>1</sup>, FELIZITAS KIRNER<sup>2</sup>, HELMUT CÖLFEN<sup>2</sup>, and LUKAS SCHMIDT-MENDE<sup>1</sup> — <sup>1</sup>Department of Physics, University of Konstanz, Germany — <sup>2</sup>Department of Chemistry, University of Konstanz, Germany

The self-assembly of anisotropic metal nanoparticles (NPs) into ordered nanostructures is a promising bottom-up approach for applications in photonics and nanoelectronics due to the unique directional

properties of the resulting structures. However, the deterministic placement and orientation of these NPs remains a challenge to this day. In this study, we apply a combination of capillary forces and lithographically patterned substrates to assemble gold nanocubes (AuNCs) with an edge length of 60 nm into linear structures. Here, the influence of trench geometry on the assembly outcome is investigated in detail, which allows to generate ordered mono- to bilayer AuNC structures with varying widths. Finally, this directed capillary self-assembly approach is used to assemble AuNC lines onto pre-fabricated electrodes to perform electrical measurements. Thus, this method can be applied to integrate anisotropic NPs into future electronic devices.

MM 22.4 Tue 11:00 C 230

**Electronic properties of transition metal dichalcogenide nanowrinkles** — ●STEFAN VELJA<sup>1</sup>, JANNIS KRUMLAND<sup>2</sup>, and CATERINA COCCHI<sup>1,2</sup> — <sup>1</sup>Institute of Physics, Carl von Ossietzky Universität Oldenburg — <sup>2</sup>Department of Physics and IRIS Adlershof, Humboldt-Universität zu Berlin

Mechanical deformations in transition metal dichalcogenide monolayers can appear both spontaneously and artificially, giving rise to structures such as nanowrinkles or nanobubbles. Such deformations have been observed to harbor localized electron states, a known prerequisite for single-photon emission, triggering theoretical studies attempting to explain these phenomena. However, fully quantum-mechanical insight given by ab initio calculations is still missing to date.

We model one-dimensional MoSe<sub>2</sub> nanowrinkles by applying uniaxial compressive strain with increasing magnitude in the plane of the monolayer. We analyze their structural properties highlighting the effects of coexisting local domains of tensile and compressive strain in the same system. We find that the electronic properties are driven by the curvature rather than strain: band gaps vary moderately in size compared to flat counterparts and remain direct: in contrast, the spatial distribution of the frontier states is affected by strain. We finally discuss transport properties through the inspection of effective masses and their correlation with wave-function distributions, showing the excellent perspectives for these systems as active components for (opto)electronic devices.

MM 22.5 Tue 11:15 C 230

**Electric field gradients at <sup>111m</sup>Cd sites in single domain and periodically poled Mg-doped LiNbO<sub>3</sub> crystals** — ●HANNES GÜRLICH<sup>1</sup>, BJÖRN DÖRSCHEL<sup>3</sup>, THIENH THANH DANG<sup>3</sup>, IAN YAP<sup>3</sup>, JULIANA SCHELL<sup>1,2</sup>, SAMUEL DOMINIC SEDDON<sup>1</sup>, BORIS KOPPITZ<sup>1</sup>, and LUKAS ENG<sup>1</sup> — <sup>1</sup>Technische Universität Dresden — <sup>2</sup>European Organization for Nuclear Research (CERN) — <sup>3</sup>Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE)

At ISOLDE-CERN, <sup>111m</sup>Cd was implanted at 30 keV into differently ferroelectric-polarized LiNbO<sub>3</sub>-5%Mg crystals in z-direction. After annealing at 600 °C, 700 °C or 800 °C for up to 30 min in an oxygen atmosphere, the samples were measured with the time-differential perturbed angular correlation (TDPAC) technique for at least 2 h at room temperature.

The results show that in the periodically poled samples, the measured electric field gradient (EFG) is strongly suppressed. While in the single domain samples, this depends strongly on the annealing temperature. At 800 °C annealing temperature, the signal is strongly suppressed, while at 700 °C the best results were found. Therefore, it is proposed, that in between those two temperatures an irreversible destruction of the unitary directed polarization occurs.

Two main frequencies were found being independent of the polarization direction: 214(5) MHz and 173(5) MHz.