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2015 J. Phys.: Conf. Ser. 647 012059

(http://iopscience.iop.org/1742-6596/647/1/012059)

Monte Carlo Study on Anomalous Carrier Diffusion in Inhomogeneous Semiconductors

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Abstract. We perform ensemble Monte Carlo simulations of electron diffusion in high mobility inhomogeneous InAs layers. Electrons move ballistically for short times while moving diffusively for sufficiently long times. We find that electrons show anomalous diffusion in the intermediate time domain. Our study suggests that electrons in inhomogeneous InAs could be used to experimentally explore generalized random walk phenomena, which, some studies assert, also occur naturally in the motion of animal foraging paths.

1. Introduction

Inhomogeneous semiconductors display distinctive electric and magnetic properties [1]. We recently demonstrated how linear magnetoresistance arises from the stochastic behavior of the electronic cycloidal trajectories around low-mobility islands in high-mobility inhomogeneous InAs epilayers [2, 3]. In an engineered inhomogeneous optical medium, Barthelemy *et al.* [4] demonstrated that light waves perform Lévy flight, a particular class of generalized random walk. Generalized random walk phenomena have been observed in nature and studied widely, ranging from electron [5, 6], photon [4, 7], and phonon [8, 9] motion in solids and gases to animal foraging paths [10–12]. Here we present Monte Carlo studies demonstrating the possibility to experimentally explore generalized random walks in inhomogeneous InAs. We adopt the Monte Carlo method because it can handle arbitrary inhomogeneous patterns more easily than analytical models [13]. In addition, it can be easily extended to study the influence of high magnetic field [2, 3].

2. Calculation Method

We consider an inhomogeneous high-mobility InAs layer containing regions with low-mobility (low-μ regions) covering a fractional area f; the remaining regions are called high-μ regions. The random spatial profile of the low-μ regions is generated from the power spectrum of the autocorrelation function $\langle\Delta(\boldsymbol{r})\Delta(\boldsymbol{r}')\rangle = \Delta^2\exp(-|\boldsymbol{r}-\boldsymbol{r}'|^2/\Lambda^2)$. Here $\boldsymbol{r} = (x, y)$ is the two-dimensional in-plane vector and Λ is the correlation length. The low-μ regions R_{low} are defined according to the relation $R_{\mathrm{low}} = \{\boldsymbol{r}|\Delta(\boldsymbol{r}) < \Delta_{\mathrm{th}}\}$ where the threshold Δ_{th} determines the low-μ coverage $f = R_{\mathrm{low}}/(R_{\mathrm{low}} + R_{\mathrm{high}})$. The scattering rate in the low-μ regions is assumed to be equal to $W_{\mathrm{i}} + W_{\mathrm{e}}$ and in the high-μ regions to W_{i}. Here W_{i} is the weak inelastic scattering rate and $W_{\rm e}$ the strong elastic scattering rate. We assume that electrons relax to thermal equilibrium at $T = 300\,\mathrm{K}$ after inelastic scattering, while the momentum vector $\boldsymbol{k}$ is randomized isotropically after elastic scattering. The non-parabolicity of the electron energy dispersion of InAs is modeled as $\varepsilon(\boldsymbol{k})[1 + \alpha\varepsilon(\boldsymbol{k})] = \hbar^2 k^2/2m_{\rm e}$ with $m_{\rm e} = 0.023\,m_0$ and $\alpha = 2.2\,\mathrm{eV}^{-1}$. Note that we consider zero-field diffusion processes in a sample with low carrier density and the non-parabolicity plays a minor role. We performed ensemble Monte Carlo simulations to obtain the mean square displacement (MSD) at zero applied electric and magnetic fields:

$$\mathrm{MSD} = \frac{1}{N}\sum_{i=1}^{N} |\boldsymbol{r}_i(t) - \boldsymbol{r}_i(0)|^2. \tag{1}$$

Here N is the number of electrons. In the following simulations, the typical number of electrons is $N \sim 100000$.

3. Results and Discussion

Figure 1 shows examples of randomly generated patterns of low-μ regions with $\Lambda = 0.5\mu$m. For $f < 0.5$, low-μ regions (colored regions) are isolated from each other and look like islands in the surrounding high-μ regions, while for $f > 0.5$, high-μ regions (white regions) look like islands. In spite of the fact that the low-μ coverage of the actual samples reported in Ref. [2] is $f \sim 0.05$, we mainly focus on high-f samples with $f = 0.8$, since we expect that relatively long range

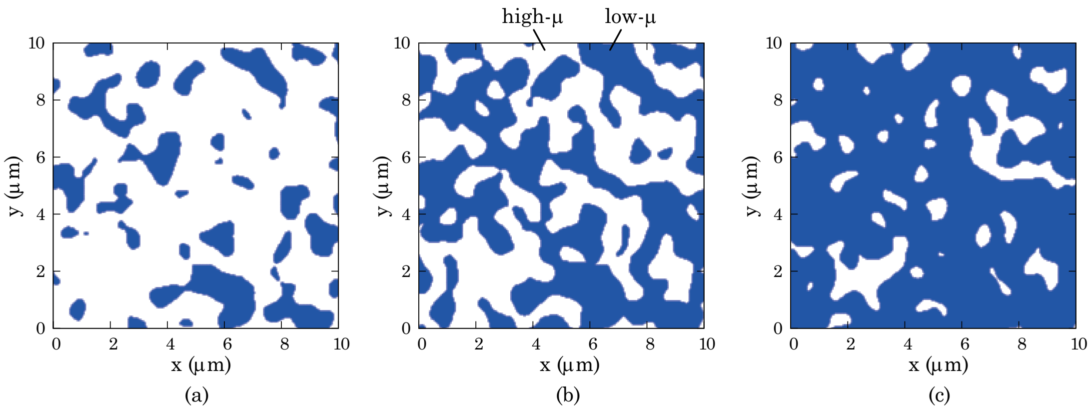

Figure 1. Examples of the generated distribution of low/high mobility islands for $\Lambda = 0.5\,\mu$m with the low-μ coverages (a) $f = 0.2$, (b) $f = 0.5$, and (c) $f = 0.8$. Colored areas represent the low-μ region.

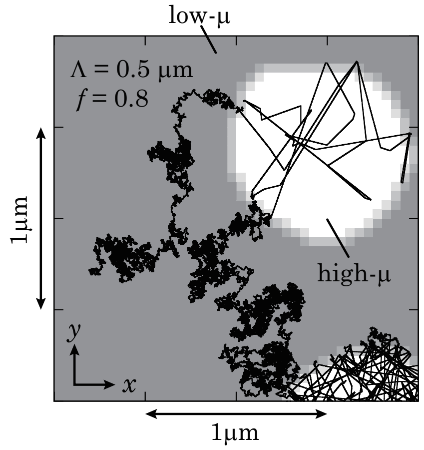

Figure 2. Example of a simulated trajectory in an inhomogeneous sample with $\Lambda = 0.5\,\mu$m and $f = 0.8$.

ballistic "jumps" occur when electrons enter the high-μ islands, which may lead to anomalous diffusion. Figure 2 shows an example of an electron trajectory in a sample with $f = 0.8$ and $\Lambda = 0.5\,\mu$m. The scattering rates are set to $W_\mathrm{i} = 1.5 \times 10^{12}\,\mathrm{s}^{-1}$ and $W_\mathrm{e} = 2.5 \times 10^{14}\,\mathrm{s}^{-1}$. Note the similarity between the trajectory and the possible Lévy motion of birds and animals – see for example Fig. 4 of Ref. [10].

Figure 3 shows the MSD for an inhomogeneous sample (solid line) compared with that for a homogeneous sample (dashed line). For the homogeneous sample, we assume that the scattering rate is given by an area-weighted average of the scattering rates in the low-μ and high-μ regions $W_\mathrm{i} + fW_\mathrm{e}$ $(= (W_\mathrm{i} + W_\mathrm{e})f + W_\mathrm{i}(1 - f))$. It can be seen that electrons move ballistically (MSD $\propto t^2$) for short times $t \lesssim 10$ fs while move diffusively (MSD $\propto t$) for sufficiently long times $t \gtrsim 1$ ns. In the intermediate time domain, electrons in the inhomogeneous sample show anomalous diffusion; MSD $\propto t^{1.65}$ (super-diffusive) for 10 fs $\lesssim t \lesssim$ 1 ps and MSD $\propto t^{0.7}$ (sub-diffusive) for 1 ps $\lesssim t \lesssim$ 1 ns.

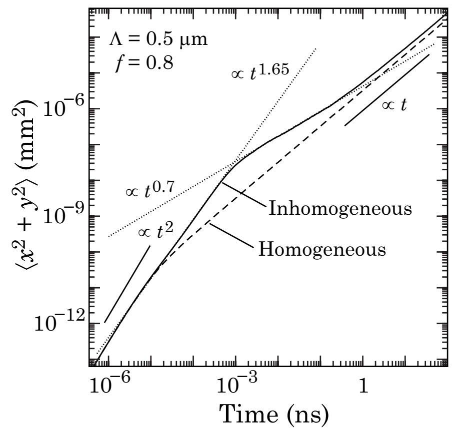

Figure 3. Mean square displacement as a function of t for an inhomogeneous sample (solid line) and a homogeneous sample (dashed line).

The transition from ballistic transport to anomalous diffusion should occur at the shortest scattering time $t_0 = (W_\mathrm{e} + W_\mathrm{i})^{-1} \approx W_\mathrm{e}^{-1} = 4$ fs. On the other hand, one can expect that the transition from anomalous to normal diffusion occurs at a time t_∞ when the long-time diffusion length becomes equal to the correlation length Λ. The crossover condition from anomalous to normal diffusion, therefore, may be written as $(Dt_\infty)^{1/2} = \Lambda$ or $t_\infty = \Lambda^2/D$. Here D is a diffusion coefficient given by $D = \ell^2/2\tau$ with ℓ being a mean free path and τ the scattering time. By assuming $\ell = v_\mathrm{th}\tau$, $\tau = W_\mathrm{e}^{-1}$, and $v_\mathrm{th} = (2kT/m_\mathrm{e})^{1/2}$, we obtain

$$t_\infty = \frac{m_\mathrm{e} W_\mathrm{e} \Lambda^2}{kT}. \tag{2}$$

To check this relation, we calculate the MSD for inhomogeneous samples with various correlation lengths Λ (see Fig. 4). In addition, to show the anomalous behavior more clearly, figure 5 plots the MSD divided by t, which corresponds to the long-time diffusion coefficient as $t \to \infty$. The down-arrows represent t_∞ given by Eq. (2). It can be seen that the transition from the anomalous to the normal diffusion can be well described by Eq. (2).

We finally consider the transition from the super-diffusive to the sub-diffusive regime. As suggested in Ref. [4], the transition occurs at a time $t_\mathrm{trans} = d_\mathrm{max}/v$, where d_max is the greatest step length and v is the velocity of the random walker. In the present case, t_trans may be written as

$$t_\mathrm{trans} = \frac{\Lambda}{v_\mathrm{th}}. \tag{3}$$

The up-arrows in Fig. 5 represent t_trans given by Eq. (3). We find reasonable agreement between the Monte Carlo results and Eq. (3).

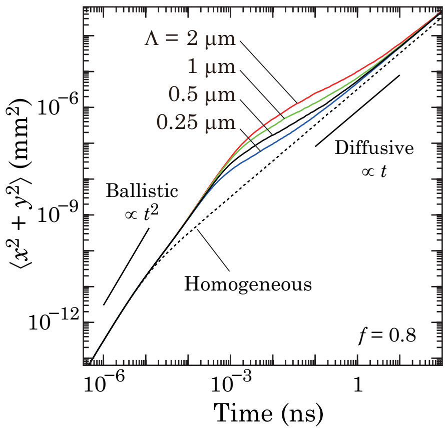

Figure 4. Mean square displacement (MSD) as a function of t for inhomogeneous samples with $\Lambda = 2$ (red), 1 (green), 0.5 (black), and $0.25\,\mu$m (blue). Dashed line shows MSD for a homogeneous samples.

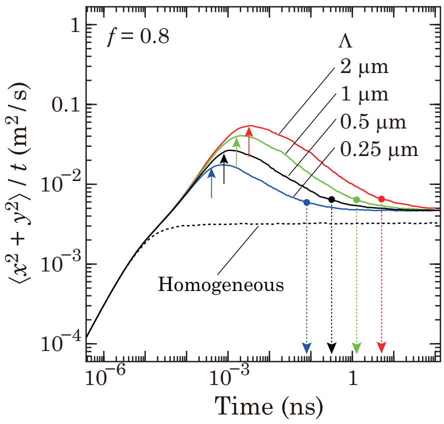

Figure 5. MSD divided by t for inhomogeneous samples with various correlation lengths Λ. Down-arrows (up-arrows) represent t_∞ ($t_{\rm trans}$) given by Eq. (2) (Eq. (3)) for $\Lambda = 2$ (red), 1 (green), 0.5 (black), and $0.25\,\mu$m (blue).

In this study, we considered inhomogeneous InAs. Other types of semiconductors, including alloys (e.g. InGaAs), may show similar behavior and are worth investigating. The anomalous diffusion presented here could be explored by measuring sample-size dependence of the carrier transmission (or conductance) to compare generalized random behavior which appears in a wide range of natural phenomena.

4. Conclusion

We have performed ensemble Monte Carlo simulations of electrons in inhomogeneous InAs layers. We find that electrons show anomalous diffusion in the intermediate time domain $t_0 \lesssim t \lesssim t_\infty$. Our study suggests that inhomogeneous InAs systems could be used to experimentally explore generalized random walk phenomena, which, some studies assert, also occur naturally in the motion of animal foraging paths.

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