Electronic Supplementary Material (ESI) for Nanoscale.

Supporting information for: Efficient, non-stochastic, Monte-Carlo-like-accurate method for the calculation of the temperature-dependent mobility in nanocrystal films

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1 Smoothing procedure to remove fluctuations in the mobility caused by the finite discretisation of the Q space

The mobility tensor components shown in Fig. 3 (black diamonds), calculated for each of the 100 energy intervals in which we divided the full miniband width, exhibit sizable fluctuations from one energy interval to the next. We attribute this behaviour to fluctuations

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in the number of states in each interval resulting from our choice for the (finite) discretisation of the Q space, and to the way these fluctuations propagate to other quantities, especially the flight times.

The number of $\vec{q}$ states with energy within a given interval $[E_i, E_i + \Delta E]$ obtained with any finite Q-space discretisation, is a numerical approximation for the density of states. The exact density of states would be theoretically obtained with an infinitely dense discretisation $Q_s \to \infty$ and with an infinitesimal width $\Delta E \to 0$ for the energy interval.

We therefore define the function

$$\zeta(E) = \lim_{\Delta E \to 0} \lim_{Q_s \to \infty} \frac{n_{\text{int}}(E, E + \Delta E)/Q_s}{\Delta E}, \tag{1}$$

where $n_{\text{int}}(E, E + \Delta E)$ is the number of $\vec{q}$ with energy within the interval $[E, E + \Delta E]$ obtained with a discretisation which divides the Q space into an infinite number of $\vec{q}$ vectors. This function is related to the fraction of the number of states within an infinitesimal interval $[E, E + \Delta E]$, divided by the total number of states. Our choice $Q_s = 51 \times 51$, although adequate to provide a suitable description of the scattering process considered here, is only a rough estimate for $\zeta(E)$. In order to obtain a better estimate for $\zeta(E)$, a more accurate calculation was therefore carried out using a 500×500 discretisation of the Q-space.

In Eq. (3) $\Gamma_{i \to f}$ is expressed in terms of the discretisation-dependent simulation parameters Q_s and ΔE. The quantity $\Gamma_{i \to f} Q_s \Delta E$ is, instead, independent of the discretisation. Using this quantity, the flight time can be expressed as:

$$t_i = \frac{\Delta E Q_s}{\sum_f \Delta E Q_s \Gamma_{i \to f}}, \tag{2}$$

where the denominator is now discretisation-independent. A more accurate estimate for the numerator would be

$$Q_s \Delta E \approx \frac{n_{\text{int}}(E, E+\Delta E)}{\zeta(E)} \tag{3}$$

which leads to the following 'corrected' expression for the flight time:

$$t_i = \frac{n_{\text{int}}(E, E+\Delta E)/Q_s}{\zeta(E)\Delta E \sum_f \Gamma_{i\to f}}. \tag{4}$$

The physical justification for this procedure is based on the substitution of the inaccurate value $n_{\text{int}}(E, E+\Delta E)/Q_s$, provided by the sparse $Q_s = 51 \times 51$ discretisation, with a more accurate value of that quantity, obtained using a denser discretisation, represented by $\zeta(E)\Delta E$.

The results of this smoothing procedure are presented in Fig. 3, where the 'corrected' mobility tensor components (red lines) are shown to exhibit a less fluctuating behaviour than the 'uncorrected' ones, as a result of the more accurate density of states in the miniband used to compute flight times and mobilities. The benefits of this procedure are especially important when calculating mobilities at low temperatures, where only the lowest energy intervals in the miniband are significantly populated. Any fluctuation in the mobility curve as a function of the energy interval greatly affects the calculation of this quantity.