TRANSIENT LOCALIZATION IN CRYSTALLINE ORGANIC SEMICONDUCTORS

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There is an important research activity to identify new classes of semiconductors for the development of novel applications in electronics. These are, by definition, "unconventional" and their study and characterization requires new tools. Examples of such materials are organic semiconductors or graphenederived materials such as graphene oxide or graphane.
In crystalline organic semiconductors, such as Rubrene, a fundamental unsettled question is whether the mechanism of charge transport can be ultimately understood from the point of view of band electrons alone, as suggested by the "bandlike" temperature dependence of the measured mobility. In these materials, the inherently large thermal molecular motions act as strong electron scatterers, leading to apparent electron meanfreepaths comparable or even smaller than the intermolecular distances [1,2].
This issue can be addressed using a general relation derived from the Kubo formula which relates the carrier diffusion to the optical conductivity [5]. In Figure 1 is shown the carrier position mean square displacement ($\Delta x^2(t) = |x(t) - x(0)|^2$) and carrier timedependent diffusivity ($D(t) = d\Delta x^2(t)/dt$) together with the corresponding optical conductivity. Data are obtained by a quantum-classical simulation of a one-dimensional tight-binding model of carriers interacting with intermolecular vibrations [1,2] of frequency ω_0.
We can conversely use the conductivity measurements below the gap frequency for Rubrene [3,4] to probe directly the time-dependent quantum dynamics of charge carriers [5]. This is shown in Figure 2 where $D(t)$ is extracted by the experimental data of ref. [4]. There is shown the phenomena of transient localization between 5 and 50 fsec. Using a phenomenological model for the carrier velocity correlation function we are also able to extract fundamental quantities such as the elastic and inelastic scattering rates, as well as the dynamical localization length scale [1,2].
In conclusion the relation between the quantum dynamics of electrons and the optical conductivity that stems from the Kubo formula, appears to be a powerful tool to analyze the charge dynamics in semiconductors with unconventional transport properties, which potentially applies to several broad classes of "bad" conductors that cannot be described by the usual Bloch-Boltzmann semiclassical description.
When applied to experimental data on crystalline organic semiconductors, it provides evidence for the role played by localization phenomena in the charge transport mechanism. The scenario emerging from the this analysis is indicative of a prominent role of the dynamical

lattice disorder associated to intermolecular vibrations, which is supported by a microscopic calculation on a onedimensional model. In analogy with our results disorderinduced weak-localization phenomena in graphene-based semiconducting systems d could be revealed by optical conductivity measurements.

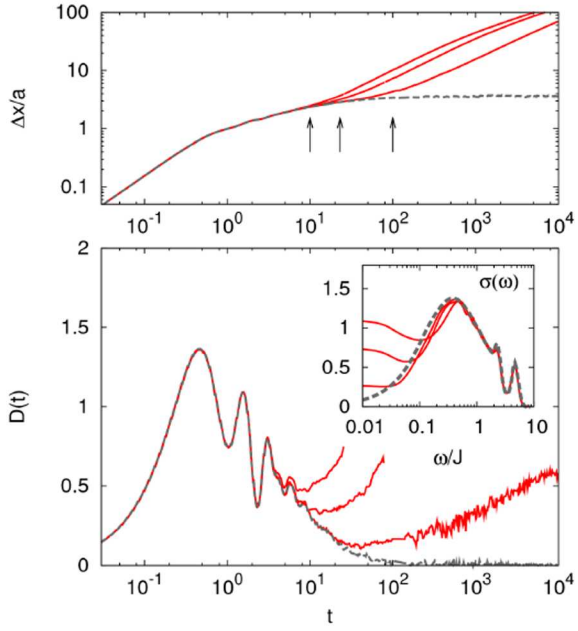

Figure 1: a) square root of carrier mean square displacement in units of the lattice spacing obtained from the microscopic model [1,2] for static (grey, dashed) as well as dynamical disorder (red, full lines: from bottom to top, $\hbar\omega_0/J = 0.01, 0.0435, 0.1$). Times are in units of $\hbar/J$ where J is the transfer integral [5]. b) The corresponding instantaneous diffusivity $D(t)$. The inset shows the corresponding optical conductivity.

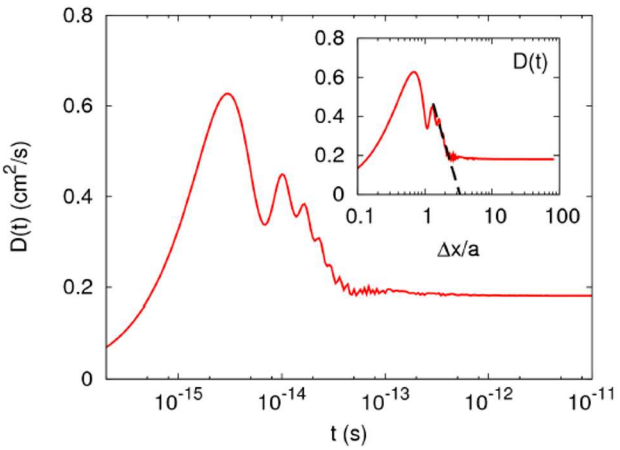

Figure 2: Time dependent electron diffusivity $D(t)$ extracted from the experimental optical conductivity of Ref. [4] in the direction of highest conduction. The absolute value is fixed by the measured mobility (7 cm^2/Vs). The inset shows the same quantity as a function of the instantaneous electron spread. The dashed line is the weak localization extrapolation.

References

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