Towards Quantum Sensing for Directional Dark Matter Detection Using Nitrogen Vacancy Centers in Diamond

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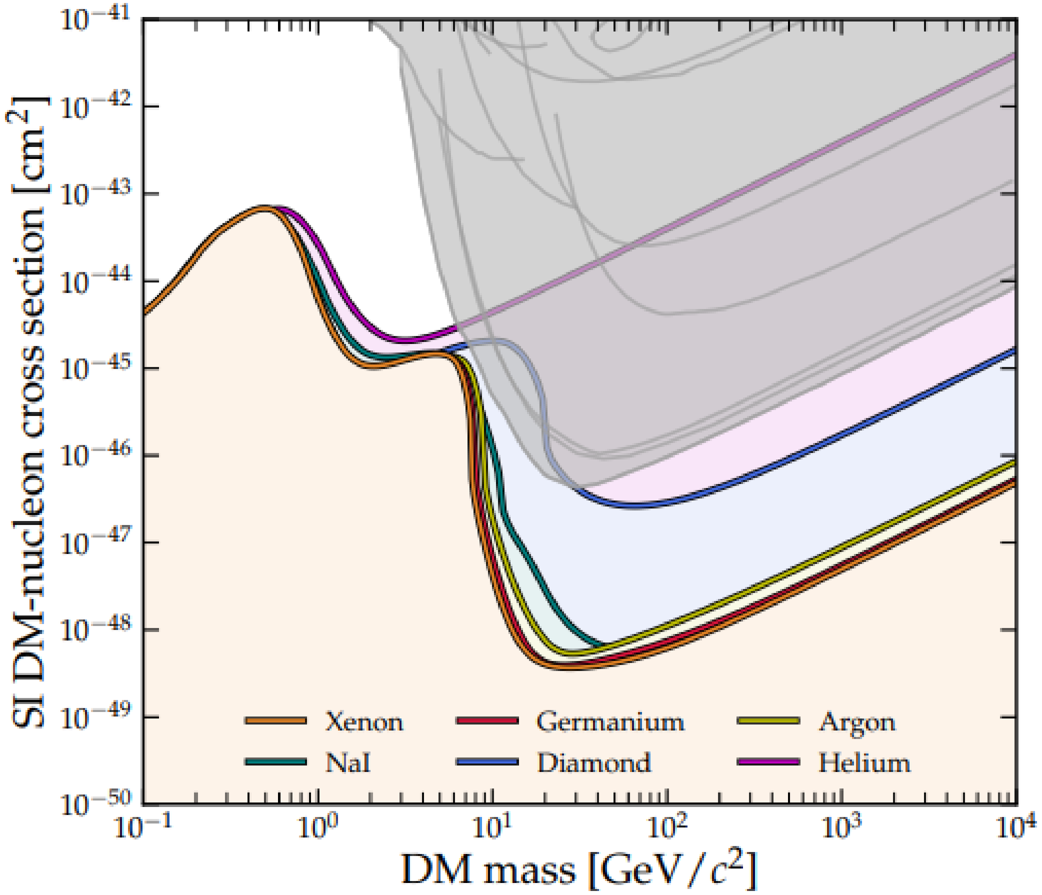
Diamond for WIMP DM detection

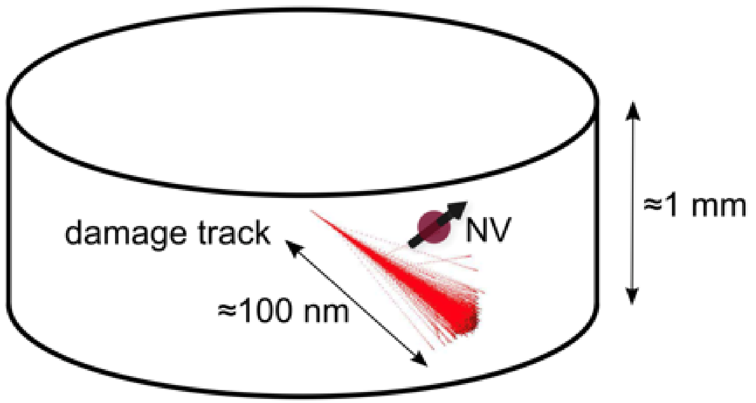
- Weakly interacting massive particles (WIMPs): a leading DM candidate
- WIMP detectors with current technology are projected to shortly reach the solar neutrino fog
- Our goal: Use nitrogen-vacancy (NV) color centers in diamond as directional DM detector to overcome neutrino fog
- Advantages:
  - Solid state → dense target mass
  - Utilize latest advances in NV quantum sensing
  - Can integrate conventional detection techniques

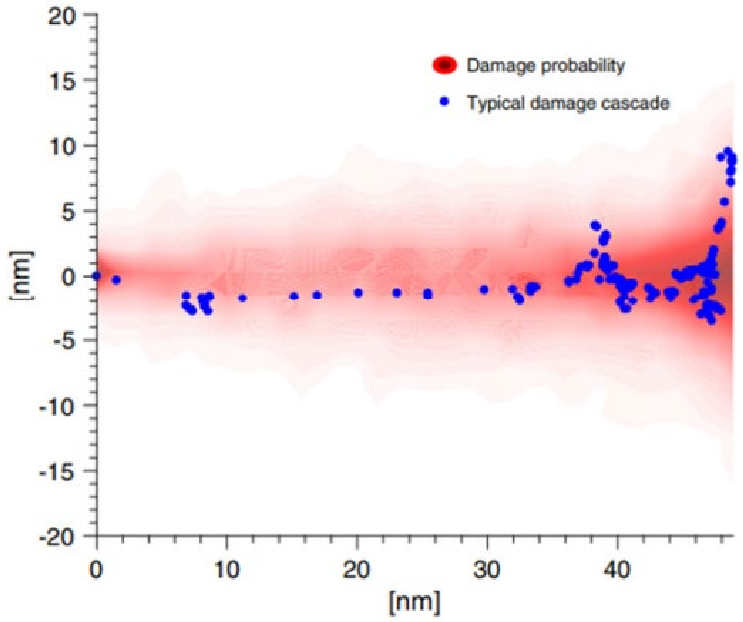


O'Hare, PRL 127, 251802 (2021)
Ebadi et al., AVS Quant. Sci. 4, 044701 (2022)

Nuclear recoil track detection with diamond

- 1-100 GeV WIMP → 10-100 keV nuclear recoil → 10-100 nm damage track in diamond
- Locate and characterize damage track w/ NV spectroscopy
  - Fluorescent track readout
  - Quantum strain readout
- Deduce initial recoil direction and distinguish between solar neutrinos vs. DM





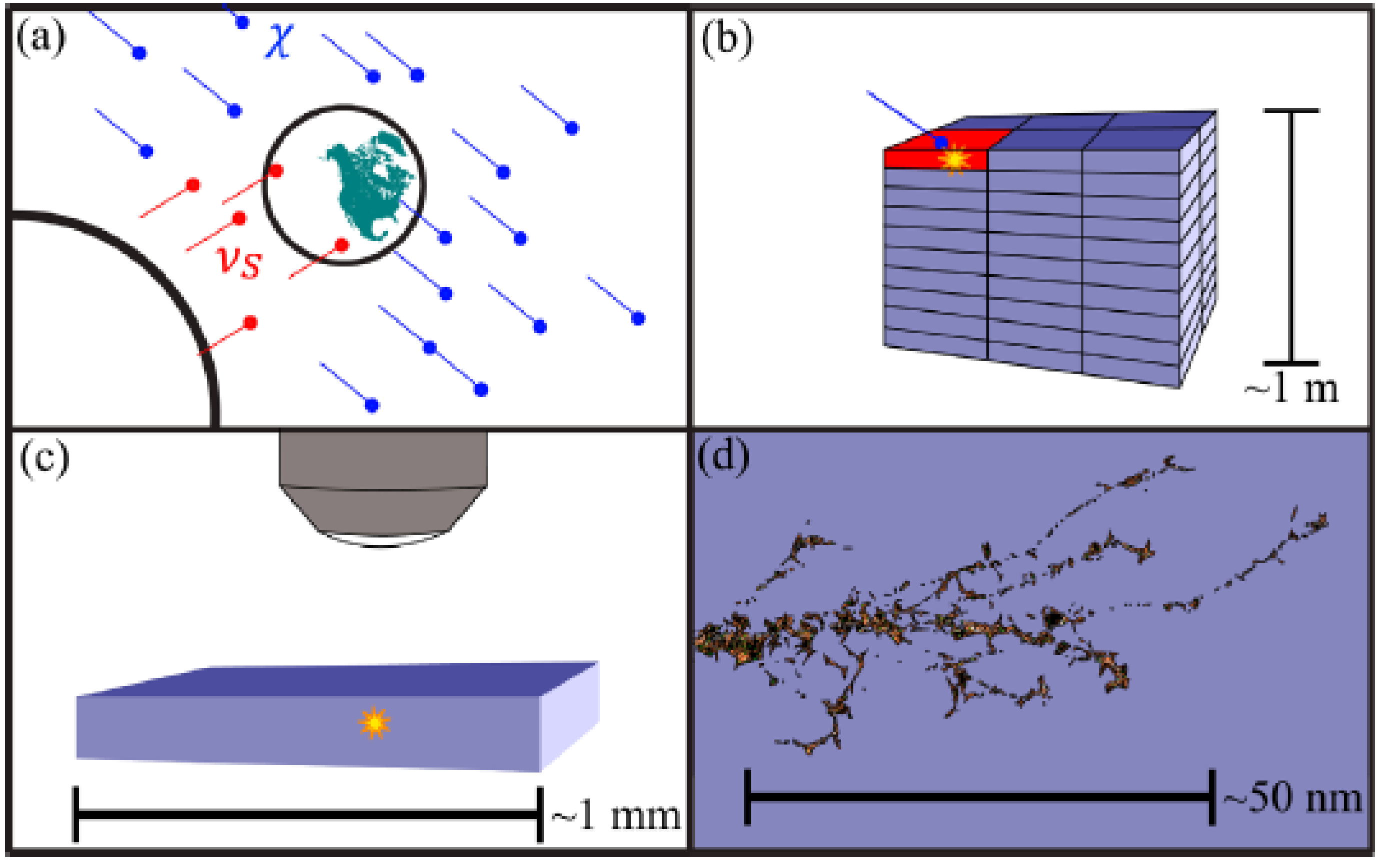
SRIM simulation for 30 keV recoil

Rajendran et al., PRD **9**, 035009 (2017)

Future directional hybrid detector scheme

- **Stage 1:** real-time event detection with conventional detectors
- **Stage 2:** micron-scale localization via NV widefield spectroscopy
- **Stage 3:** nanoscale imaging to determine track characteristics
- Correlate stage 3 with stage 1 data to interpret event
- Requires **rapid, precise, robust imaging capabilities at all scales (micro & nano)**

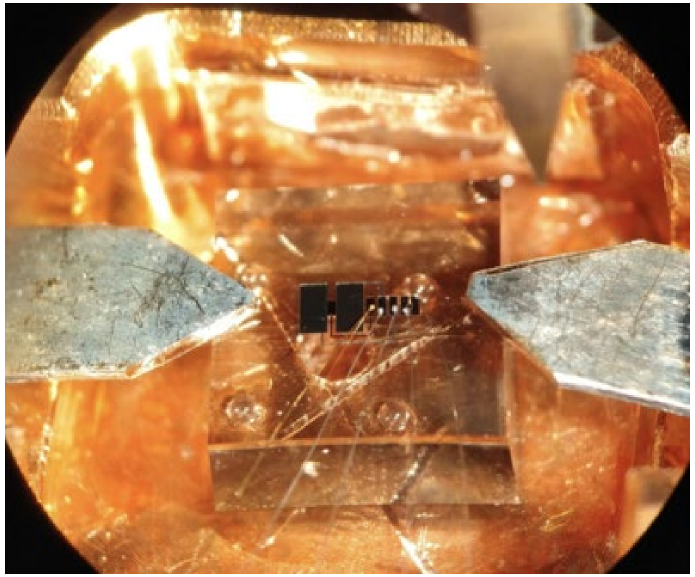
Stage 1



Stage 2 **Stage 3**

Diamond as a conventional DM detector

- Several favorable properties:
  - Semiconductor with wide bandgap (5.4 eV)
  - Lower mass compared to other solid-state detectors – can access underexplored low mass DM regions
  - Can be manufactured with high purity
- Charge, phonon, or scintillation detection possible
  - Active research efforts: CRESST, LLNL/SLAC, U. Tsukuba, etc.
- Open research questions:
  - Background characterization and suppression
  - Practical implementation (engineering) issues
  - Improve signal localization



CRESST diamond-based phonon detector

Abdelhameed et al., Eur. Phys. J. C 28:851 (2022)
Umemoto et al., NIMS A 1057, 168789 (2023)
G. Angloher et al., Eur. Phys. J. C 84:324 (2024)
Kim et al., arXiv:2409.19238 (2025)

Natural diamond as a paleodetector?

- Advantages:
  - Exposure ages of ~1-3 Gyr
  - Intrinsic radiopurity (<1 ppb U-238)
  - In nitrogen-rich diamonds, color center (NV) readout potentially possible
  - Widely mined, synthetic diamond available for R&D
- Principal challenge:
  - Kimberlite host rock carries ~1 ppm U
  - Samples must exceed a few cm in size or sourced from select locations
- Requires better understanding of
  - Anticipated track spectra
  - Track formation and readout
  - Measurements of typical local U/Th in kimberlite environments

Cramers, EPS Lett. 42, 58-70 (1979)

Research strategy

- **Study all aspects of the formation and imaging of tracks in diamond for fundamental physics applications**
- Three major areas of research:

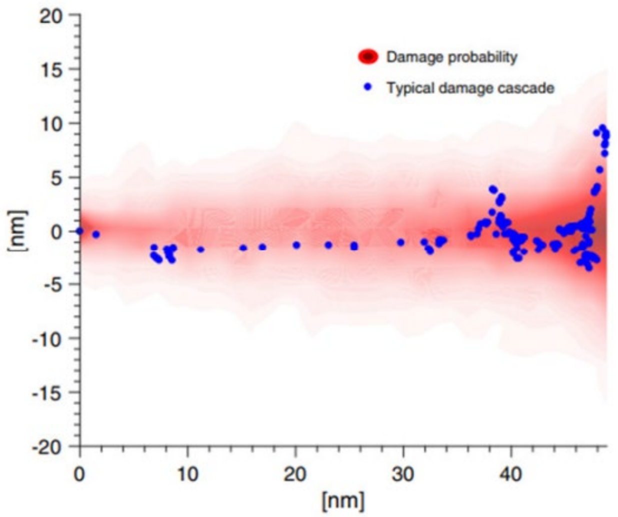
1. Modelling nuclear recoil-induced tracks in diamond
2. Experiments with artificial damage tracks
3. Development of new imaging techniques:
    - Microscale imaging
    - Nanoscale imaging

1. Track simulations

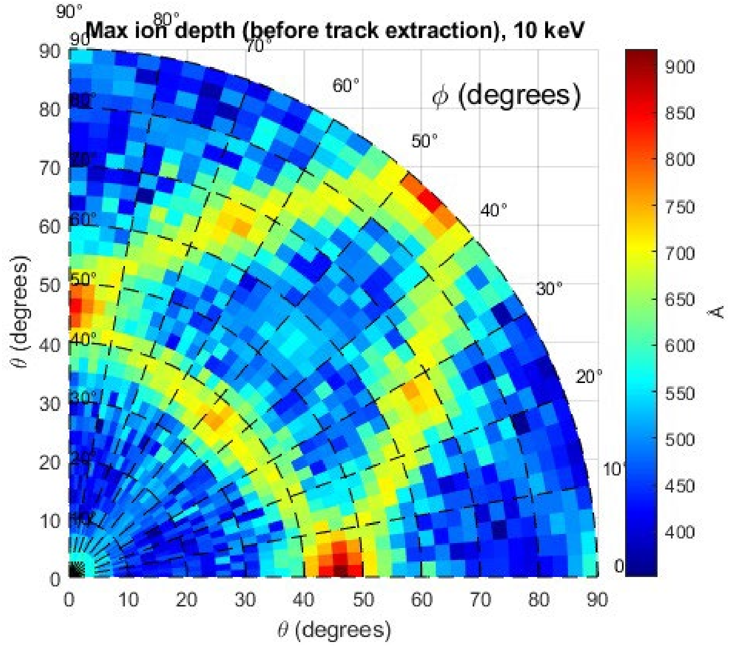
work done with
Max Shen

BCA simulations

- Modelling nuclear recoil damage tracks is crucial for designing and understanding mineral detectors
- Binary Collision Approximation (BCA): approximate ion trajectory by experiencing a sequence of independent binary collisions
  - Not fully atomistic, inaccurate at low energies
  - Low computational requirements, very fast
- Initial studies for diamond dark matter used SRIM
  - No lattice structure
- Recently switched to SIIMPL, which allows modelling lattice structure and thus observe channeling effects
  - https://github.com/msjanson01/siimpl



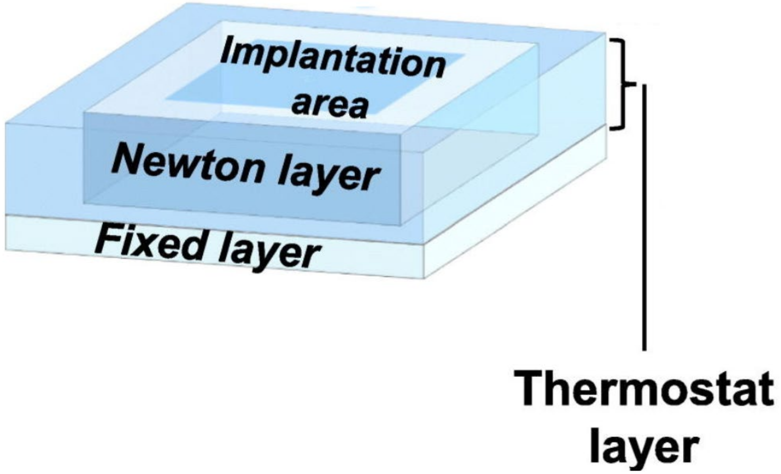
SRIM simulation for 30 keV recoil



Ion penetration vs angle (SIIMPL)

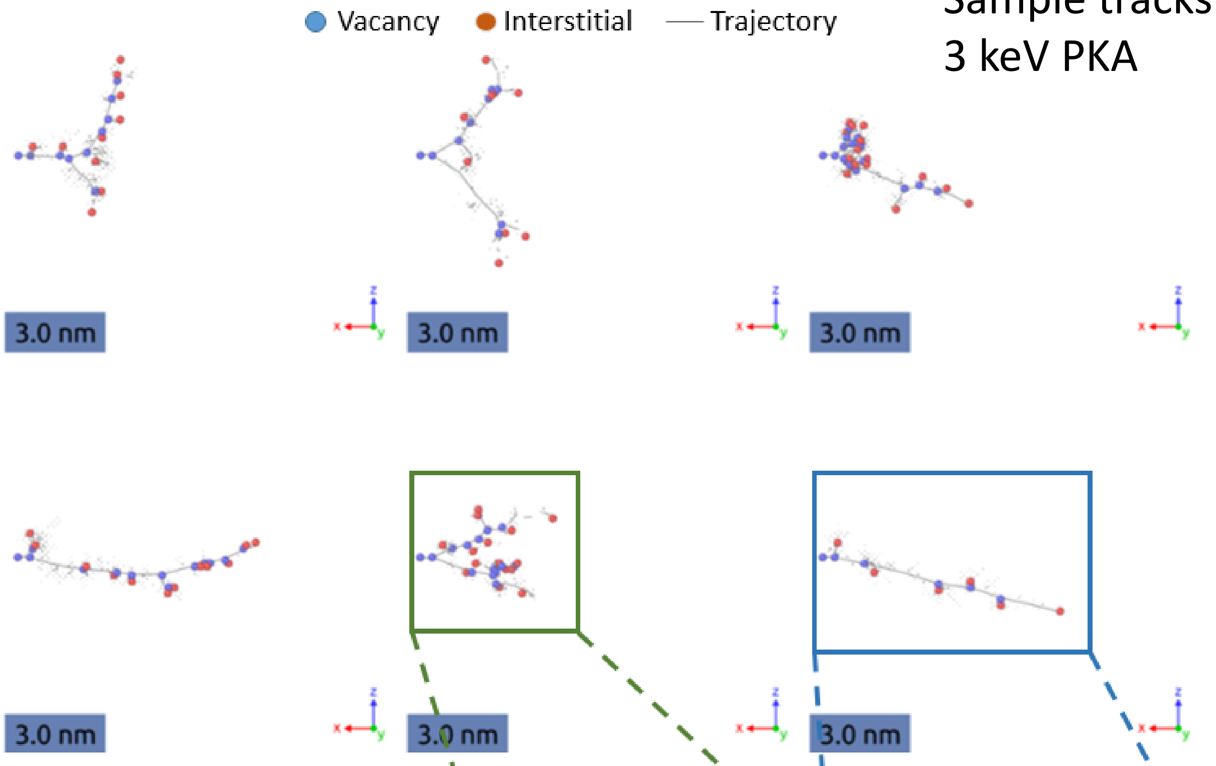
Molecular dynamics simulations

- Molecular dynamics allows fully atomistic simulations
  - Fully model channeling, recombination, phonons, etc.
- Implement standard techniques in LAMMPS to ensure physicality of simulation:
  - Thermal and fixed layers
  - Nuclear repulsion at close distances (ZBL)
  - Bonding potential at medium distances (EDIP, following Buchan et al. 2015)
  - Electronic stopping (ESPNN)
  - Wigner-Seitz analysis

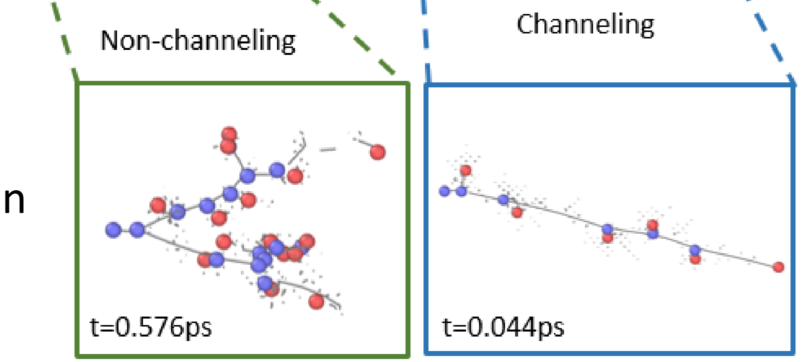


Buchan et al., J. Appl. Phys. 117, 245901 (2015)
Zhao et al., Dia. Rel. Mat. 132, 109683 (2023)
Haiek et al., J. Appl. Phys. 132, 245103 (2022)

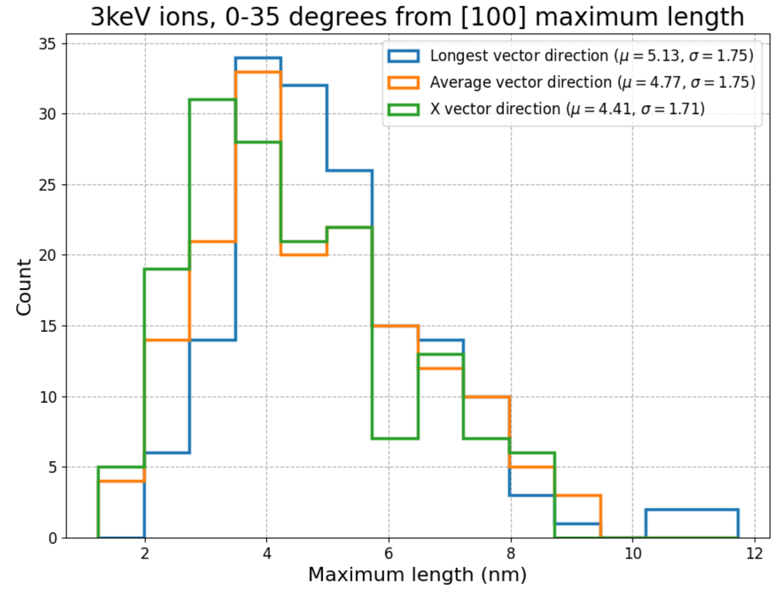
Some MD results

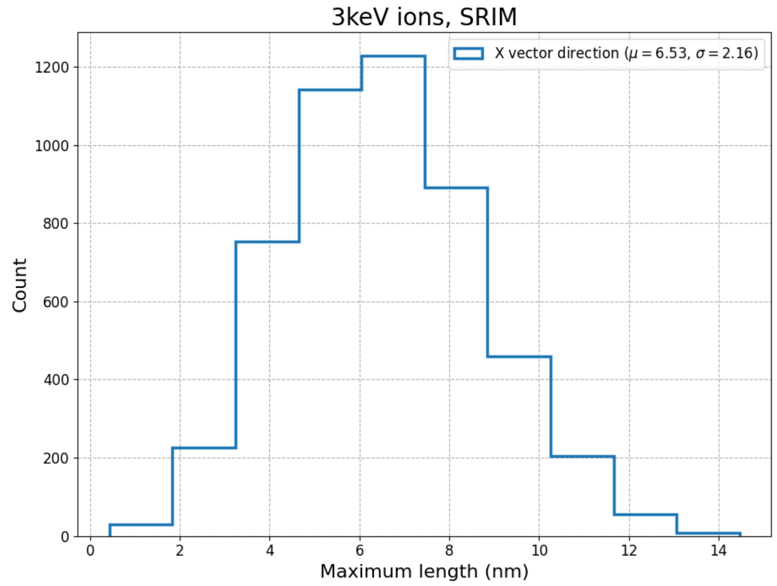


Sample tracks from
3 keV PKA



Results match SRIM within
a factor of ~2

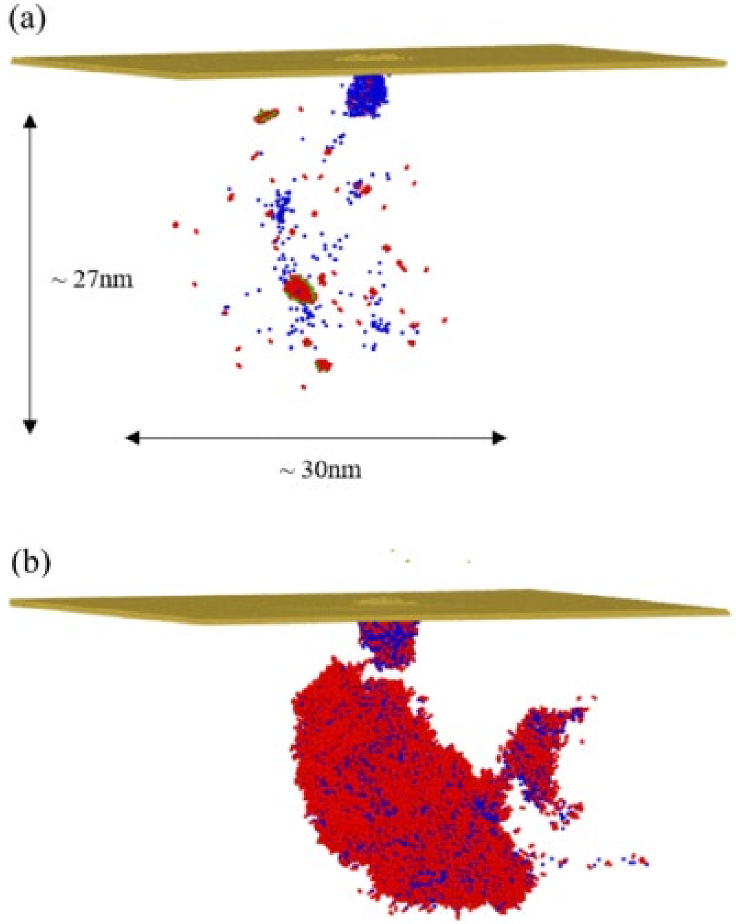




Comparison with SRIM

Lessons learned from MD

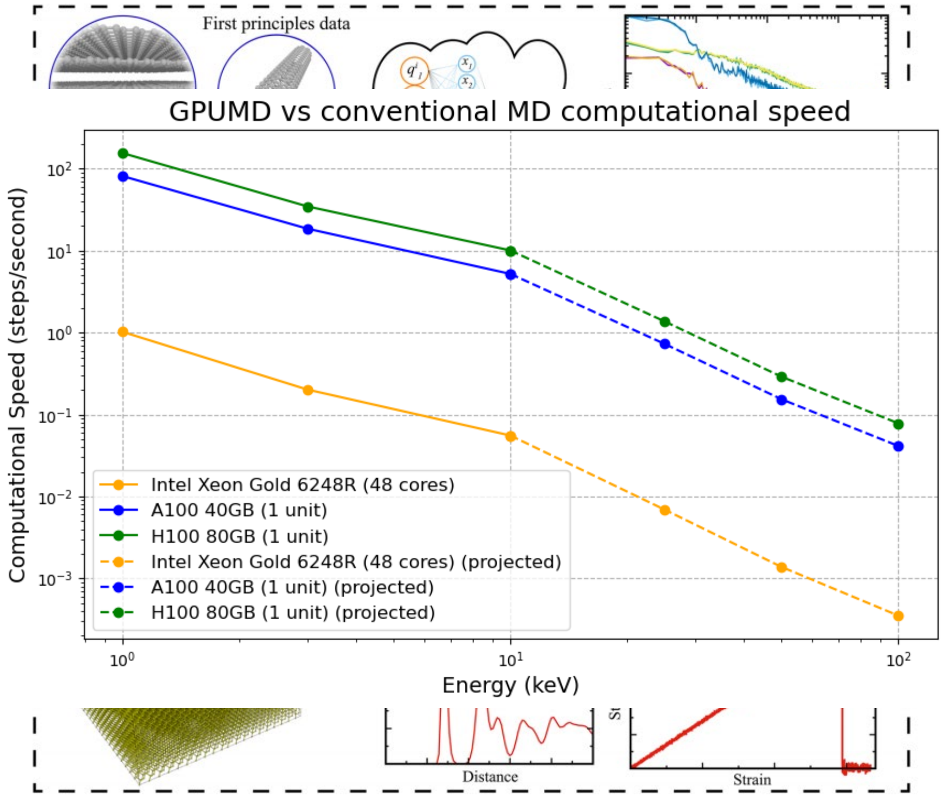
- Lack of clear benchmarks for simulation accuracy
  - 50+ possible interatomic potentials for carbon in the literature (+ many other simulation options)
  - Highlights the need for **empirical benchmarking** through imaging of artificial tracks
- Computational power limits
  - Variations in track size and shape show the need for statistics (>100 tracks)
  - With conventional MD, 40^3 lattice (3 keV) already takes ~4 days per track
  - Cell-based methods (e.g. CMDC) not applicable
- Prospect of ML-enhanced MD methods (GPUMD)
  - Can be run on GPUs
  - Allows for ~10-100x speed up
  - Has been used for up to 200 keV recoils in tungsten



Fan et al., J. Chem. Phys. 157, 114801 (2022)
Liu et al., PRB 108, 054312 (2023)

GPUMD: machine-learned, GPU-compatible potentials

- Use GPUMD package and neuroevolution potential (NEP) following Fan et al. (2022)
  - NEP is optimized for massively parallel GPU execution
  - Allows training on DFT-generated data
- Train NEP potential on diamond crystal structures with interatomic forces
  - Base training dataset from Derringer & Csanyi (2017)
  - Supplement with custom close-range data generated with standard DFT packages (GPAW)
- Preliminary runs indicate ~100x speedup
  - Possible to scale to >50 keV implantations
  - Will likely be limited by GPU RAM



Fan et al., J. Chem. Phys. 157, 114801 (2022)
Derringer & Csanyi, PRB 95, 094203 (2017)

Outlook

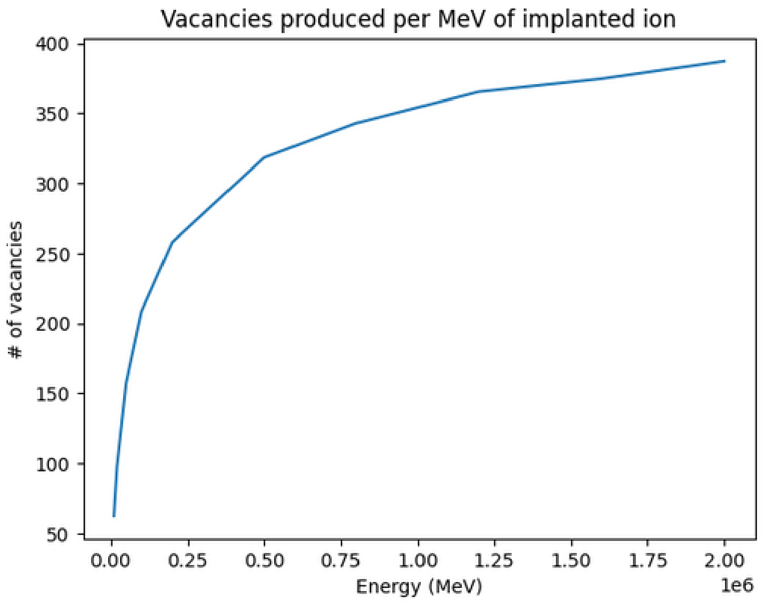
- Track metrics and classification + implications for dark matter detection
- Inverse problem
  - Given a certain track, how accurately can we predict the properties of the original recoil?
- Linking vacancy distributions to experimental observables
  - Annealing and NV formation (see next section)
  - Diamond lattice strain (relevant for NV strain sensing)
- Modelling of cosmogenic, radioactive, and other backgrounds
- Ongoing group discussions on MD with U Michigan

2. Experimental studies of artificial damage tracks

work done with
Jiashen Tang

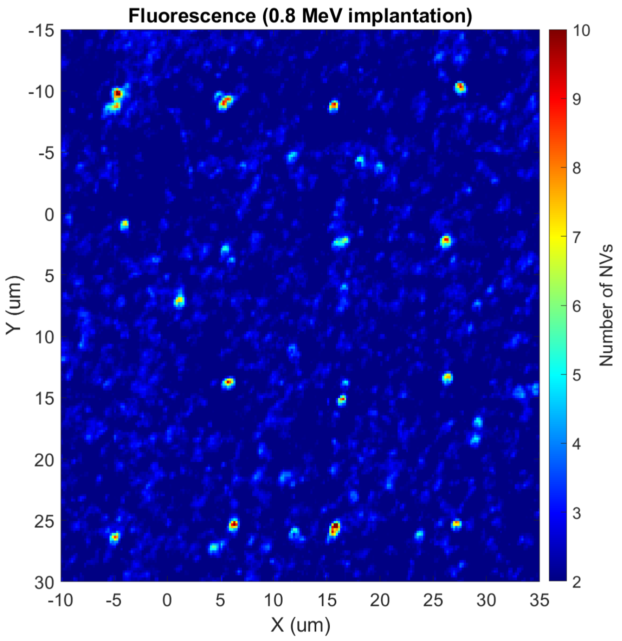
Fluorescent track studies

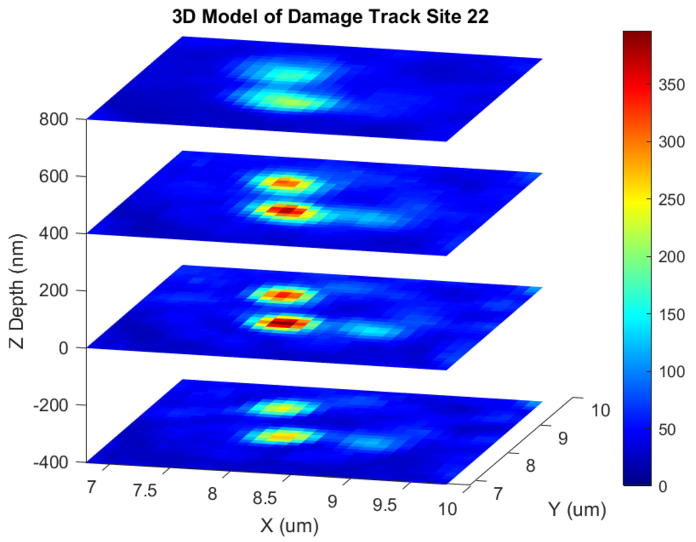
- Goals:
  - Emulate effect of DM/neutrino-induced nuclear recoils
  - Also relevant for potential paleodetector studies
- Precision single carbon ion implantation @ SNL
- Use Type 1b diamonds with high (~200 ppm) nitrogen
- Super-polish diamond surface (Ra < 1 nm)
- Implantation at ~1 MeV with 6-10 um spacing
  - SRIM predicts ~200-400 vacancies formed
- Annealing (2 hrs @ 800 C) results in vacancies meeting nitrogen atoms and forming bright nitrogen vacancy centers (NVs)
- **What is the vacancy conversion rate?**
  - Enable us to predict the minimum detection threshold

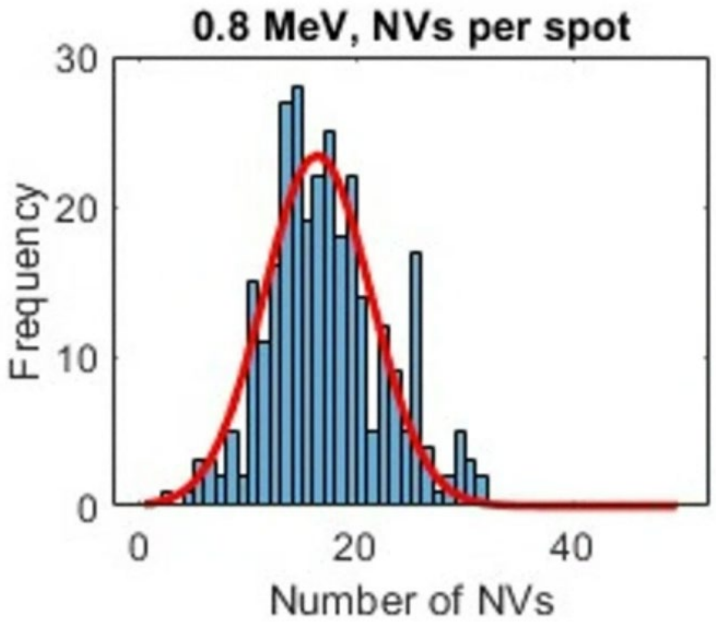


SRIM prediction

- Scan ~300 implantation sites with confocal microscope, ~1 um below the surface
  - Typical background is ~3 NVs
  - Polishing damage results in some regions with high backgrounds
  - Graphitization on surface after annealing, difficult to clean due to gold alignment markers
- Observed 17(5) NVs per single ion impact site







Interpreting the results

- Understanding the data requires connecting track simulations (SRIM/MD) with observables

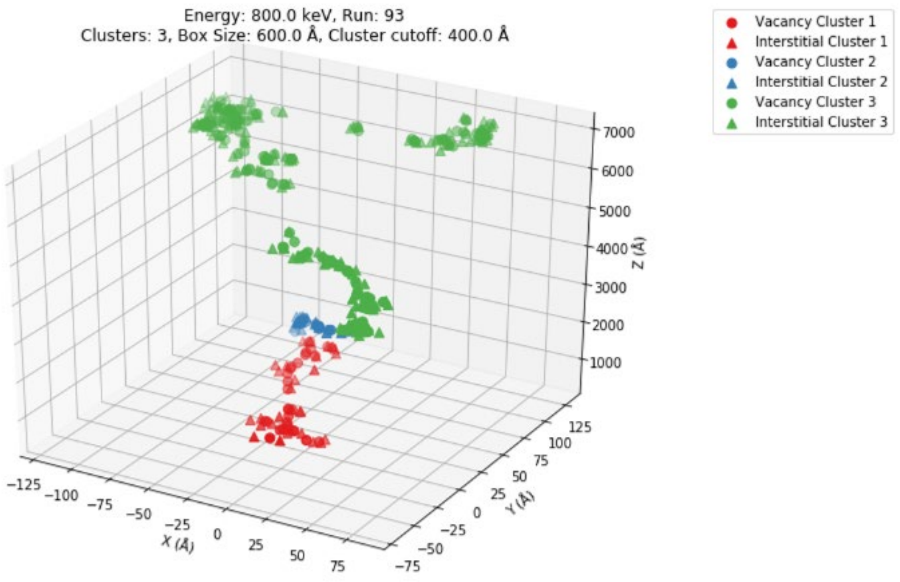
$$N_{NV} = N_V\,(E) * P_{conv}\,([N_s], \rho_{vac}(r), t_{anneal}, T, D, \dots)$$

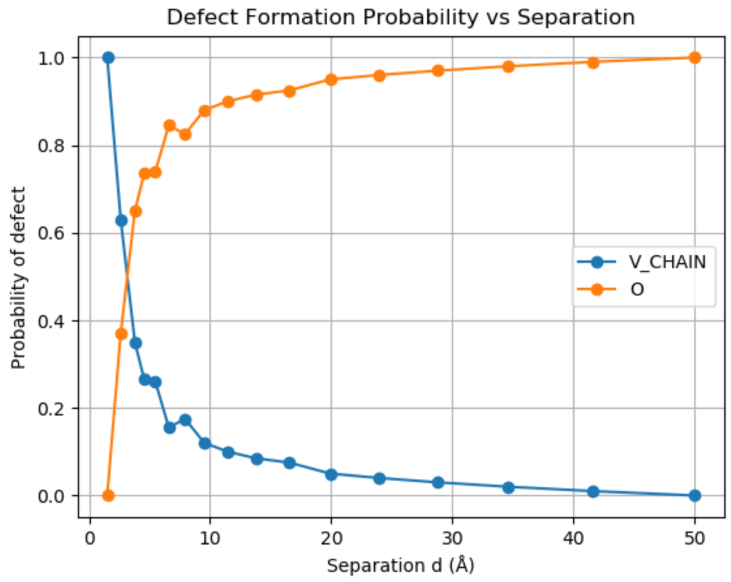
Empirical observable — **Obtained via SRIM/MD** — **Outcome of annealing process**

- Dependent variables important for modelling annealing process:
  - Nitrogen concentration $[N_s]$: measured via SIMS @ Rice University & EAG ~ 185 ppm
  - Vacancy spatial distribution $\rho_{vac}(r)$: import from SIIMPL
  - Annealing time t_{anneal} : verified that we “annealed to completion”
  - Temperature T: 800° C
  - Diffusion constant D and other variables: use literature values

NV formation simulation

- Not feasible to model full annealing with MD
- Currently performing Kinetic Monte Carlo (KMC) simulation with SPPARKS software package
  - Native support for MPI parallelization
- Import vacancy distribution from SIIMPL (~0.5-1 um long)
  - Memory limitations necessitates dividing damage track into clusters that fit within <200^3 atom lattices
- Processes modelled:
  - Vacancy & interstitial diffusion
  - NV formation
  - Vacancy-interstitial recombination
  - Vacancy clustering
  - Vacancy escaping to the surface



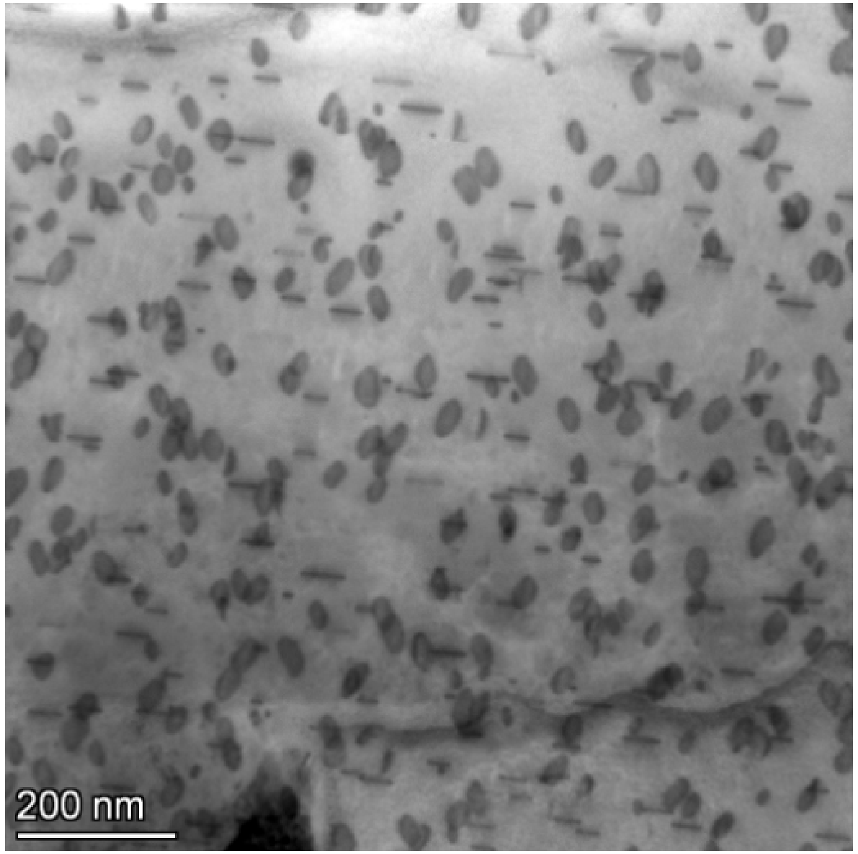


Oliveira et al., Nat. Comms. 8, 15409 (2017)

Outlook

- Could we perform quantum measurements with formed NVs?
  - Planning to measure coherence time (T2)
  - Potential to apply Fourier-based super-resolution techniques to resolve track size and shape (see later)
- Implantations at lower energies
  - Improve sample surface preparation via chemical etching to reduce background
- Neutron irradiation @ NIST
  - Irradiated natural diamond at 14 MeV
  - Performed preliminary TEM imaging at U Michigan, observing dislocation loops – likely because of high irradiation energies

Credit: Kai Sun, Emilie Lavoie-Ingram (U Mich)



U Michigan TEM image showing dislocation loops

3. Development of quantum imaging techniques

Team:

Mason Camp
(Rapid microscale imaging)

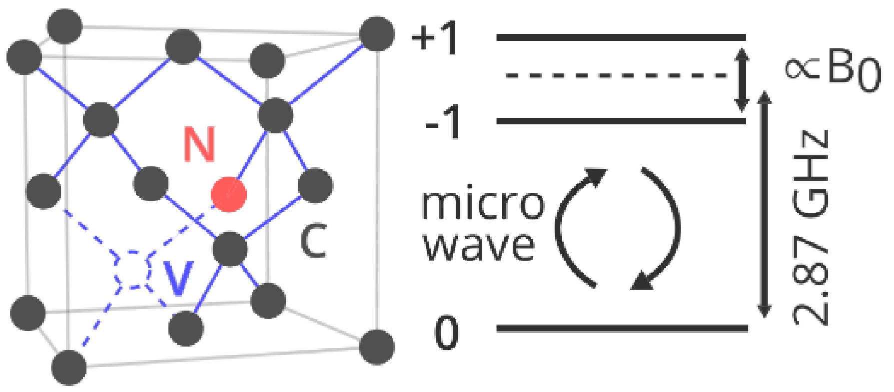
Max Shen Gavishta Liyanage

(Nanoscale imaging)

Limitations of NV fluorescent readout

- Annealing may alter track shape, compromising directional detection performance
- High nitrogen impurities in diamond (~200 ppm) may make integration with conventional detection methods (e.g. charge or phonon readout) difficult in a full-scale DM detector
- **Alternative readout method**: use low-N, NV-rich (~1-10 ppm) CVD diamond to perform **precision strain sensing** with NV quantum sensors to detect a nearby track
  - No annealing required

Overview of NV quantum sensing



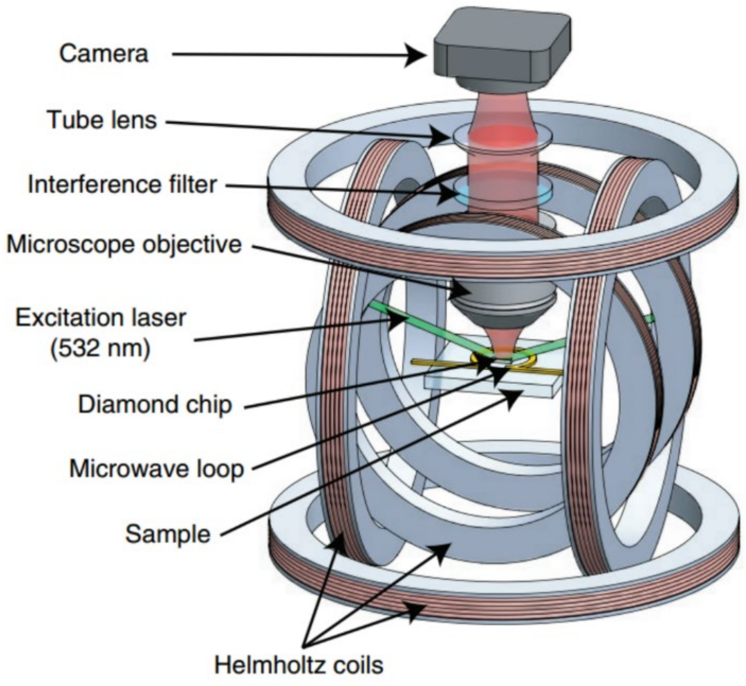
$$H = (D + M_z)S_z^2 + \gamma B_z S_z$$

Temperature-dependent

Crystal strain

Magnetic field

Shifted by presence of DM-induced damage track



Quantum diamond microscope

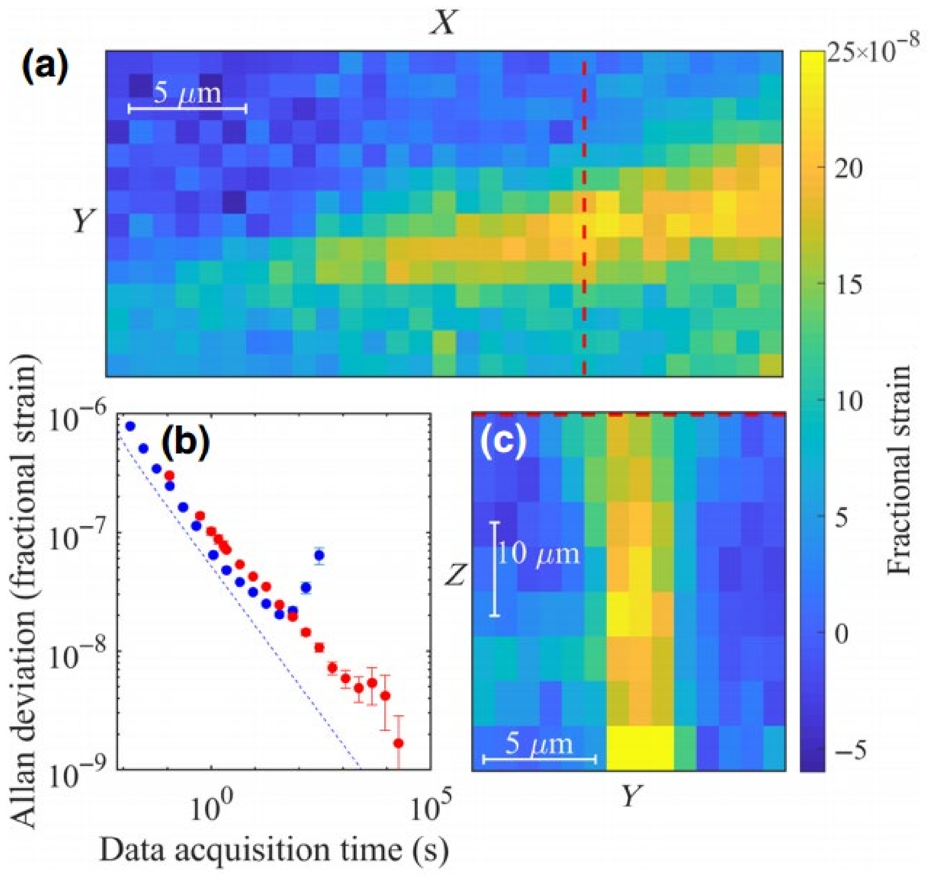
Figure adapted from Levine et al., Nanophotonics 8(11): 1945-1973 (2019)

Previous work in NV strain imaging

- 2022: Demonstrated NV strain sensing in confocal QDM with sensitivity

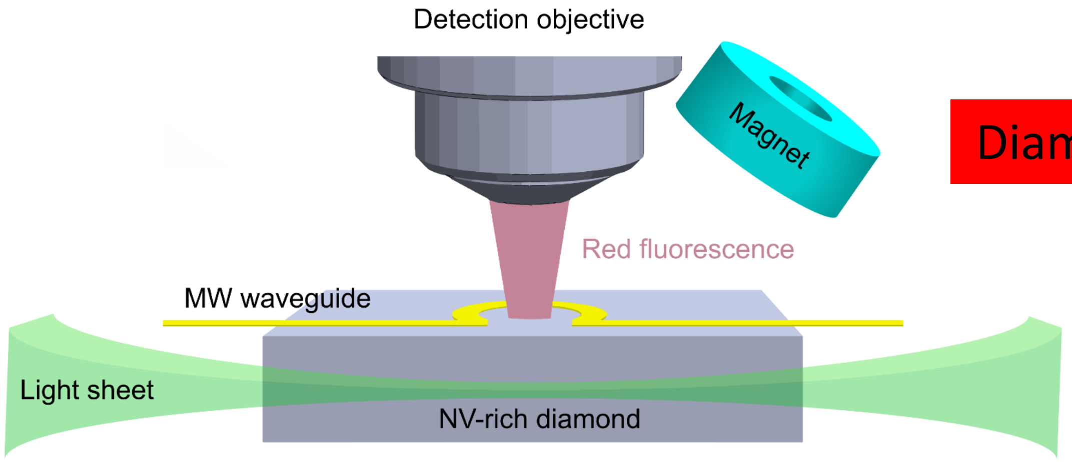
$$5(2) \times 10^{-8}/\sqrt{Hz\ \mu m^{-3}}$$

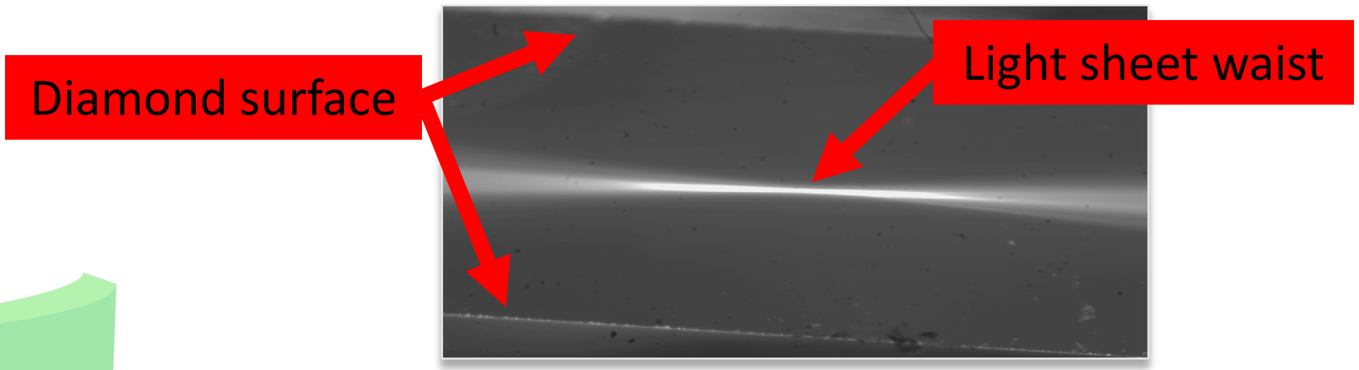
- Fulfills DM detection requirement
- However, confocal scanning speed is too slow to keep up with anticipated event rate
- Widefield imaging has also been done, but only in 2D



M. Marshall et al., PR Applied **17**, 02401 (2022)

Solution: light sheet quantum diamond microscope

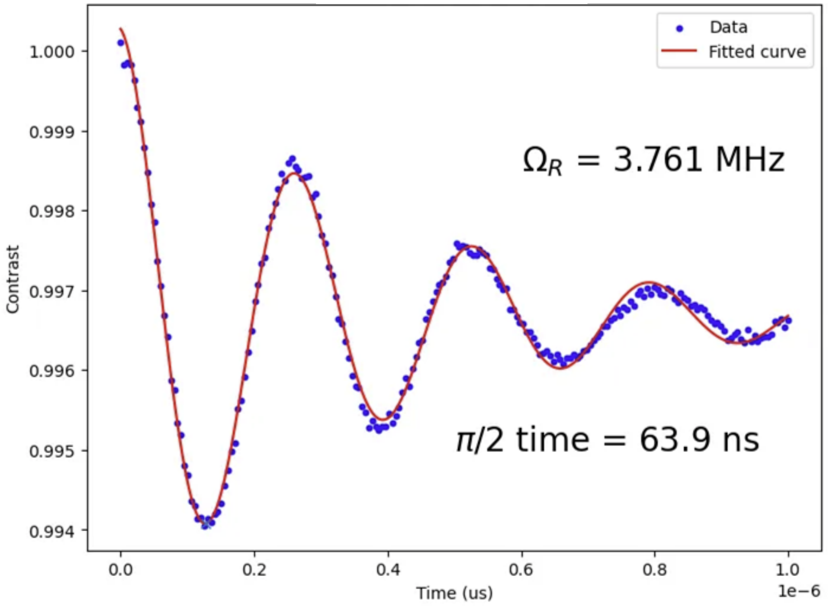




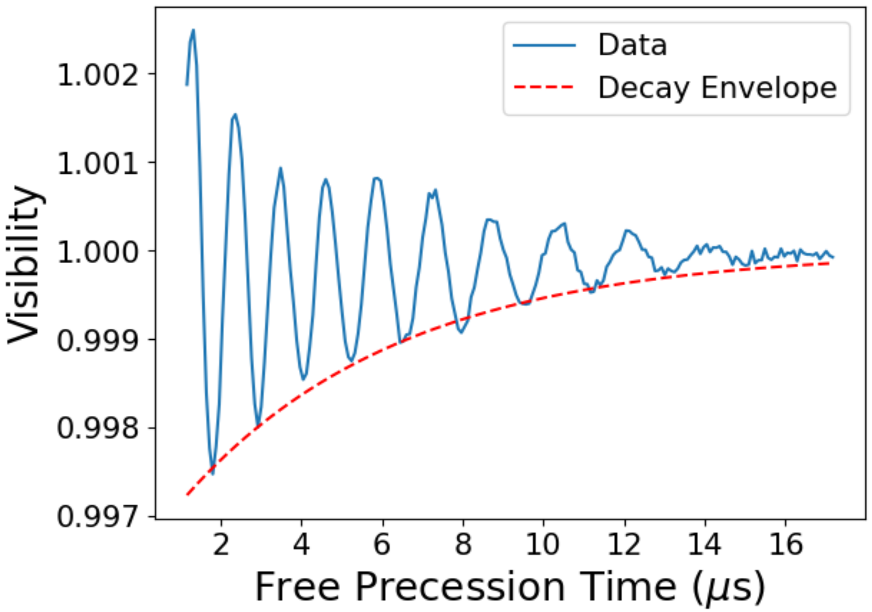
- Currently building 1st gen LS-QDM (9 µm Gaussian light sheet, ~100 μm^2 FoV)
- Technical challenges:
  - LS alignment in diamond (due to high refractive index)
  - Making a robust MW waveguide with LS-compatible geometry
- Goals for 2025:
  - Demonstrate strain sensitivity
  - Image neutron-irradiated sample

Preliminary LS-QDM quantum measurements

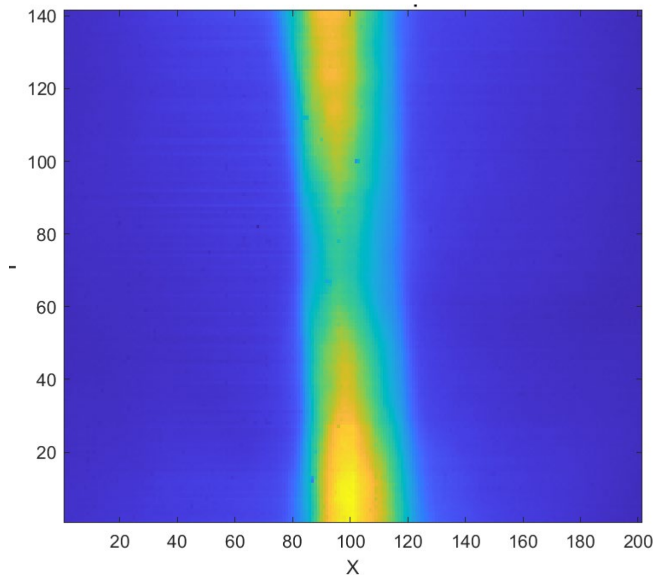
Rabi driving



Strain-CPMG protocol



Rabi oscillation amplitude (TIRF illumination)

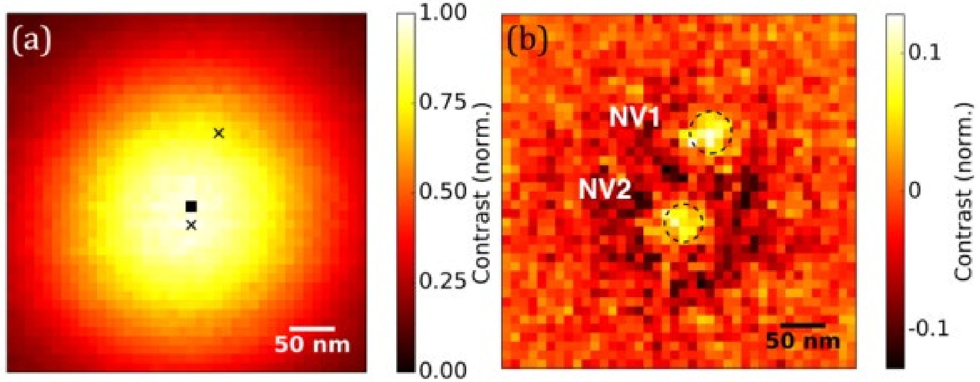


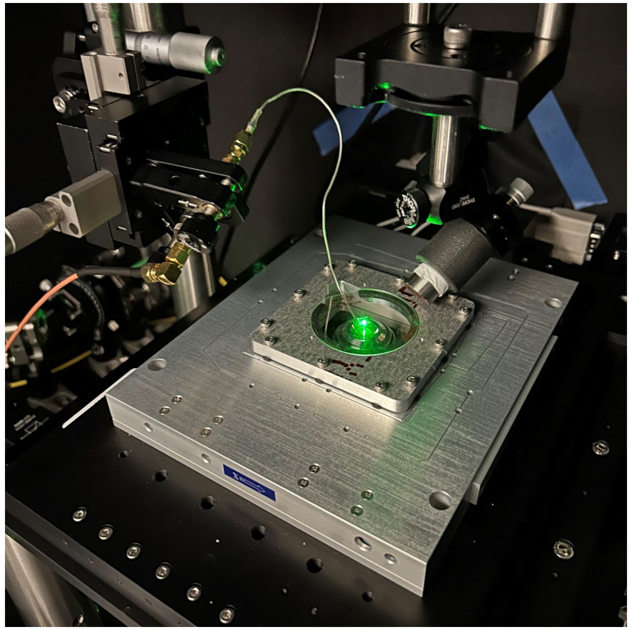
Longer term outlook: aim to be able to determine location of a damage track to 1 µm within <1 week

- Improve to 1 µm light sheet (will likely require non-Gaussian beam)
- Redesign MW delivery

Nanoscale imaging

- Need to find and image track within 1 μm^3 volume with nm-scale precision
- Possible: X-ray diffraction imaging
  - 2022: performed diamond strain studies at sufficient sensitivity @ ANL
- **NV super-resolution spectroscopy techniques**
  - Spin-RESOLFT: utilize doughnut laser beam to only retain NV spin information at the center of the beam
  - Fourier sensing: nanoscale addressing and sensing of NVs with strong magnetic field gradients
- Currently building a new confocal setup to explore these techniques

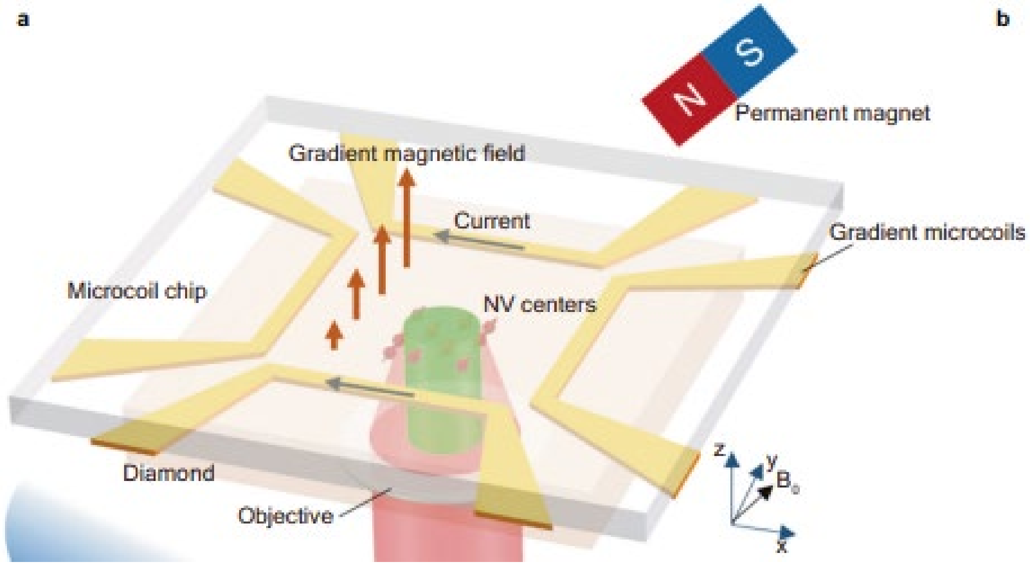


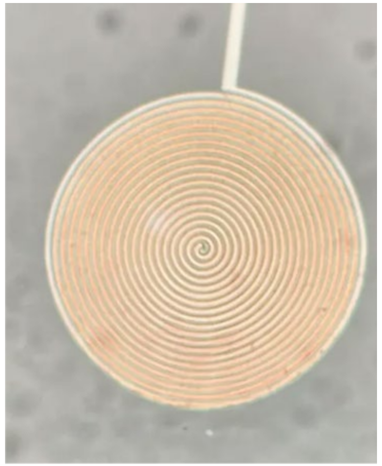


Marshall et al., PR Applied 16, 054032 (2021)
Jaskula et al., Opt. Express 25, 11048 (2017)
Arai et al., Nat. Nano. 10, 859–864 (2015)
Zhang et al., NPJ Quantum 3:31 (2017)

Fourier nanoscale imaging

- Previous experimental demonstrations primarily along XY
  - Amawi et al. (2024): 3D imaging with <10 nm axial resolution only to a depth of 6 µm
- Practical track detection also requires imaging at depth (along Z)
  - Cutting and etching could be used to relax depth requirements
- Aiming to produce 1-10 G/µm gradients (based on expected T_2)
- Collaborating with LPS (UMD) to design and fabricate microcoils on diamond





Spiral Z coil design

Arai et al., Nat. Nano. 10, 859–864 (2015)
Zhang et al., NPJ Quantum 3:31 (2017)
Amawi et al., NPJ Quantum 10:16 (2024)
Guo et al., NPJ Quantum 10:24 (2024)

Summary and conclusion

- Diamond has exciting potential for mineral track detection
  - Directional WIMP DM detection with synthetic diamonds (enhanced with NV quantum sensing)
  - Paleodetection with natural diamonds
- Substantial recent progress in studies of track formation and detection in diamond
  - Computational studies of track formation (BCA, MD, KMC)
  - Artificial damage track studies: observed ~1 MeV NV tracks in nitrogen-rich diamond
  - Microscale imaging: building LS-QDM for 3D quantum strain sensing
  - Nanoscale imaging: building new confocal for NV super-resolution imaging
- Many exciting opportunities for mutual collaboration in all the above

UMD Dark Matter team

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Other collaborators (past and present)

- Emilie LaVoie-Ingram, Kai Sun, Kathryn Ream (Josh Spitz group @ Michigan)
- Michael Titze, Ed Bielejec (Sandia)
- Shannon Hoogerheide, Hans Mumm (NIST)
- Tanguy Terlier, Juehang Qin (Rice)
- Nigel Marks (Curtin Univ.)
- Surjeet Rajendran, Reza Ebadi (JHU)
- Johannes Cremer, Mason Marshall, Mark Ku, David Phillips, Pauli Kehayias (Harvard)
- Martin Holt, Nazar Delegan, F. Joseph Heremans (Argonne)
- Arianna Gleason (SLAC)

Graduate students:

Jiashen Tang

Mason Camp

Max Shen

Gavishta Liyanage

Andrew Gilpin
(undergrad)

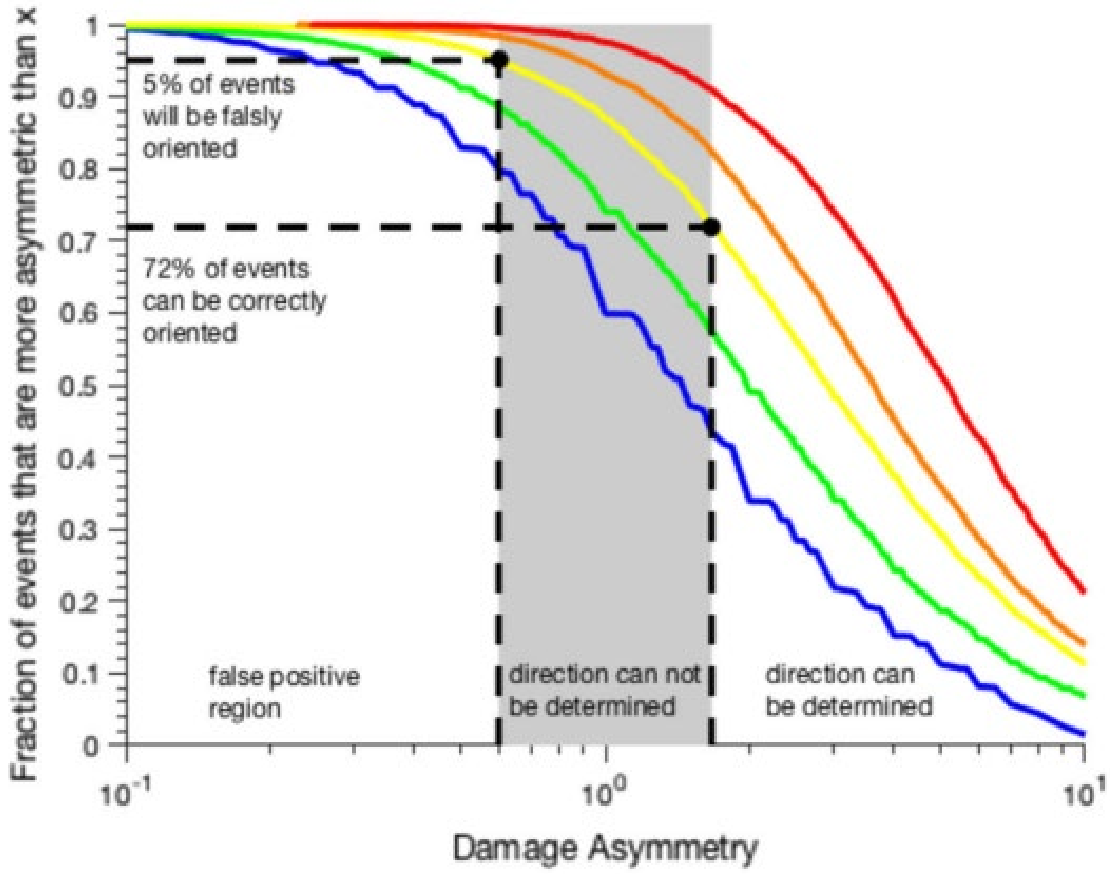
Funding:

- Argonne National Lab
- Department of Energy
- Army Research Laboratory
- UMD QTC and Clark School of Engineering

Thank you for your attention!

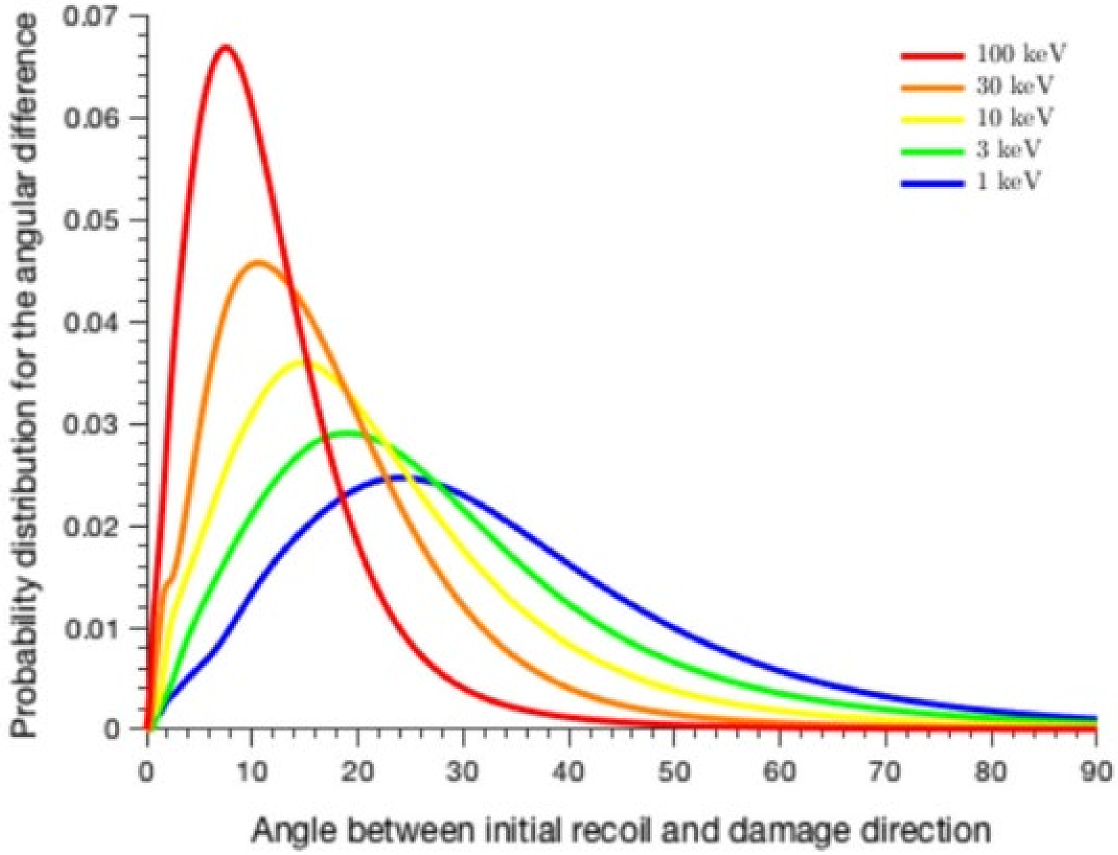
Estimated directional performance

Based on SRIM simulations



Head/tail identification

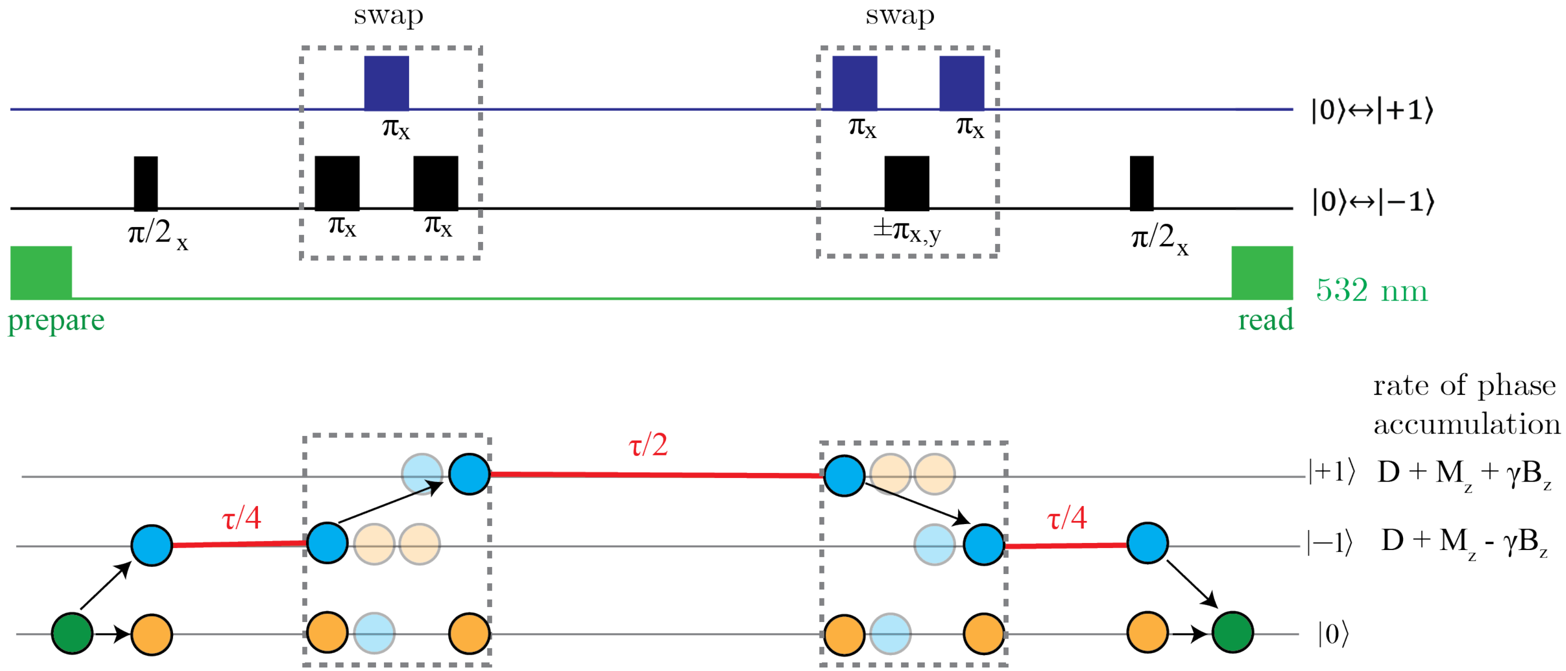
Angular difference to initial recoil



Rajendran et al., PRD **9**, 035009 (2017)

Strain CPMG pulse protocol

- By spending equal time in $|\pm 1\rangle$ states, B_z term is cancelled out
- Need to ensure temperature is constant



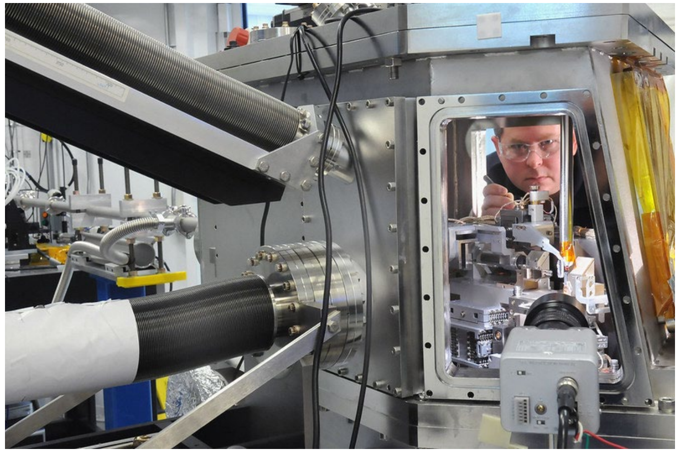
$$H = (D + M_z)S_z^2 + \gamma B_z S_z$$

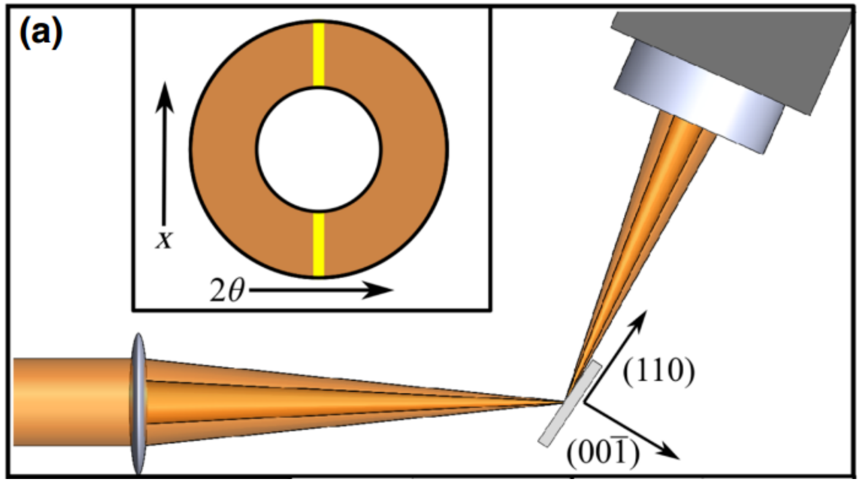
$$M_z = A_1 \epsilon_{zz} + A_2(\epsilon_{xx} + \epsilon_{yy})$$

M. Marshall et al., PR Applied **17**, 02401 (2022)

Nanoscale X-ray imaging

- Scanning X-ray diffraction microscopy @ ANL Hard X-Ray Nanoprobe
- X-ray beam focused to ~10 nm spot
- Detect Bragg diffraction pattern which encodes local crystal structure
- Extract strain by comparing readings from nearby positions in the sample
- Scans at different sample angles allow for 3D reconstruction
- $\sim 1.6 \times 10^{-4}$ strain sensitivity
  - 10 keV WIMP expected to produce similar strain levels

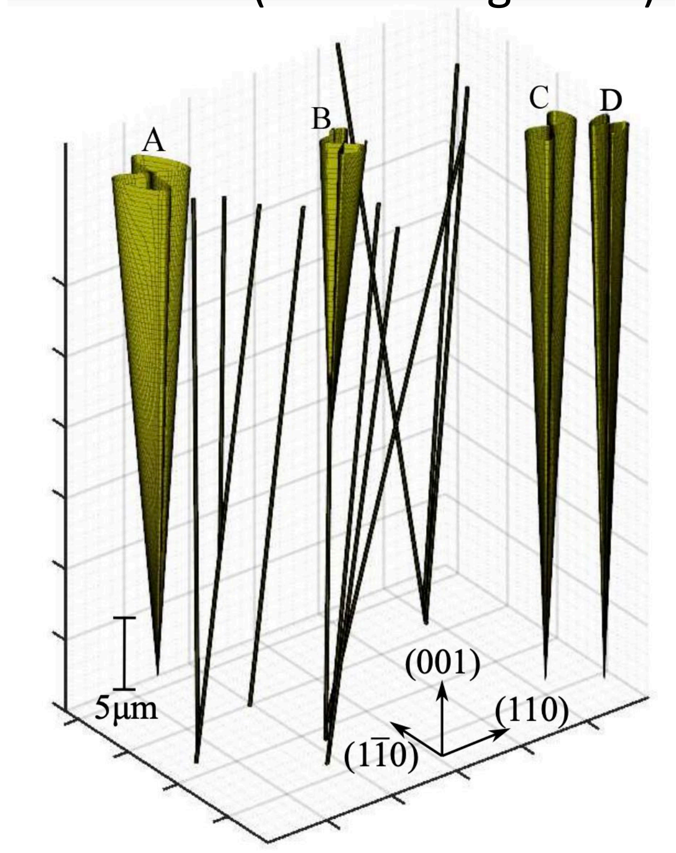


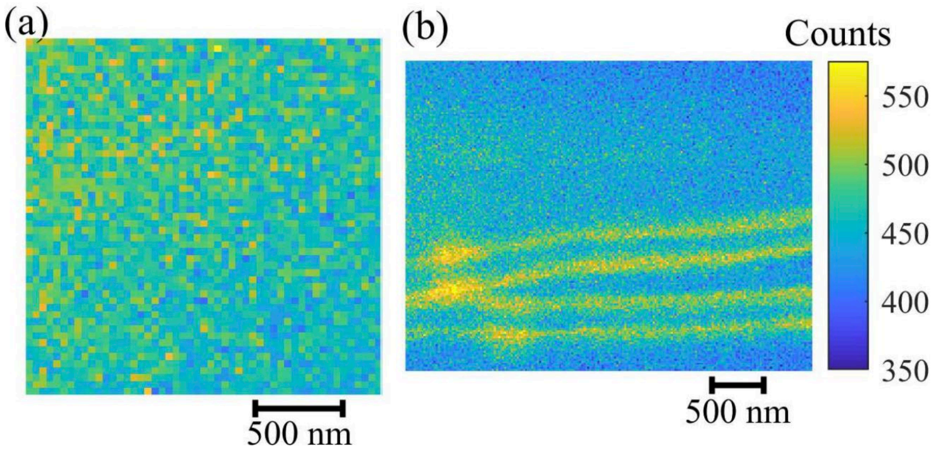


Marshall et al., PR Applied **16**, 054032 (2021)

- Low strain regions exhibit no natural features that could be mistaken for WIMP damage tracks
- Future: repeat SXDM scans with implanted samples
- Con:
    - Only a few SXDM facilities available in the world
    - Danger of sample contamination during transport

3D reconstruction of pre-existing strain features (from CVD growth)





Low strain regions

Marshall et al., PR Applied **16**, 054032 (2021)