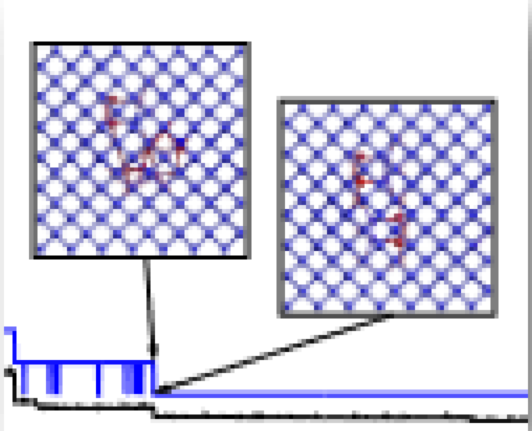
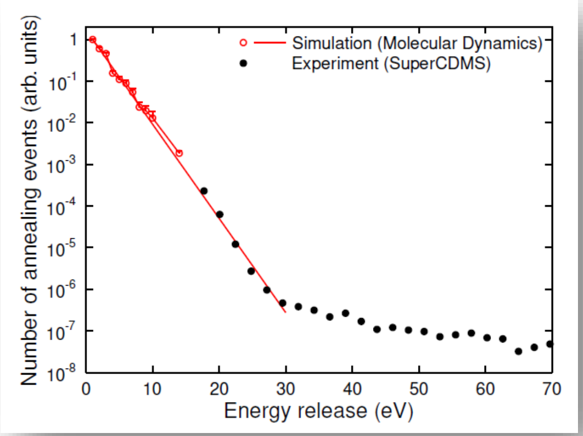
Energy release from recrystallization of amorphous pockets and low-energy excess signals





Kai Nordlund, Fanhao Kong, Flyura Djurabekova, Matti Heikinheimo, and Kimmo Tuominen

Department of Physics,
University of Helsinki, Finland

Nader Mirabolfathi

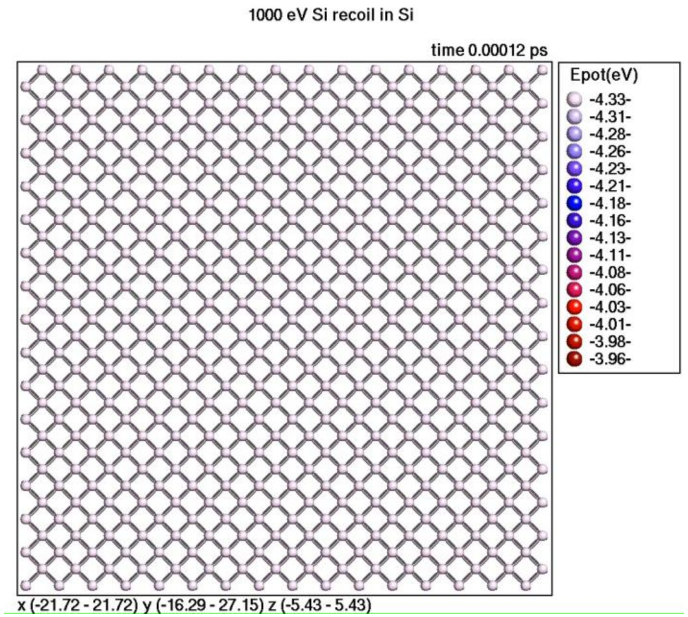
Texas A&M University, USA

Contents

- Radiation damage in semiconductors: a very brief overview
- Results
  - Damage recombination at ns times after a cascade
  - Energy release spectrum of events
  - Avalanche mechanism of annealing
  - Time scale of annealing events at cryogenic temperatures
- Conclusion

Radiation damage in semiconductors: it is not Frenkel pairs

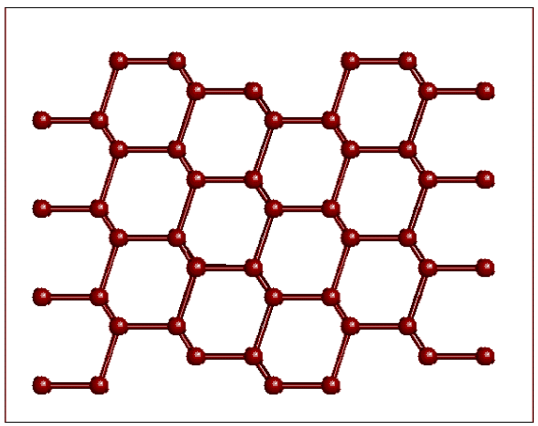
- We have studied damage in a wide range of metals, semiconductors and ionic material over the last 30 years
- For semiconductors, key message: primary damage is practically never simple Frenkel pairs (vacancies and interstitials)

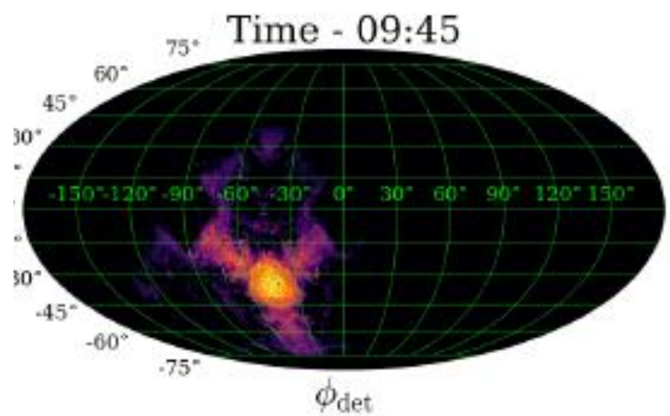


[K. Nordlund *et al*, Phys. Rev. B 57, 7556 (1998); K. Nordlund *et al,* J. Nucl. Mater. 512, 450 (2018)]

Our previous works on relation of defects and dark matter

- We have previously shown that DM interactions with a single crystalline detector of known orientation may lead to a distinct daily variation in DM observations

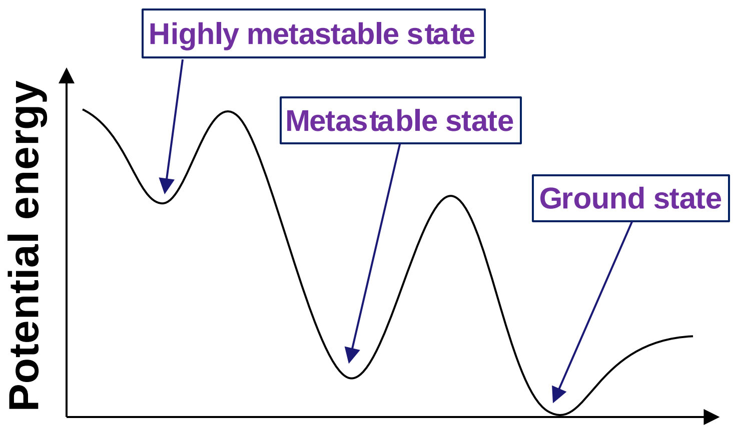


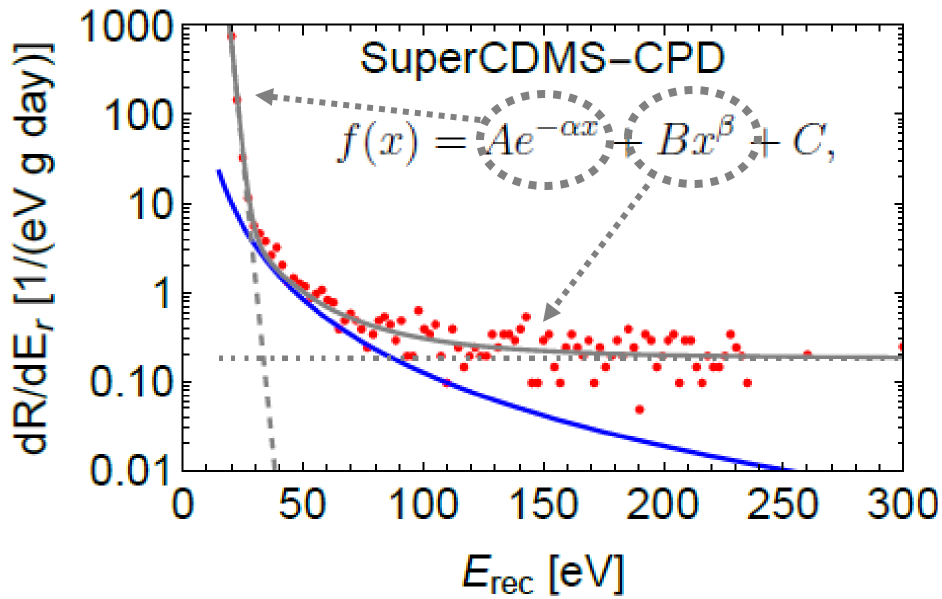


[F. Kadribasic et al,, Phys. Rev. Lett. 120, 111301 (2018); F. Kadribasic et al, Journal of Low Temperature Physics 5-6, 1146 (2018); M. Heikinheimo et al,, Phys. Rev. D 99, 103018 (2019); S. Sassi et al, Phys. Rev. D 104, 063307 (2021); S. Sassi et al, Phys. Rev. D. 106 (2022) 083009 M. Heikinheimo et a, Phys. Rev. D 106 (2022) 083009]

Recent observations: low-energy excess and defects in solids??

- Defects produced by radiation or other means store energy in solids
  - Could the DM excess signal be somehow related to this?





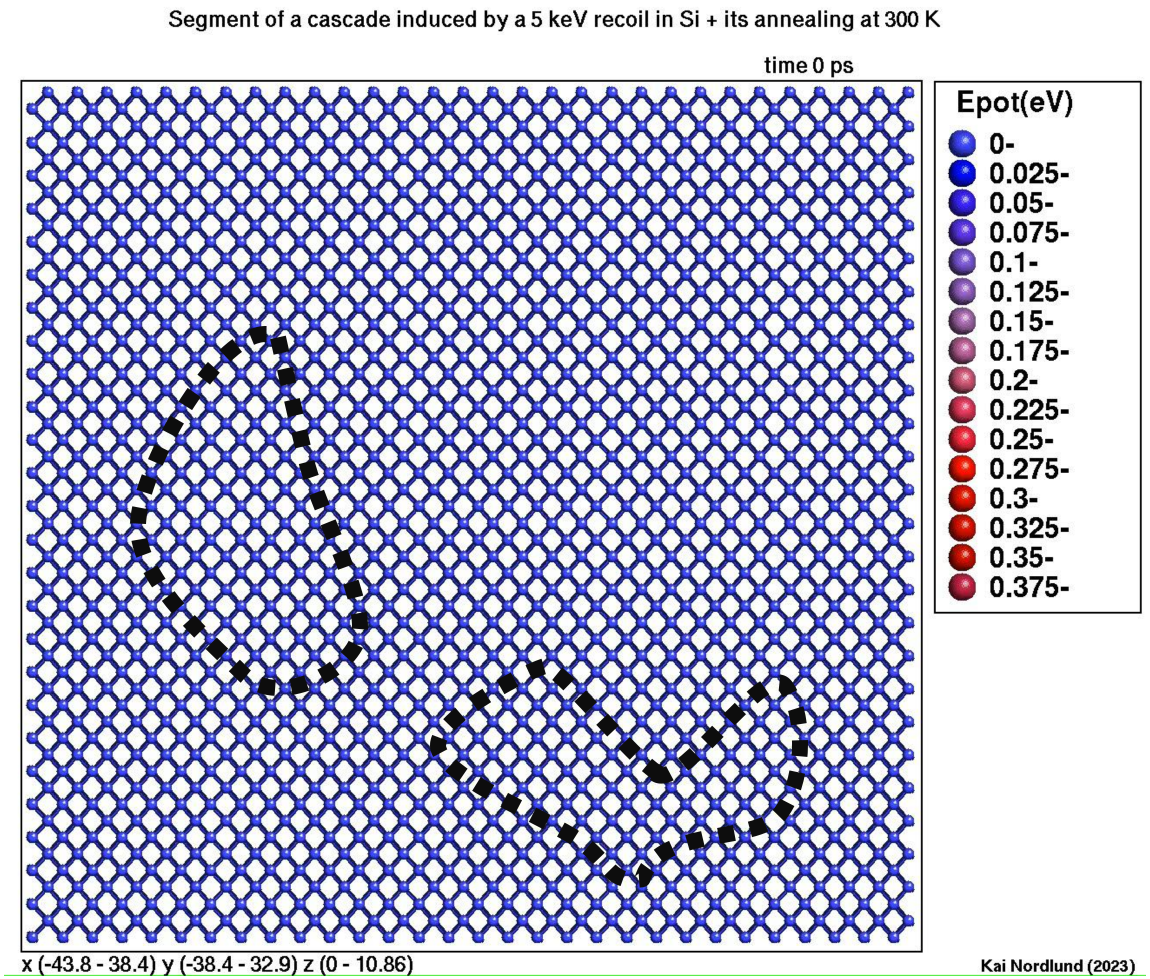
[M. Heikinheimo et al, Phys. Rev. D **106**, 083009 (2022)]

Our hypothesis to be tested

- Could recombination of damage induced by radioactive impurities in the materials or surroundings be a source of energy release
  - Decay of radioactive impurity isotopes are a known source of background signal in detectors
  - Radioactive impurities are practically impossible to avoid
  - Could there be a delayed signal from the damage production?
- We set out to test this systematically, using our best understood material Si as a basis

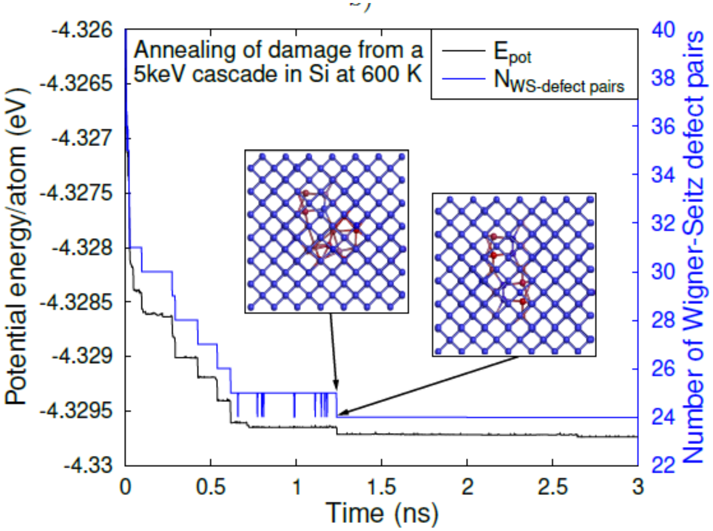
Annealing simulations, example animation

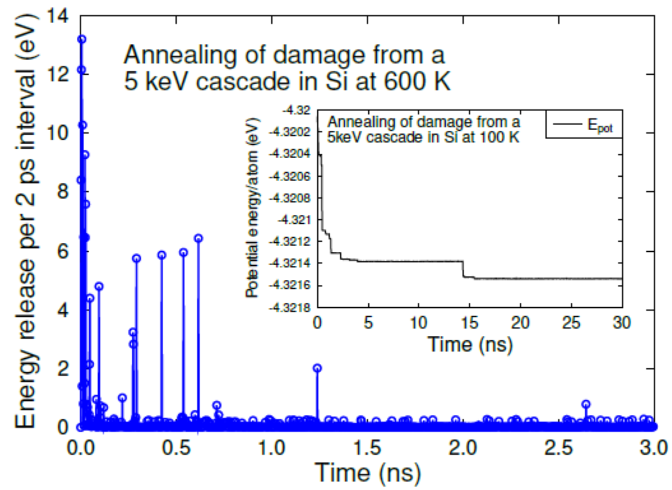
- Cascade + its annealing at 300 K for 3 ns
  - Extent of damage after cascade shown with dashed lines
- Major annealing observed in the time intervals
  - 20-30 ps
  - 50-60 ps
  - 200-300 ps
  - 900 ps – 1 ns



Systematic analysis of annealing energy release

- The annealing runs were systematically analyzed for number of defects and potential energy
- The results show rapid annealing within first ~ 100 ps from damage event, but after that continued intermittent annealing events for as long the simulations were ran – up to 100 ns

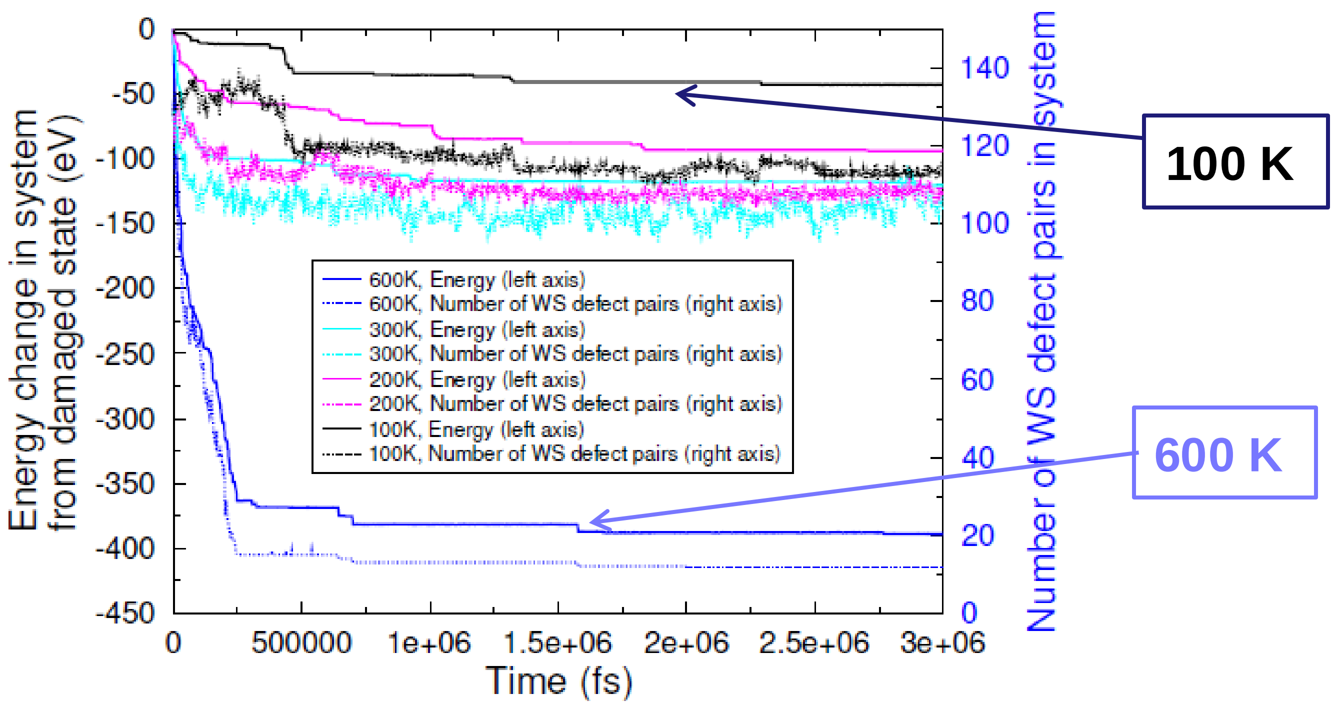




c)

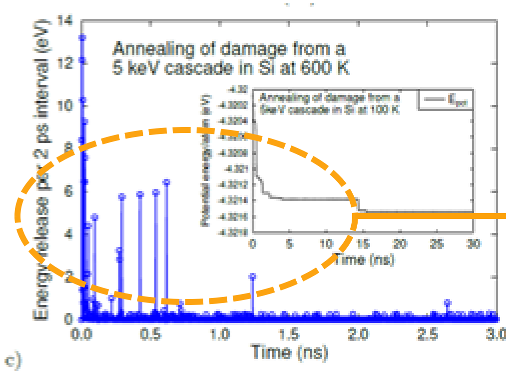
Temperature dependence

- At 600 K such annealing as been reported many times before
- What was surprising was that similar annealing events were observed even at 100 K and below!

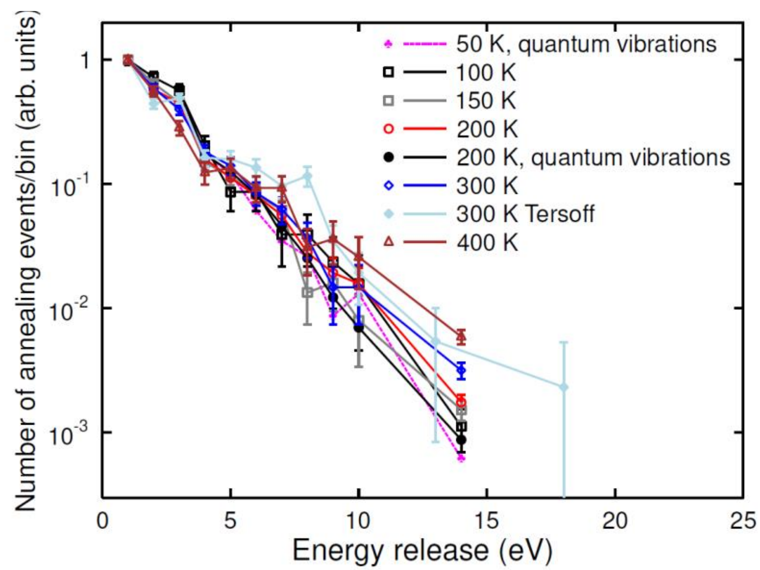


Statistics of energy release

- Taking the energy release peaks from all the independent annealing+quenching runs, one can get a statistical distribution of the energy release
  - Remarkably, the slope almost independent of temperature
  - Slope also remains the same when the quantum mechanical zero point vibrations are taken into account

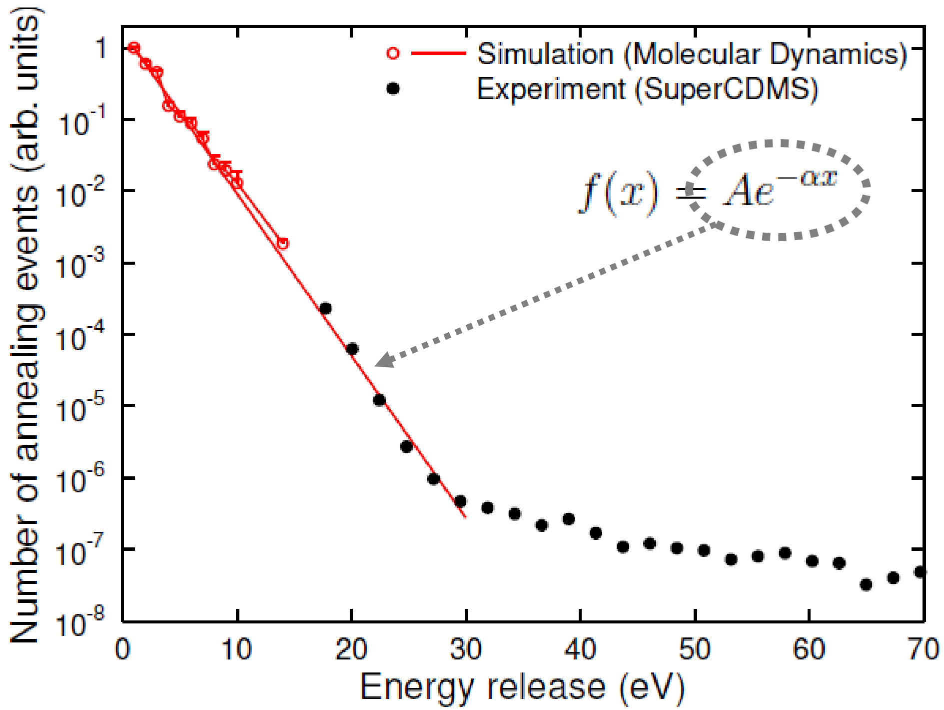


50-5000 runs



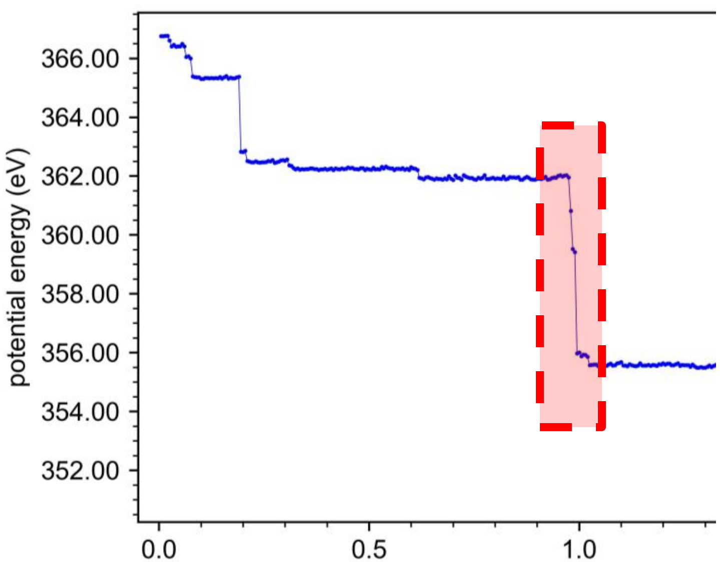
Statistics of energy release: comparison with experiments

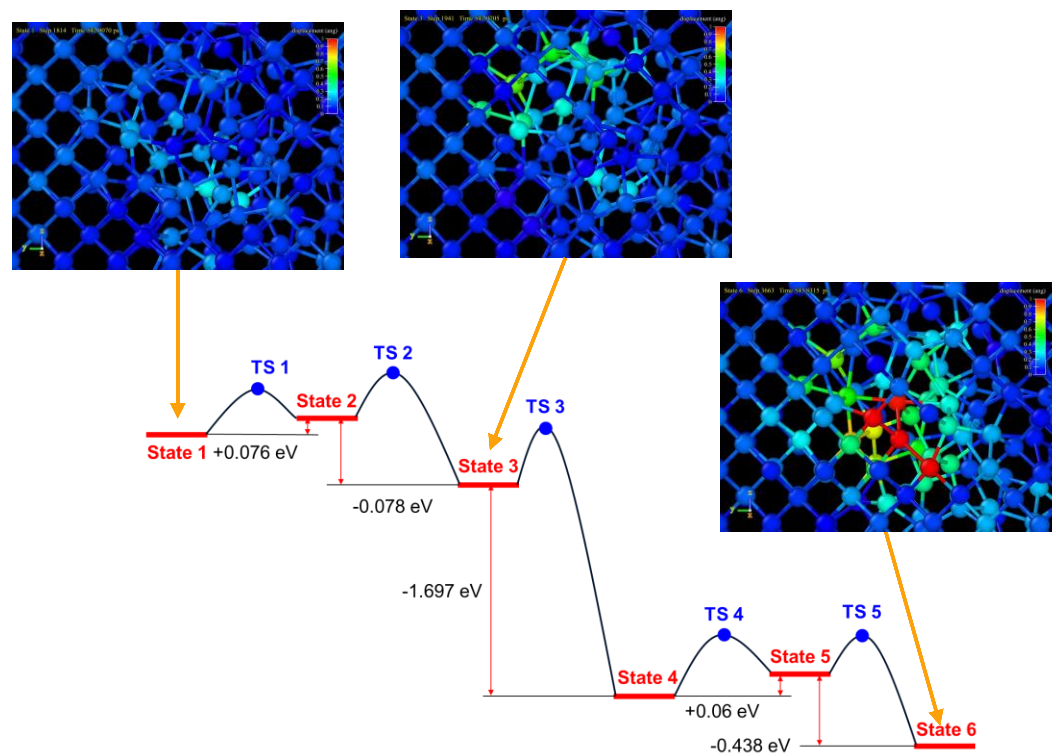
- This data can be compared directly with the experimental low-energy excess exponential tail
  - Outstanding agreement!



Why is the statistics of energy release independent of temperature?

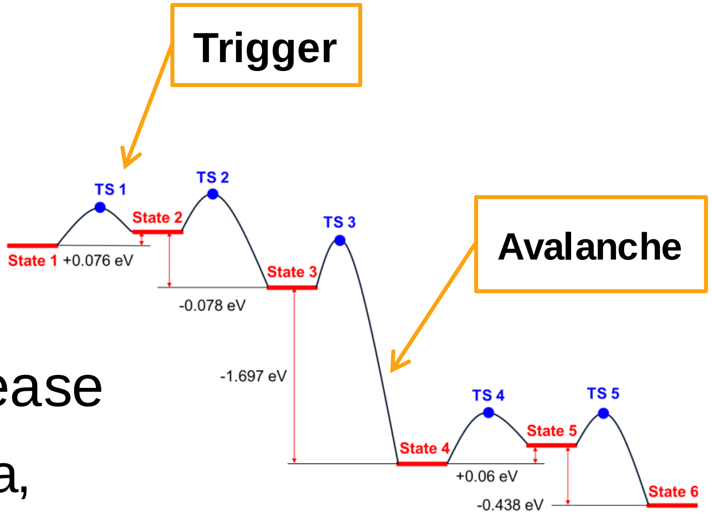
- To understand why the energy release has practically no dependence on temperature, we analyzed in detail some individual recombination events
  - Atoms plotted with displacement color scale





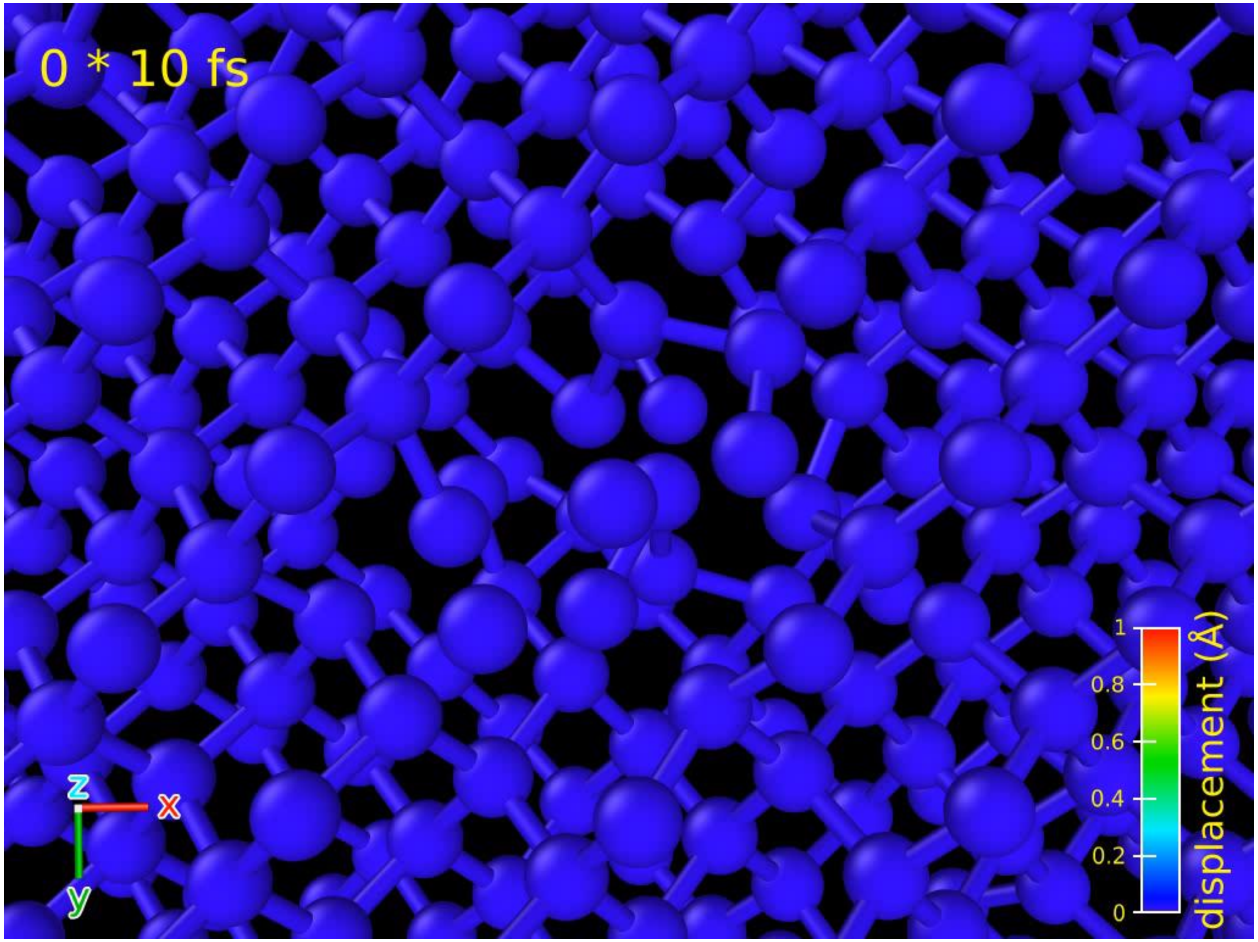
A recombination avalanche

- We observed that the large energy release events are always at low-temperatures preceded by crossing a very small (~ 0.1 eV) barrier
- This initial small rearrangement of atoms slightly heats up the immediate surroundings, which can **trigger** a much larger atom rearrangement and hence energy release
  - This is analogous to critical phenomena, such as avalanches in sand piles or snow



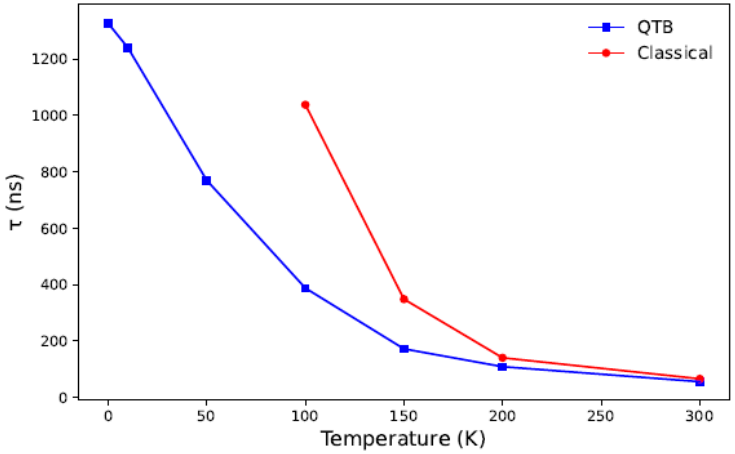
- We hence call this a “recombination avalanche” effect
  - Such events are observed up to the maximum simulation time of 30 ns – no reason there would be an upper time limit

Animation of recombination avalanche



Timescale of events

- In purely classical molecular dynamics, the rate of energy release does slow down with temperature
- At the cryogenic detector temperature of 0.04 K, the rate would be astronomically high (pun intended)
- However, taking into account quantum vibrations, we observe annealing effects even at 0.05 K with a decay time constant of the order of microseconds
  - If the **entire macroscopic** detector e.g. undergoes a radioactive decay **anywhere** at rates < 1 event/microsecond, this predicts a roughly constant signal if the time resolution of the detectors is above microseconds

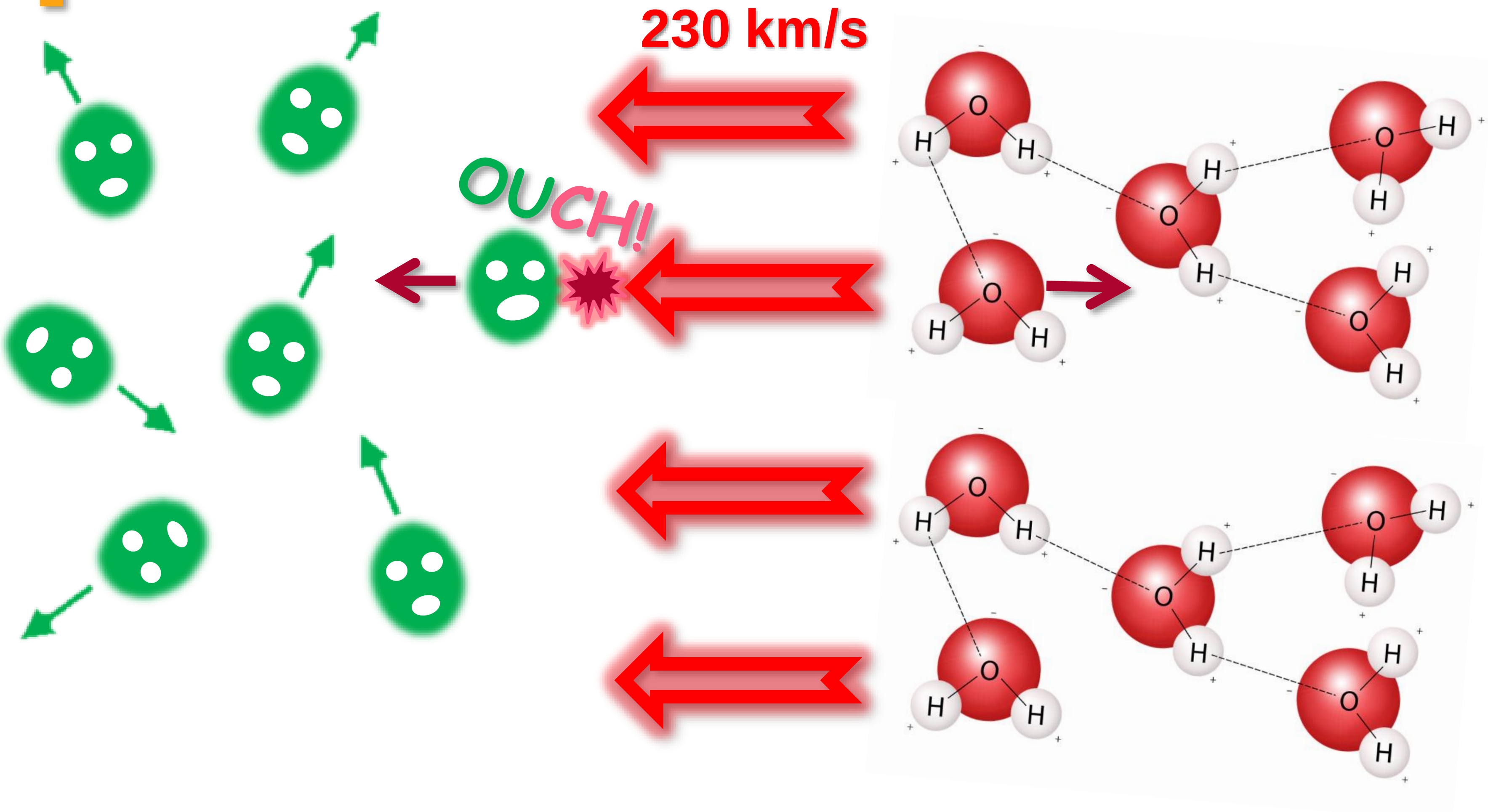


Conclusion

- Energy release from defects in Si follow a very similar exponential energy dependence as the experimentally observed “low-energy excess” in semiconductor detectors
  - Defects could be induced by radiactive impurities or possibly also be associated with cracks or other inherent defects
- The energy release is almost independent of temperature due to a “recombination avalanche” effect
- Outlook: nanocalorimetry and/or pulsed ion beam experiments could be used to confirm the effect?

Backup slides

Actually: we are the energetic particles hitting the dark matter!



Kinetic energy transfer from dark matter to ordinary atom nucleus

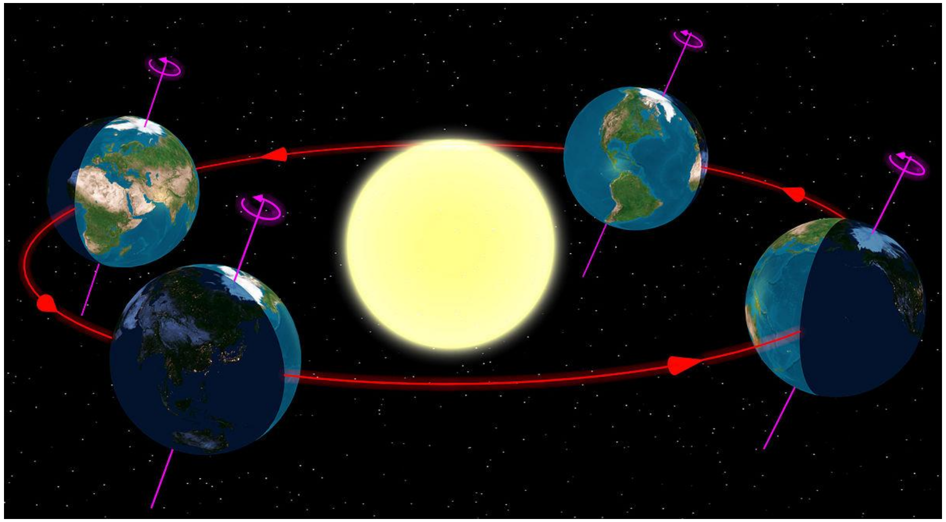
- Estimation of order of magnitude of energy transfer:
- **Assume** dark matter particle of mass m_1= 1 GeV/c^2
- 220 km/s corresponds to E_{DM} = 269 eV
  - A typical low-energy ion gun energy!
  - From DM density of ~ 1 GeV/cm^3 given by astronomical models, we can deduce our bodies pass **through 30 billion DM particles per second.**
- Then we can calculate the energy transfer in a head on collision from basic kinematics to a Si atom (m_2=28 u):

$$T = \frac{4m_1m_2}{(m_1+m_2)^2}E_{DM} = 38\ \text{eV}$$

- This is in the range of threshold displacement energies in Si!

Relative movement effects

- The motion of the sun around the galaxy would give a constant level of recoil energies to ordinary matter from the “WIMP wind”
  - This would be difficult to distinguish from any number of regular background radiation sources
- However, any position on earth rotates around its axis
  - This should give a daily variation in the signal if measured **in a direction sensitive way** from a crystal fixed on earth
- Moreover: the earth rotates around the sun at 30 km/s
  - This should give an annual variation in the signal in a given direction



[Fig: wikipedia]

Key idea: utilize the threshold displacement energy in detection

- In case it so happens that the energy transfer from dark matter to ordinary matter is **around the threshold displacement energy**, then:
  - If you make a single-crystal highly sensitive detector, and fix it on earth, the dark matter detection signal should vary daily!
    - Simplified argument: if the relative motion of the detector w.r.t. the dark matter background is in a direction such that the energy transfer is just below the threshold, no signal, above: clear signal
  - In reality if is of course a convolution of the kinetic energy distribution of dark matter itself, the movement of the earth and the threshold displacement energy surface

Our work: systematic analysis of effect

- Formulate a way to calculate transfer of dark matter particles to ordinary ones
- 1. Distribution of dark matter particle velocities (with galactic escape velocity truncation) in galaxy

$$f_{\rm gal}(\mathbf{v}) = \begin{cases} \frac{1}{N_{\rm esc}(2\pi\sigma_v^2)^{3/2}} \exp\left[-\frac{\mathbf{v}^2}{2\sigma_v^2}\right] & \text{if } |\mathbf{v}| < v_{\rm esc} \\ 0 & \text{if } |\mathbf{v}| \geq v_{\rm esc} \end{cases}$$

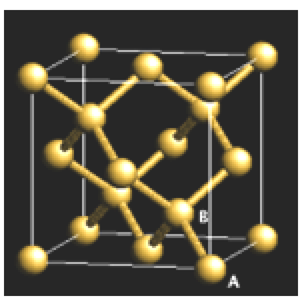
- 2. Radon transform to get to lab coordinates on Earth from motion and rotation of Earth, and movement of solar system around the galaxy

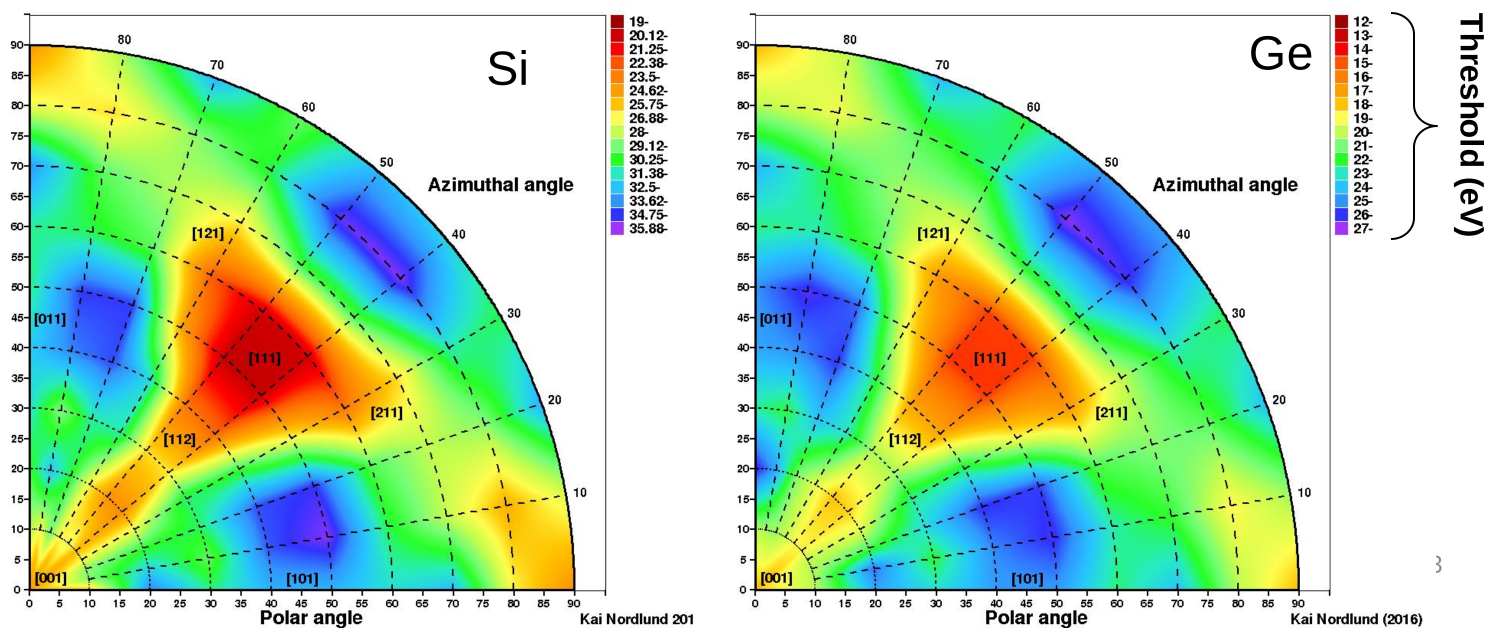
$$\hat{f}_{\rm lab}(v_{\rm min}, \hat{\boldsymbol{q}}; t) = \frac{1}{N_{\rm esc}\sqrt{2\pi\sigma_\nu^2}} \times \left[\exp\left(-\frac{|v_{\rm min} + \hat{\boldsymbol{q}} \cdot \boldsymbol{v}_{\rm lab}|^2}{2\sigma_\nu^2}\right) - \exp\left(-\frac{v_{\rm esc}^2}{2\sigma_\nu^2}\right)\right]$$

[F. Kadribasic, N. Mirabolfathi, K. Nordlund, A. E. Sand, E. Holmström, and F. Djurabekova, Phys. Rev. Lett. **120**, 111301 (2018)]

Our work: full 3D surface from classical potentials

- We used the DFT results to find which classical interatomic potentials are closest to them
  - For Si original Stillinger-Weber potential, for Ge Stillinger-Weber potential modified by Nordlund in 1998
- Then systematic simulations of 85 000 directions in Ge, 24 000 in Si and 5000 in diamond. Results:

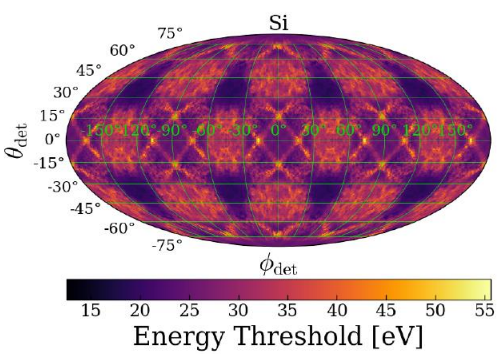


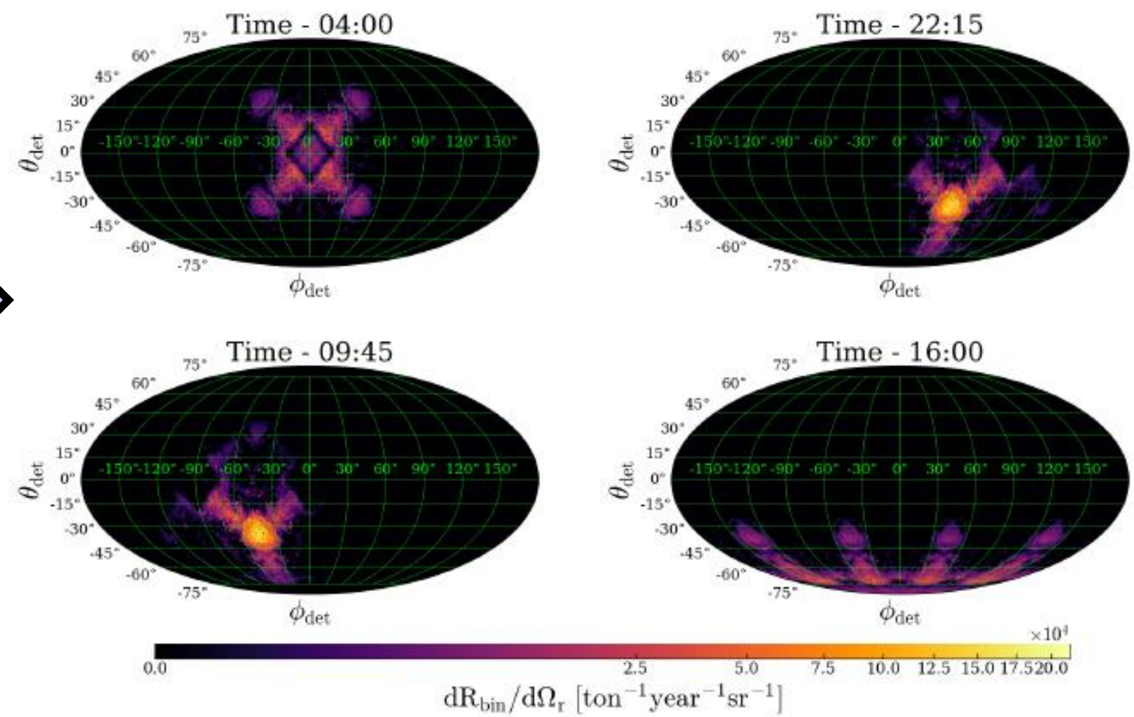


From threshold to signal

- A computer code implementing the numerical convolution integrals 1-4 then allows predicting the dark matter signal for a given (assumed) mass
  - Note major differences per time of day

Same Si data in Mollweide plot





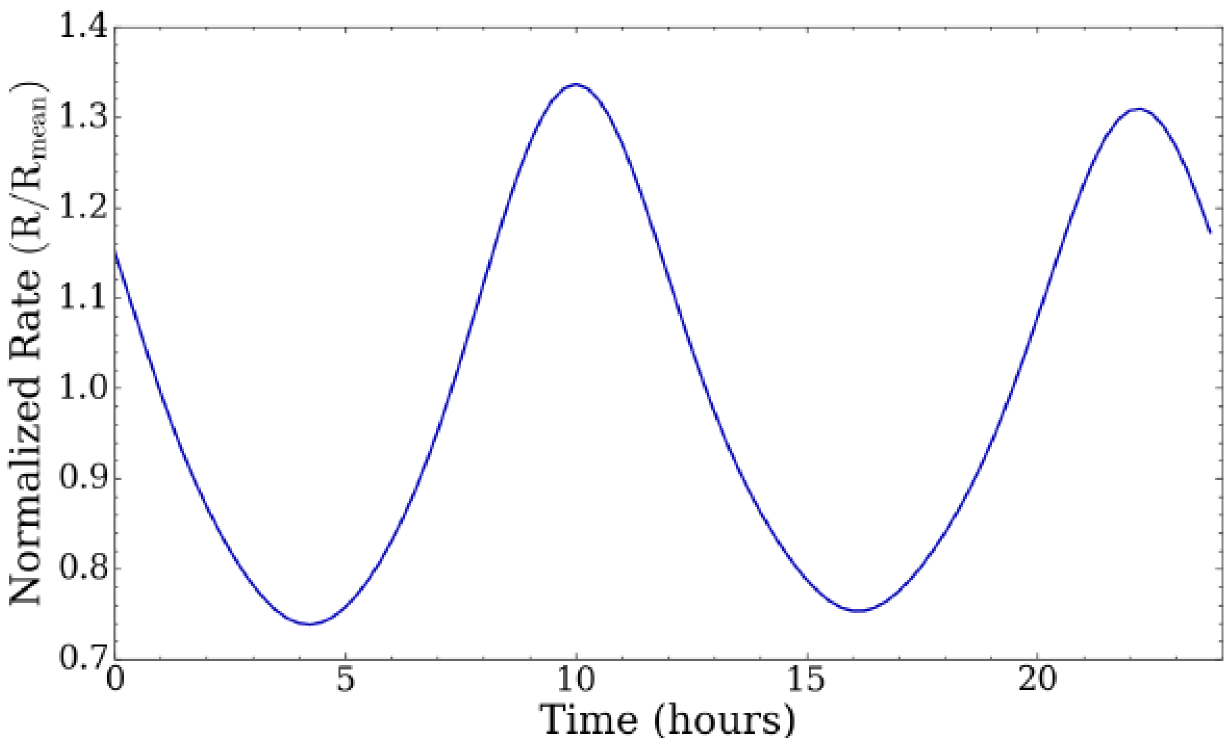
HELSINGIN YLIOPISTO
HELSINGFORS UNIVERSITET
UNIVERSITY OF HELSINKI

Faculty of Science
Department of Physics
Prof. Kai Nordlund

[F. Kadribasic, N. Mirabolfathi, K. Nordlund, A. E. Sand, E. Holmström, and F. Djurabekova, Phys. Rev. Lett. **120**, 111301 (2018)]

Daily variation

- Example for 300 MeV/c^2 dark matter particle



[F. Kadribasic, N. Mirabolfathi, K. Nordlund, A. E. Sand, E. Holmström, and F. Djurabekova, Phys. Rev. Lett. **120**, 111301 (2018)]

Conclusion

- **If:**
  - Dark matter exists
  - It is composed of particles
  - The particles interact with ordinary matter with other means except gravity
  - The interaction follows Newton's law of momentum transfer
  - The interaction cross section is large enough
  - The dark matter particle mass is roughly in the 100 MeV/c^2 to 10 GeV/c^2 range
  - The detector can actually be built
  - **Then:** the approach we developed should be able to detect dark matter, and distinguish it from other particles thanks to a distinct diurnal variation
  - **Else:** even if dark matter is never detected, **the detectors developed are incredible and will certainly be useful for other purposes!**

Probability??

- 99%
- 99%
- 1%
- 99%
- 1%
- 4%
- 99%

$= 4x10^{-6}$

[F. Kadribasic et al,, Phys. Rev. Lett. 120, 111301 (2018); F. Kadribasic et al, Journal of Low Temperature Physics 5-6, 1146 (2018); M. Heikinheimo et al,, Phys. Rev. D 99, 103018 (2019); S. Sassi et al, Phys. Rev. D 104, 063307 (2021); S. Sassi et al, Phys. Rev. D. 106 (2022) 083009 M. Heikinheimo et a, Phys. Rev. D 106 (2022) 083009]