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Sparse Sampling in Scanning Probe Microscopy

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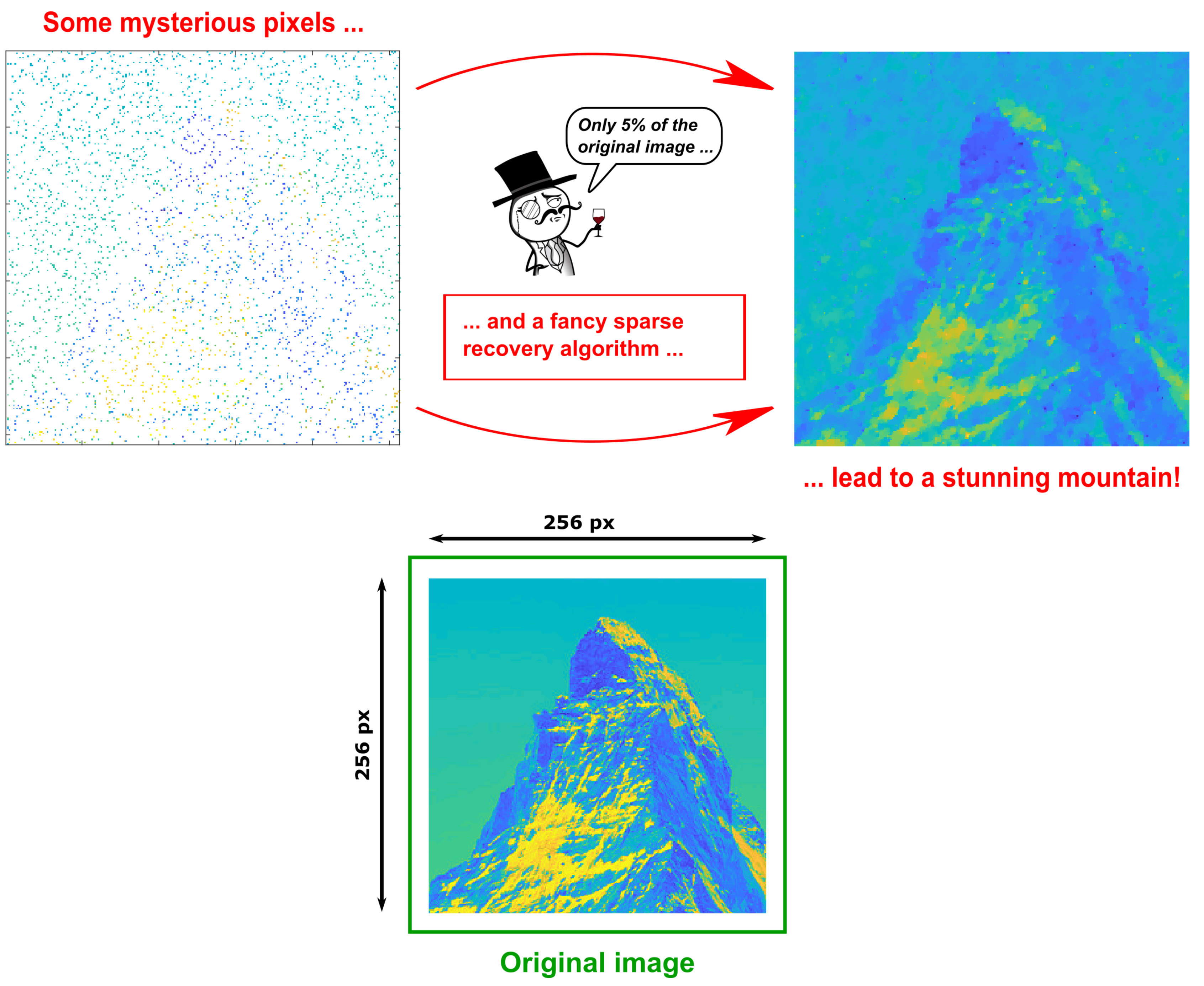

Fig.1: Compressive Sensing (CS) can be used to reconstruct a signal, here a 2D image, by using just a fraction of the total data points. Original image in black-white by Menno Boermans.

Application in Scanning Tunneling Microscopy (STM)

- **Massive decrease in measurement time of Quasi-particle interference (QPI): assuming *5% measurement data* is sufficient for the sparse recovery, a *5-day measurement could be done in about 6 hours* as shown by the method of Oppliger and Natterer [2]**
- **The usage of a pre-calculated near optimal open Traveling Salesman path which connects the random measurement locations leads to a further time reduction**
- **Compressive Sensing in an STM is here achieved by the sparsity of the signal (in this case seen as wave vectors) in Fourier space**
- **The sparse recovery itself has been handled by the large-scale sparse reconstruction algorithm SPGL1 [3]**
- **Robust denoising of the sparse signal recovery includes effects like white noise, drift, creep or a change of the STM tip**

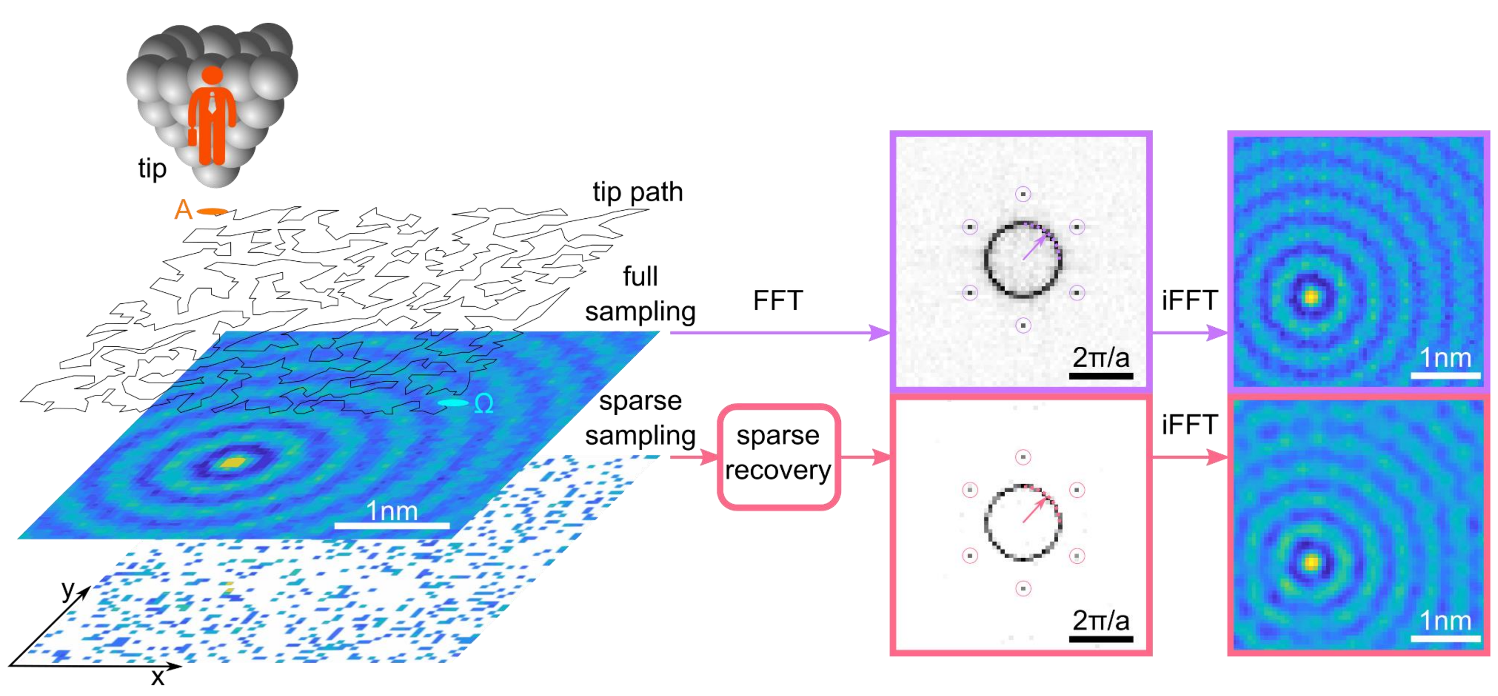

Fig.2: The simulated Cu(111) surface states with underlying FCC atomic structure can be fully recovered by measuring a small fraction of the total Local Density of States (LDOS) (here: 20%) which is represented on a 64x64 pixel grid. The Bragg Peaks are clearly visible and a near optimal tip path is shown for completeness as shown by Oppliger and Natterer [2].

Compressive Sensing: sparse signal reconstruction

- **Representing a signal with $K \ll N$ sparse (non-zero) coefficients in a vector domain where N represents the total signal length**
- **Requires incoherent m measurements with $K \ll m < N$**
- **ℓ_1 minimization subject to $\|Ax - b\|_2 < \sigma$**
- **Random measurement matrix $A \in \mathbb{R}^{m \times N}$: sparse recovery for $m \geq cK\, log(N/m)$ [1]**
- **Achieves sampling rates much lower than stated in the Nyquist theorem**

Random sampling and Informed sampling

- **Informed sampling: sampling the regions near the scattering sites with a higher probability than further away using a Lorentzian line shape**
- **Informed sampling leads to better a reconstruction probability at very low measurement rates as shown by Oppliger and Natterer [2]**
- **"Inverse Informed sampling" can be used to avoid certain regions in order to minimize and exclude the influence of effects which provoke a STM tip-instability like mask point impurities or step-edges**

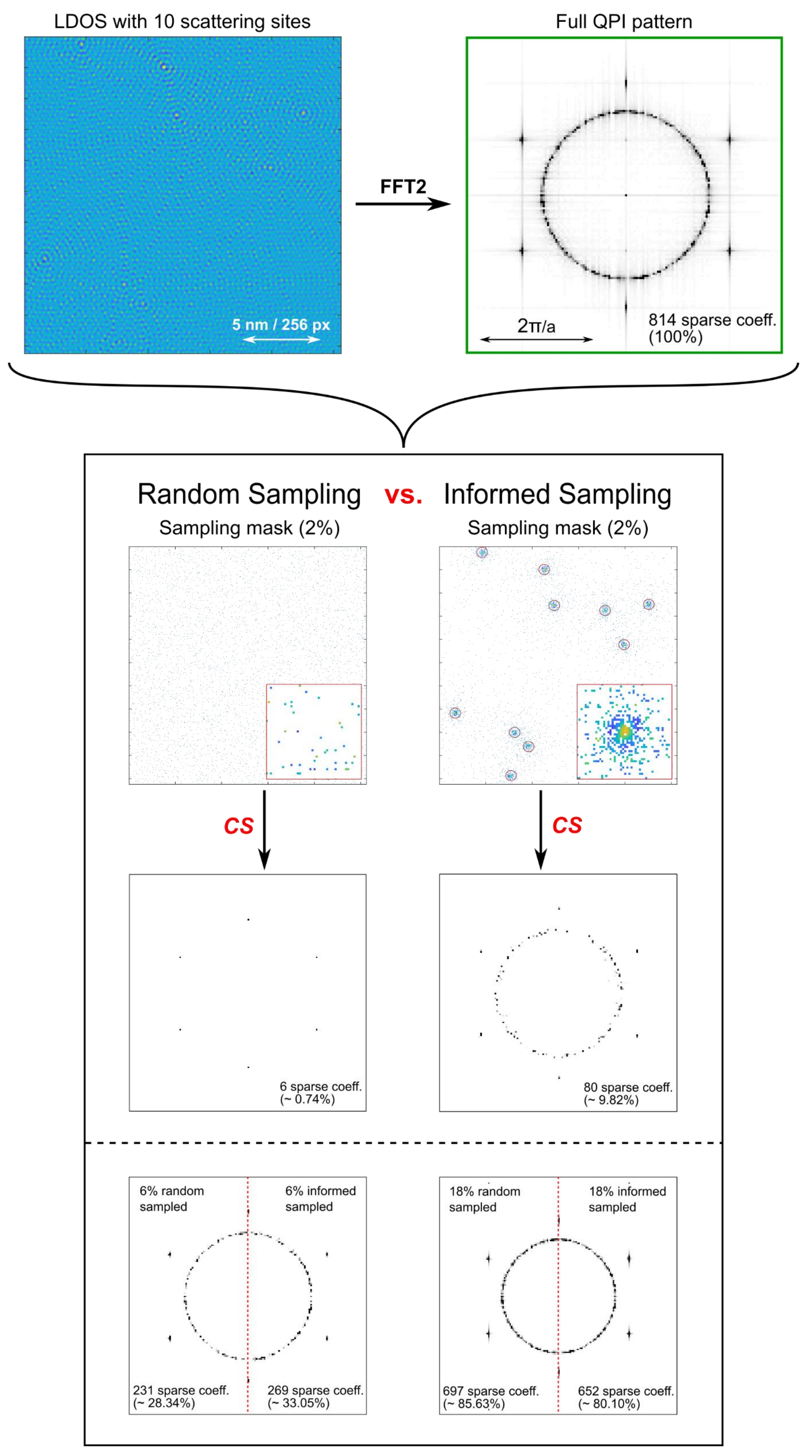

Fig.3: Comparison between two different data sampling approaches on a 1024x1024 pixel grid using the technique of general random sampling and informed sampling by Oppliger and Natterer [2].

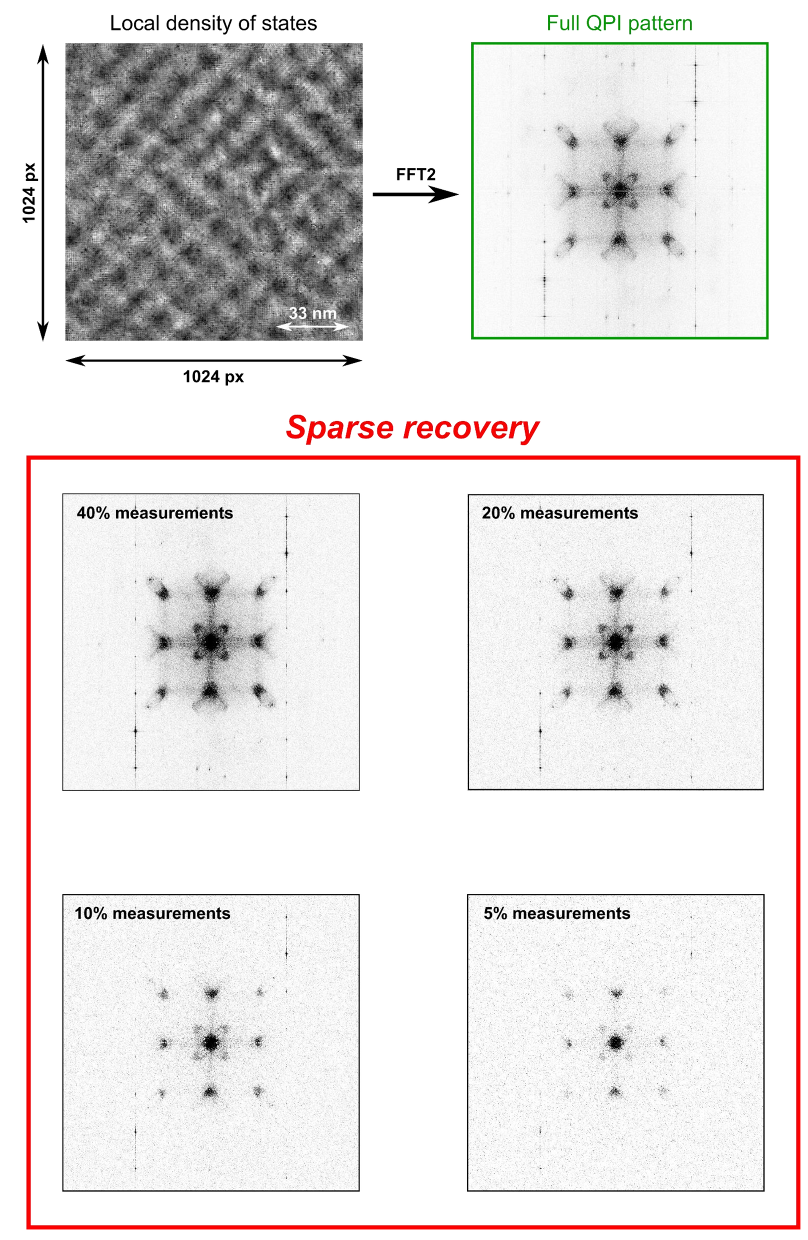

Fig.4: The surface state of a topological insulator made from SnTe at 104 mV represented on a 1024x1024 pixel grid [4] and its corresponding full QPI pattern (by measuring 100% of the data) compared to the sparse recovery of the same by using only a fraction of random measurements.

Conclusion / Outlook

- **Applying compressive sensing in the field of STM quasi-particle interference can be used to massively reduce the time needed to resolve parts of the band structure by using the property of sparse signals and incoherent measurements**
- **The usage of an open Traveling Salesman path can be utilized for further measurement time reduction**
- **Time saving factors of 5 – 50 can be reached which means ...**
  - ✓ **More different LDOS energies can be probed**
  - ✓ **Higher resolution measurements can be recorded to reveal more details in momentum space**
  - ✓ **Less wasted measurements since surface areas with bad artifacts can be skipped without loosing sparse information**

References

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3. Berg, E. van den & Friedlander, M. P. Probing the Pareto frontier for basis pursuit solutions. SIAM J. Sci. Comput. 31, 890–912 (2008)
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4. Original data by I. Zeljkovic et al., Nature Nanotechnology 10, 849 (2015)

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