ESRF	**Experiment title:** **Electron-phonon coupling in the doped graphitic system KC_8**	**Experiment number**: **HS-4112**
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Report:

Although potassium intercalated graphite (KC_8) was discovered to superconduct over 40 years ago, [1] the nature of the superconductivity remains controversial. Angle-resolved photo-emission (ARPES) measurements find "kinks" in the electronic bands at energies of about 160 meV below the Fermi surface, which are analysed in terms of strong, anisotropic electron-phonon coupling [2]. This is in direct contrast to first principles calculations that predict a far weaker, and isotropic, electron-phonon coupling [3], and there have been several suggestions as to why ARPES might overestimate the electron-phonon coupling in doped graphite systems [3]. A precise determination of the $\boldsymbol{q}$ dependence of the phonon modes and electron-phonon interaction in this test-case material should shed light on the exact mechanism for superconductivity in this, and other related graphitic superconductors such CaC_6. Moreover since KC_8 has the same electronic structure as doped monolayer graphene [2], this study could also point the way to inducing superconductivity in doped graphene systems in the future

Experiment:

KC_8 samples were synthesized from natural flake graphite at University College London using the vapour transport method [4]. These samples were transferred into a high purity glove box and loaded into a beryllium dome at the ESRF, which was sealed using indium wire. The high sample purity was confirmed using diffraction on ID28. The high energy in-plane graphitic phonons in KC_8 were measured throughout the a-b plane in reciprocal space.

Results:

The left-hand panel of Fig. 1 shows a typical measured phonon spectrum at the K-point of the Brillouin zone. All the spectra were fitted using Lorentizian functions to obtain the measured phonon dispersions depicted in the right-hand panel of Fig. 1. The data are plotted within the graphene Brillouin zone and are compared to those of graphite [5]. We observe that the phonons in KC_8 are significantly softened with respect to those in graphite. Currently theoretical calculations of the phonon dispersions are underway at IMPMC, Paris. These

calculations employ a newly developed theoretical method [6] that accounts for non-adiabatic electron-phonon interactions, which have been shown to be important in doped graphitic systems. Experimentally the deconvolved intrinsic phonon linewidths are typically <1 meV. Currently we can obtain an upper limit on the electron-phonon coupling contribution to the linewidth, but we wish to compare our results to the theoretical calculations in order exclude other contributions to the linewidth such as anharmonicity and finite momentum resolution.

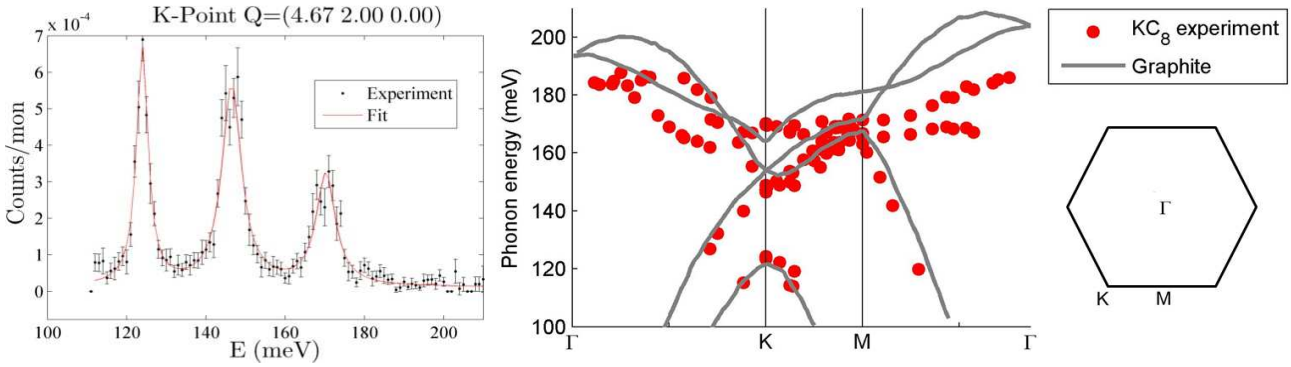

Figure 1: Left an example of the measured measured phonon peaks at the K-point of the Brillouin zone, the experimental resolution is 3 meV. Right: The dispersion relations of the KC_8 phonons compared with those of graphite.

The electron-phonon coupling contribution to the phonon linewidth $\gamma_{\mathbf{q}\nu}$ for mode ν with wavevector $\boldsymbol{q}$ and energy $\omega_{\mathbf{q}\nu}$ is related to the electronic density of states at the Fermi level $N(0)$ = 0.6 states/(cell eV spin) and the electron-phonon coupling constant $\lambda_{\mathbf{q}\nu}$ by [7]

$$\gamma_{q\nu} = 2\pi N(0)\omega_{q\nu}^2 \lambda_{q\nu} .$$

APRES obtains anisotropic electron-phonon coupling values summed over all the phonon modes of λ=0.2-0.6 [2]. Using these values we obtain predicted linewidths of

$$\Sigma_\nu \gamma_{q\nu} = 17 - 51 \;\; meV .$$

where the sum should be performed over all 27 phonon modes. However ARPES suggests that the majority of the coupling comes from the high energy phonons in the region 155-165 meV. The theoretical phonon calculations are required to determine the number of indepent phonon modes over which the sum should be performed, as the experimentally observed phonon peaks are likely to correpond to several degenerate modes. However, the results thus far suggest that the real electron-phonon coupling might be significantly weaker than is currently thought.

In summary, we have obtained the first measurement of the high-energy phonon dispersions in KC_8, demonstrating that the phonons are significantly softened with respect to the graphite phonons from which they are derived. The phonon linewidth analysis should allow a detailed measurement of the electron-phonon coupling as a function of $\boldsymbol{q}$ and the different phonon modes, with significant implications for the physics of doped-graphitic systems. These results will form the basis of a publication, which is currently in preparation.

References

[1] N. B. Hannay, et al., *Phys. Rev. Lett.* **14**, 225 (1965)
[2] A. Grüneis et al., *Phys. Rev. B* **79**, 205106 (2009); Z.-H. Pan et al., *arXiv:1003.3903*
[3] M. Calandra and F. Mauri, *Phys. Rev. Lett.* **95**, 237002 (2005) & *Phys. Rev. B* **76**, 161406(R) (2007); C.-H. Park et al., *Phys. Rev. B* **77** 113410 (2009) & *Phys. Rev. Lett.* **102**, 076803 (2009)
[4] M. S. Dresselhaus and G. Dresselhaus, *Adv. in Phys.* **51**(1), 1 (2002)
[5] M. Mohr et al., *Phys. Rev. B* **76**, 035439 (2007)
[6] M. Calandra, G. Profeta and F. Mauri *arXiv:1007.2098* (2010)
[7] P. B. Allen, *Phys. Rev. B* **6**, 2577 (1972); P. B. Allen and R. Silberglitt, *Phys. Rev. B* **9**, 4733 (1974)