PHONON LIFETIME AND THERMAL CONDUCTIVITY IN IRRIDIATED GRAPHENE MOMOLAYER

Georges Bouzerar
Simon Thébaud and Ch. Adessi
CNRS & Université Lyon 1, Villeurbanne FRANCE
Georges.bouzerar@univ-lyon1.fr

In the literature, the disorder contribution to the scattering rate, an essential and crucial ingredient for the determination of the thermal conductivity $\kappa(T)$, is often obtained from second order perturbation theory (together with a standard virtual crystal approximation in alloys). Although, such an approximation is reasonable for isotopic disorder, it is highly questionable for non-perturbative defects such as vacancies. Here, we present (i) the effects of vacancies in disordered/irradiated graphene on the phonon spectrum, (ii) on the quasiparticle linewidth for various branches LA, TA, ZA, and (iii) on the T dependent thermal conductivity calculated beyond the Relaxation time approximation and including properly the effects of anharmonicity (3 phonons scattering processes 'U' and 'N'). To allow both large scale (beyond 10^7 atoms) and accurate calculations, we employ an exact representation of the Green's functions in terms of Chebyshev Polynomials that properly includes both quantum interference effects and phonon localization. The realistic input parameters characterizing the graphene monolayer (with and without vacancies), the interatomic force constants and the T dependent phonon–phonon collision rates are calculated within Density Functional Theory (SIESTA and VASP). Hence, our approach has no adjustable parameters. We compare our theory to both available Boltzmann Transport Equation simulations, to Molecular Dynamics and to existing experimental data.

Figures

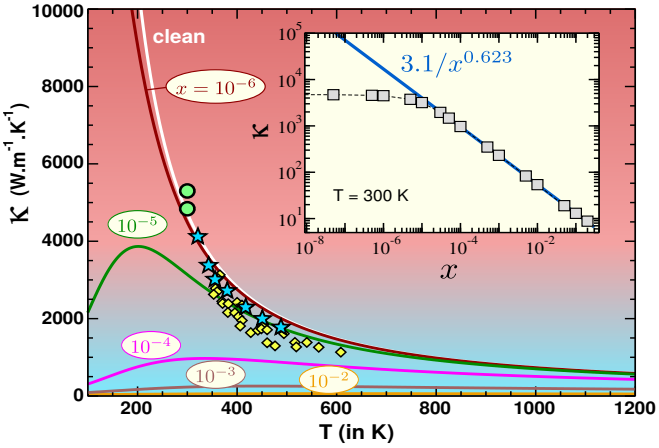

Figure 1: Thermal conductivity as a function of temperature in Graphene for various concentration x of C vacancies (continuous lines). The symbols (circles, diamonds and stars) are experimental data from various groups. The inset shows κ (T=300 K) as a function of x. Notice that 0.1% of vacancies is enough to suppress the conductivity by a factor 25.