Diffraction of 80 eV hydrogen through suspended graphene

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Synopsis We have investigated theoretically the possibility to diffract hydrogen atoms through a suspended graphene single layer. Using quantum and semi classical approaches we evaluate the momentum and energy exchange to the electronic and vibrational system and estimate their influence on the coherence and spot size.

Classical trajectories of H-graphene deflection have been determined using molecular dynamics (MD) based either on TDDFT or, more extensively, to DFT potential [1]. Both calculations yield generally similar results : a barrier of $3.8 \pm 1.3eV$ for atomic hydrogen to penetrate graphene at the center of the hexagonal ring, and a sputterization threshold of $82.5 \pm 2.5eV$.

The H-graphene potential energy landscape is approximated as being proportional to the electrostatic potential of the graphene sheet with a coefficient fitted to explicit DFT potential along the axes through the center of the hexagon.

Diffraction pattern has been determined within the eikonal approximation, whose validity has been shown to be excellent at the considered energy ($80eV$) by comparison with an exact 3D wavepacket calculation. When no decoherence effect is taken into account, a perfectly periodic hexagonal graphene layer gives rise to point like diffraction spots with an intensity distribution dominated by the Airy disk associated with the size of the central ring and elongated branches associated with the reduced repulsion perpendicular to the $C-C$ bound.

The main source of decoherence is expected to arise from the momentum spread induced by thermal movement of the lattice (Debye Waller factor). The diffraction pattern is calculated using a super cell of 256 unit cells distorted by the thermal displacements and convoluted by the beam parameter. The diffraction spot now acquires an additional broader contribution with a width increasing with the distance to the specular peak. The decoherence due to electronic excitation was estimated from TDDFT. For central trajectory, it indicates an electronic energy of $\sim 3.5eV$, significant but lower than the $\sim 4.7eV$ of the lowest in-plane plasmon. This later has a wavelength of $\sim 7nm$, encompassing hundreds of lattice cells and is expected to have a limited contribution to decoherence.

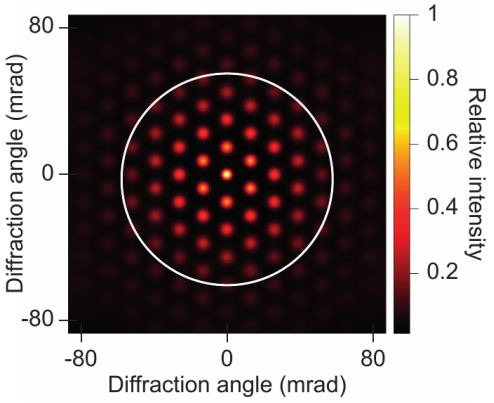

Figure 1. Diffraction pattern including decoherence effects. Around 8% of the atoms are diffracted by less than 52 mrad (white circle). The predicted signal-to-background ratio reaches up to 140.

The study suggests the possibility of constructing an ultra compact interferometer. Graphene technology is well advanced and slit with mono atomic thickness have already been demonstrated [2]. If space budget is less stringent, diffraction at crystal surfaces under grazing incidence can also provide a beam splitter with comparable deflection power and very limited decoherence [3] as the projectile is reflected above the surface with a reduce Debye-Waller factor and electronic excitation can be quenched by using wide band-gap insulator.

References

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