PCSI

Room Keahou I - Session PCSI-WeM1

Point Defects (for Quantum Information Applications) I

Moderator: Kai-Mei Fu, University of Washington

8:30am **PCSI-WeM1-1 Room Temperature Optically Detected Magnetic Resonance of Single Spins in GaN**, ***Gregory Fuchs,*** Cornell University **INVITED**

High contrast optically detected magnetic resonance (ODMR) is a valuable property for reading out the spin of isolated defect color centers at room temperature. Spin-active single defect centers have been studied in wide bandgap materials including diamond, SiC, and hBN; each with associated advantages for applications. We report the discovery of ODMR in two distinct species of bright, isolated defect centers hosted in GaN [1]. In one group, we find negative ODMR of a few percent associated with a metastable electronic state, whereas in the other, we find positive ODMR of up to 30% associated with the ground and optically excited electronic states. We examine the spin symmetry axis of each defect species and we establish coherent control over a single defect's ground-state spin. Given the maturity of the semiconductor host, these results are promising for scalable and integrated quantum sensing applications.

[1] J. Luo, Y. Geng, F. Rana, and G. D. Fuchs, "Room temperature optically detected magnetic resonance of single spins in GaN," *Nat. Maters* **23**, 512 (2024).

9:10am **PCSI-WeM1-9 UPGRADED: Er Sites in Si for Quantum Information Processing**, ***Sven Rogge,*** UNSW, Australia

Rare-earth ions in a solid-state host exhibit low homogeneous broadening and long spin coherence at cryogenic temperatures, making them promising for a range of quantum applications, such as optical quantum memories and optical-microwave transductions. Emitters with long electron spin and optical coherence in Si, a leading material platform for electronic and photonic technologies, are especially attractive for quantum applications. Here, we report on the observation of eight Er sites in Si that have both long optical coherence and electron spin lifetime. We measured 1 ms spin coherence for two sites in a nuclear spin-free silicon crystal (<0.01% ^{29}Si), which appeared to be instrumentally limited. Using Alternating-Phase CPMG sequence, we extended the spin coherence of one of the sites to 40 ms. Measurements with naturally abundant Si revealed that the Er electron spin coherence was limited by coupling to ^{29}Si nuclear spins. The measured homogeneous linewidths of all 8 sites are below 100 kHz, and inhomogeneous broadening approaches 100 MHz [1, 2]. These results were achieved for Er implanted from 200 and 700 nm from ^{28}Si surface at 10^{16} cm^{-3} level. The Er homogeneous linewidth and spin coherence were addressed using optical comb-based spectral hole burning and optically detected magnetic resonance techniques. To enhance Er emission collection efficiency, samples were directly positioned atop specially fabricated superconducting single photon detectors and resonantly excited via fibre optics. The demonstration of a long spin coherence time and narrow optical linewidth in multiple sites show that Er in ^{28}Si is an exceptional candidate for future quantum information and communication applications and can be used for single photon frequency multiplexing schemes. Finally, integration into silicon on insulator nanophonic devices is discussed.

[1] Ian R. Berkman et al. arXiv:2307.10021v2 (2023).

[2] B.J. Suh et al. Journal of Magnetic Resonance, Series A, **110** (1), 58-61 (1994).

9:30am **PCSI-WeM1-13 Simulating X-STM Images of Iso-Electronic Dopants in Semiconductors Using DFT**, ***Thomas Verstijnen,*** *Douwe Tjeertes, Edoardo Banfi, Paul Koenraad,* Eindhoven University of Technology, Netherlands

The sizes of devices and active regions in semiconductor devices are reaching the atomic scale. This requires us to have an understanding and control over defects at this level as well. A technique that is very well suited to investigate semiconductors at this scale is Cross-Sectional Scanning Tunneling Microscopy (X-STM). We employ this technique to study iso-electronic dopants in III-V semiconductors. We study these dopants since they can locally modify band gaps and other electronic characteristics of a semiconductor which makes them interesting for device fabrication. These X-STM images that we generate can be difficult to interpret however, since the Local Density of States (LDOS) of a material is probed rather than the topology of the material surface alone. For this reason we combine this experimental technique with Density Functional Theory (DFT). We have developed a method to simulate LDOS planes above a surface supercell which can be more directly compared to the X-STM images we generate. This can help us understand the underlying topology of the X-STM images as well as helping us understand what it is that we are seeing when starting X-STM measurements on unknown materials or dopants.

This combination of techniques is applied to three different doped materials: N doped InAs, B doped GaAs and Tl doped GaAs. The N doped InAs and B doped GaAs were used to test the technique since a lot of data about both of those systems studied with X-STM is available. [1] The Tl doped GaAs however, is a material which is not measured before with X-STM and therefore the DFT simulations have helped with the interpretation of the X-STM data. In all three cases we find a strong correspondence between the X-STM and DFT results as seen in Figure 1.

9:35am **PCSI-WeM1-14 GaAsGe Ternary Alloys Studied by Cross-sectional Scanning Tunneling Microscopy**, ***Aurelia Trevisan,*** *Wout van Lierop,* Eindhoven University of Technology, Netherlands*; José M. Ripalda,* Spanish National Research Council (CSIC), Instituto de Microelectrónica de Madrid, Spain*; Yolanda González,* Spanish National Research Council (CSIC) · Instituto de Microelectrónica de Madrid, Spain*; Pablo Caño, Enrique Navarro,* Spanish National Research Council (CSIC), Instituto de Microelectrónica de Madrid, Spain*; Raghavendra Juluri, Ana M. Sanchez,* University of Warwick, UK*; Paul M. Koenraad,* Eindhoven University of Technology, Netherlands

Similarly to Si, Ge exhibit an amphoteric behavior when used as dopant in GaAs, i.e. it can substitute both Ga and As atoms [1]. In molecular-beam-epitaxy-(MBE)-grown GaAsGe, at low doping concentration, Ge preferentially substitute either Ga or As atoms depending on the growth condition, i.e. the As2 to Ga ratio in the molecular beams [2]. However, at high doping concentration, Ge is expected to substitute Ga and As atom to the same extent [1],[3]. A GaAs/GaAs:Ge structure comprising of seven 50 nm-thick GaAs:Ge layers with decreasing Ge concentration (5% - 0.01% Ge) grown by MBE was analyzed by cross-sectional scanning tunneling microscopy (X-STM). All the layers aside the 5% Ge one were imaged by X-STM. In filled-states X-STM images, the Ge atoms appear as bright features with different shapes depending on where they are located in the GaAs lattice, i.e. whether they are sitting on a Ga or As site and at what depth below the cleaved surface (0th layer). Several features are identified in the layer at lower Ge concentration (0.01% Ge, L7). Of these features we assume that some correspond to a Ge atom sitting on a Ga-site located at different depth below the cleaved surface. Similarly, some other features are related Ge atoms on As-sites located at different depth below the surface. These different features have been classified and related to the Ge position below the cleaved surface through symmetry considerations taking into account the contribution of the different surface states to the X-STM images, namely the A4 and A5 state located in the valence band and the C3 and C4 located in the conduction band [4], [5]. Other observed features are given by Ge located deeper below the cleaved surface (5th layer or lower), interstitial atoms and vacancies that can be either intrinsic or caused by the cleave of the sample. Additionally, we calculated the Ge concentration in the measured layers and we compared it to the nominal concentration. We found that for most the layers, the experimental concentration is comparable to the nominal one. With this study, we aim to gain further insight into the preferential incorporation of Ge in GaAs, which is difficult to determine with other techniques.

[1] C. M. Wolfe, G. E. Stillman, Appl. Phys. Lett. 27, 564–567 (1975)

[2]A. Y. Cho and L. Hayashi, *J. Appl. Phys.* 42, 4422–4425 (1971)

[3]R. J. Baird *et al., J. Appl. Phys.* 69, 226–236 (1991)

[4]Ph. Ebert, *Surf. Sci. Rep*. 33, 121-303 (1999)

[5]D. Tjeertes *et al., Phys. Rev. B.* 104, 125433 (2021)

9:40am **PCSI-WeM1-15 Imaging Rare-Earth Dopant Clusters in SiC in 3D Using Multislice Electron Ptychography**, ***Shake Karapetyan,*** *Malcolm Thomas,* Cornell University*; Ute Kaiser, Johannes Biskupek,* Ulm University, Germany*; David Muller,* Cornell University

There has been a long-standing interest in exploring rare-earth dopants and clusters within wide-bandgap materials as a platform for quantum computing [1]. Atomic-scale characterization of these dopants is crucial for understanding activation mechanisms and optimizing doping strategies. Multislice electron ptychography (MEP) is a new approach capable of imaging the atomic distribution of dopants inside a material, offering sub-Ångstrom lateral resolution and a few nanometers depth resolution,

making it possible to visualize atomic-scale vibration envelopes and single dopants [2, 3]. Here, we use MEP to image the effects of implanting Sm and Co atoms in SiC, a prototypical host whose rare-earth-doped defect centers display promising photonic and spintronic functionality [4].

Figure 1 presents a region of SiC containing Sm dopant clusters, comparing MEP with conventional Annular Dark Field (ADF) imaging. The MEP reconstruction reveals depth dependent features showing that the Sm atoms occupy Si positions inside the sample and displace nearby C and Si atoms, even whole columns (yellow arrow) – details that ADF fails to capture. This new capability to study atomic defects in 3D not only deepens our understanding of defect behavior in complex materials but also allows us to tackle such problems in the actual device structures needed for optoelectronic and quantum computing.

[1] G. Wolfowicz et al., Nat Rev Mater **6**, 906 (2021).

[2] Z. Chen et al., Science **372**, 826 (2021).

[3] Z. Chen et al., *arXiv preprint arXiv:2407.18063* (2024).

[4] U. Kaiser, D. A. Muller, J. L. Grazul, A. Chuvilin, and M. Kawasaki, Nature Materials **1**, 102 (2002).

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9:45am **PCSI-WeM1-16 Controlling with External Fields the Quantum-Mechanical Core-Hole Manganese Spin in III-V Semiconductors***, **Julian Zanon**,* Eindhoven University of Technology, Netherlands*; Michael E. Flatté,* University of Iowa

For applications in quantum devices the control of spin-degree of freedom has been one the major goals in semiconductor physics in the past few years. In III-V semiconductors (e.g., in GaAs or InSb) this could be achieved with manganese impurities. Manganese forms a complex, where a J = 3/2 hole from the host aligns antiferromagnetically with the 5/2 spin of the 3d5 manganese core [1]. STM images with theoretical calculations showed the potential to characterize the spatial structure of a single manganese [2] and the exchange interaction between manganese pairs [3]. Classically treating the manganese core spin, its orientation would affect the spatial structure of the manganese complex [2]. In our work, based on previous ESR measurements [1], we show a new pathway to treat the manganese core fully quantum-mechanically and, using an analytical treatment to treat the hole part of the wavefunction, we suggest a coherent manipulation of spatial structure of a single manganese in bulk III-V semiconductors. We also investigate how a surface affects the spatial structure.

[1] J. Schneider, U. Kaufmann, W. Wilkening, et al., Phys. Rev. Lett. 59, 240 (1997).

[2] A. M. Yakunin, A. Y. Silov, P. M. Koenraad, et al., Phys. Rev. Lett.92, 216806 (2004)

[3] D. Kitchen, A. Richardella, J.-M. Tang, et al., Nature 442, 436 (2006).

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