Towards atom diffraction through graphene

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Knowledge for Tomorrow



From matter wave experiments to microscopy

G.P. Thomson's electron diffraction experiment (1927)



Transmission Electron Microscopy (TEM)



Uni-ulm.de, Zubeltzu et al, Phys. Rev. B 88, 245407 (2013)

From matter wave experiments to microscopy

T.H. Johnson's hydrogen diffraction experiment (1930)



Scanning Helium Microscopy





M. Bergin PhD thesis University of Cambridge (2018)

Atom transmission through 2D Material



2D Material of Choice: Graphene

- Robust
- Commercially available
- Interesting for numerous applications
- Small lattice spacing: 246 pm

Window for atom transmission through graphene:

- Energy above potential barrier For hydrogen: E > 3.75 eV, v > 27 000 m/s
- Energy below sputtering threshold For hydrogen: E < 80 eV, v < 121 000 m/s

$$\lambda_{dB} = \frac{h}{\sqrt{2mE}} = 3.2 - 14.7 \, pm$$

Brand et al., New J. Phys. 21 033004 (2019)



Atom transmission through graphene

Coherent transmission



Results of ab initio calculations of molecular dynamics within the Born-Oppenheimer approximation



Brand et al., New J. Phys. 21 033004 (2019)

Experimental principle



Brand et al., New J. Phys. 21 033004 (2019)

Simulated detector signal



Brand et al., New J. Phys. 21 033004 (2019)

Information extracted from diffraction pattern

- Lattice constant and periodicity
 - Of radiation-sensitive materials
 - Of organic membranes
- Atom-membrane interaction:
 - Energy dependent transmission propability
 - Coupling to membrane's degrees of freedom
- Temporal evolution of membrane
 - Doping
 - Milling
 - Defect dynamics





PG

Stone-Wales defect



Single vacancy

Double vacancy

Lin. PhD thesis Aix Marseille Universite (2014)



DLR

Atom beam preparation

Ion Gun

- 5 to 3000 eV ion energy
- 100 nA ion current
- Operated with variable gases



Charge Exchange Cell

- Resonant Charge Exchange with buffer gas (Ar)
- Beam steering and collimation



P. Loeffler, Nonsequitur Technologies, 2022

Diffraction grating

- Membranes mounted on TEM grids
- 2.5µm diameter holes of free standing graphene
- Probe mount:
 - 5 axis manipulation
 - liquid nitrogen cooling
 - heating up to 700°C
- Laser cleaning of membranes







Plano-em.de, Trentino et al., Nano Lett. 21 5179 (2021)



Detection

- Multi-Channel-Plate detector stacked onto Phosphor screen
- CMOS camera recording events
- Single event detection for background-free reconstruction of diffraction pattern
- Count rate of up to $5 \times 10^4 \frac{\text{atoms}}{\text{s}}$ expected





Summary



- Transmission of neutral atoms through 2D materials
- Complimentary microscopy approach at low energies without ionizing radiation
- Detailed analysis of the coupling between atoms and 2D materials





Thank you for your attention!



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Jakob Bühler



www.dlr.de/qt

Scattering of hydrogen atoms





Excitation of electronic system

c) BOMD 80 Kinetic energy (eV) 78-TDDFT 76 8 10 2 6 4 Time (fs)

Energy dependent diffraction pattern



Bulk materials

2 layers of graphene:





Ion Flux



