Bond defects in graphene created by ultralow energy ion implantation

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Ultralow energy (ULE) ion implantation is increasingly being applied to the modification of 2D materials, in particular, for substitutional doping and intercalation of graphene[1][2]. Implantation-induced defects, whether desired or not, have a strong impact on the properties of graphene[3]. While significant research has been devoted to vacancy-related defects, disorder induced by ion irradiation in the ULE limit, that is, for energies below the vacancy-formation threshold, remains poorly understood. Here, we focus on that regime and report the formation of defects resulting from the breaking of C-C sp2 bonds and formation of C-substrate bonds (figure 1). The bond defect density is found to increase with increasing energy and atomic number of the implanted element [figure 2]. These findings significantly advance our understanding of disorder induced in graphene by ULE ion implantation, while simultaneously revealing the potential for exploiting such bond defects for physical or chemical functionalization. In particular, these bond defects can be generated with a high degree of selectivity, since they occur in the low-energy limit (at least down to 15 eV), significantly below the energies required to form stable vacancies.

References

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Figures
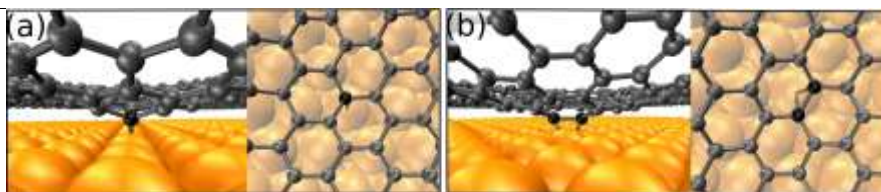
Figure 1: Snapshots of MD simulations after ion impact depicting the bond defects formed when the C-C sp2 bonds (grey) are broken and the displaced C atoms (black) form new bonds with the Pt surface (orange). Examples with side and top view of (a) one and (b) two bond defects.
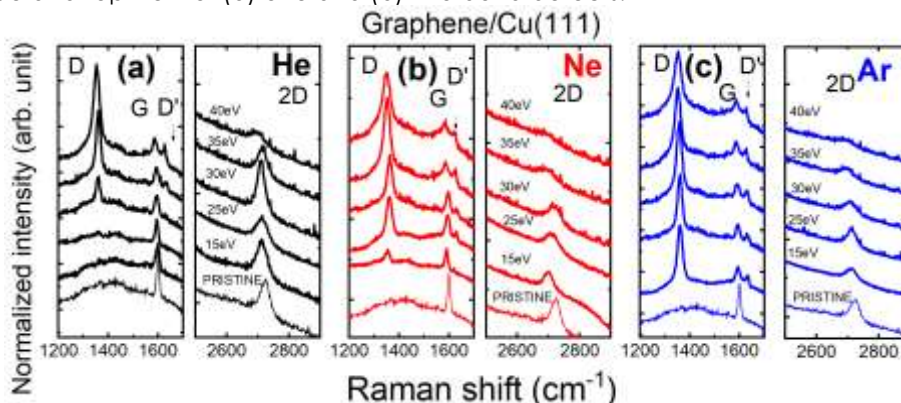
Figure 2: Raman spectra for Gr/Cu, pristine and implanted with He, Ne and Ar, for implantation energies between 15 eV and 40 eV. The implantation energies and the positions of the D, G, D' and 2D bands of graphene are indicated (D band corresponds to defective Graphene).