Suppression of thermal conduction and enhanced thermoelectric figure of merit in disordered carbon systems

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Graphitic allotropes of carbon are known to have extremely high mechanical strength and stiffness which give rise to ultra high thermal conduction through these materials [1]. Isotopic or Anderson-type disorder can reduce thermal conductivity in quasi-one-dimensional forms of carbon, namely carbon nanotubes and graphene nanoribbons, which are of special importance because of their potential in device applications [2]. Using non-equilibrium Green function methods and also developing an order-N method for phonons we investigate thermal transport properties of graphene nanoribbons with edge-disorder. We find that edge-disorder suppresses phonon transport very strongly so that elastic mean free paths are considerably short (Figure 1) and thermal conduction can be reduced by orders of magnitude [3,4]. Of special importance is graphene nanoribbons with zigzag edges where the outstanding electronic transport properties are weakly affected by edge-disorder [5]. We show that edge-disorder can separate electronic and phononic degrees of freedom very effectively in zigzag graphene nanoribbons and a “phonon glass-electron crystal” is achievable for narrow systems. We also show that thermoelectric figure of merit (*ZT*) can be enhanced at the edge of the first conduction plateau and can reach the values up to 4 at room temperature [3].

References

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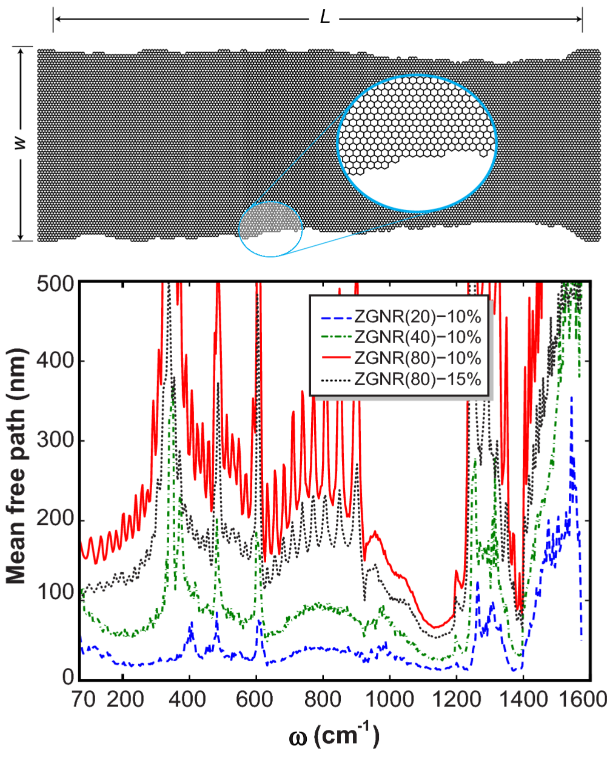

Figure 1:
Upper panel: short portion of an edge disordered GNR (width *w*=17.04 nm, length *L*~ 50 nm and disorder density of 10%).
Lower panel: elastic MFP for ZGNR of widths N_z=20, 40, and 80 (4.26, 8.52, and 17.04 nm, respectively) with disorder density of 10%, and also for the N_z=80 and 15% disorder for comparison.