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Irradiation-induced Modifications and Beam-driven Dynamics in Low-dimensional Materials

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Irradiation-induced phenomena open a plethora of pathways for material modifications far beyond the thermal equilibrium and which are beyond the reach of direct synthesis. By using electron beams, such modifications can be induced and simultaneously observed at the atomic level. Moreover, in the analysis of 2-D materials, the position of every atom (rather than the atomic column) can be discerned in a high-resolution image.

For example, the introduction of multi-vacancy defects in graphene can be readily observed under 100kV aberration-corrected HRTEM [1], and the combination of vacancy creation and bond rotations can be used to convert graphene into two-dimensional amorphous carbon (Fig. 1) [1,2]. Atom loss can be directly counted in the images as a function of dose and in this way we have measured the knock-on sputtering cross sections for carbon atoms in graphene [3]. Recently, we have carried out a statistical analysis of the 2-D amorphous carbon (or carbon glass) structures with variable degree of disorder [4], enabled by an automated image analysis. For the first time, this provides atomic configurations for a continuous transition from a crystalline to an amorphous state, which were used for a statistical analysis such as the radial distribution functions shown in Fig. 1e.

At lower energies, the formation of defects in the pristine lattice is less likely, but existing defects convert from one configuration to another and also migrate under the beam. Fig. 2 shows results from a 60kV STEM experiment under ultra-high vacuum conditions where double vacancies in graphene are extraordinarily stable; meaning that they neither convert into higher-numbered vacancies nor trap carbon and convert back to a pristine lattice, for long sequences of images. Nevertheless, the defects rapidly move via beam-driven bond rotations. Fig. 2 shows a trajectory that is obtained from a long sequence of di-vacancy migration steps, displaying a random walk or a beam-activated diffusion [5].

Although beam-driven dynamics are useful to modify materials under direct observation, these effects are also a major obstacle for the analysis of the pristine state of the sample. Using simulated data, we have shown a new approach to extract information from very low dose exposures [6]. If this can be achieved also with experimental data, it may provide a novel route to circumvent the limitations of radiation damage in the analysis of materials.

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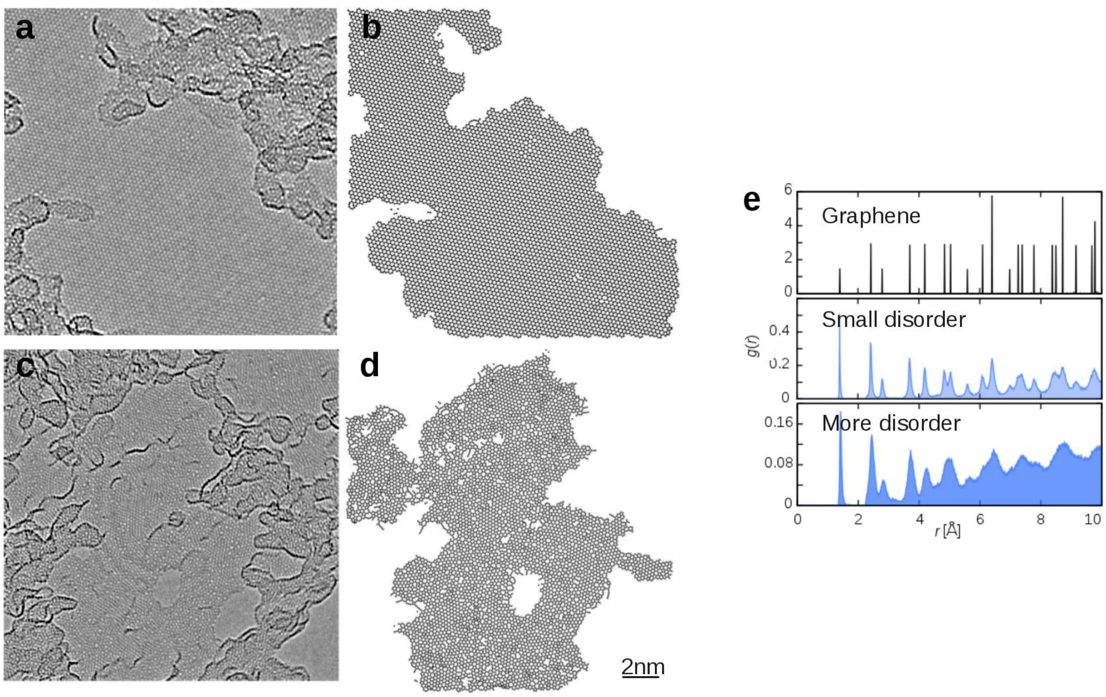

Figure 1. Conversion from graphene (a,b) to two-dimensional amorphous carbon (c,d) under electron irradiation. (a,c, AC-HRTEM images, b,d corresponding atomic structure). (e) Part of the statistical analysis of 2-D amorhous carbon, showing the radial distribution function (RDF) extracted from the experimentally observed atomic coordinates [4].

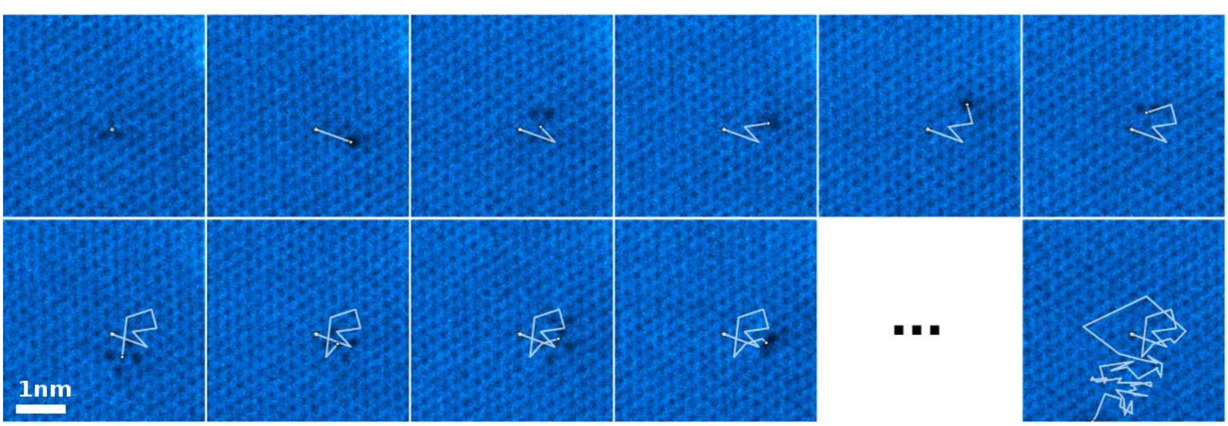

Figure 2. Beam-driven diffusion of a di-vacancy in graphene; showing the first 10 and final frame from a sequence of 50 images [5].

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