Supplementary Materials: Modeling of Heat Propagation in Anisotropic Heterogeneous Polymer-CNT Composites

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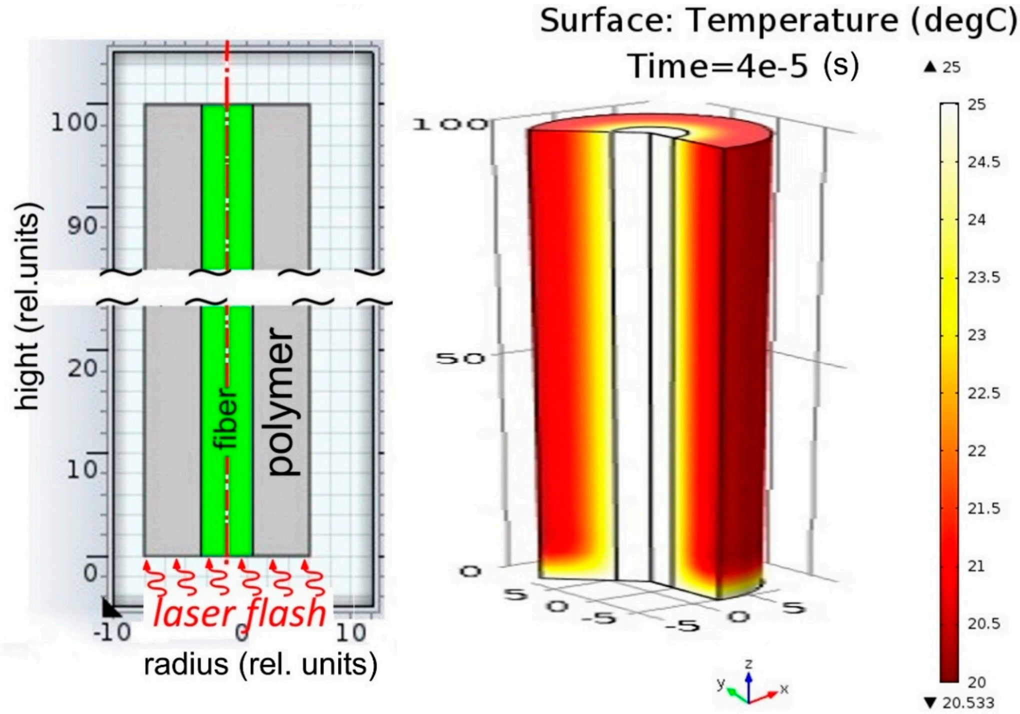
Heat propagation in the inhomogeneous PM-VANT media was simulated, using COMSOL Multiphysics code applying several approximations, using a model which we call the coaxial cylinder (CC) model. A simplified geometry of the unit cell in the CC model is shown in Figure S1a.



(**a**) (**b**)

Figure S1. (**a**) Geometry of the unit cell, consisting of the fiber and surrounding polymer in a volume proportion as estimated from the experimental data analysis; **(b)** a momentary temperature distribution in the cell as calculated with the zero interface thermal resistivity at 40 µs after laser flash start.

The CNT was substituted by a homogeneous fiber, thus ignoring the internal structure of the CNTs. The simulation is performed in a unit cell consisting of the coaxial cylinders, the fiber, and the surrounding polymer, with the cylinders height being equal to the sample thickness, the radius of the fiber neing equal to the external radius of the CNTs in the experiment, and the volume of the surrounding polymer cylinder corresponding to the volume of the unit cell in the composite. We assume that the laser pulse energy uniformly absorbed in a thin layer with the thickness of the order of light absorption length of about 50 nm at the bottom surface, i.e., well within the 5 µm graphite coating. This justifies that we ignore the absorption depth distribution, taking the step-like increase of the temperature at the bottom and start the heat propagation right after the pulse duration of 0.3 ms. The magnitude of the step is small, of the order of 1–5 °C, in order to avoid nonlinearities in heat propagation. The parameters of the system assumed in the calculation were as follows: polymer thermal conductivity 0.2 W/(m·K); polymer density 1200 kg/m^3; polymer heat capacity 1200 J/(kg·K); fiber thermal conductivity 300 W/(m·K) (also calculations were done with 3000 W/(m·K)); fiber density 2230 kg/m^3; fiber heat capacity 700 J/(kg·K). Simulation shows that the heat propagates very fast in the fiber and slowly in the polymer according to the thermal conductivity. The dynamics of the temperature increase at the top surface depends on the difference in the thermal conductivity of the fiber and polymer and on the thermal resistivity on the fiber/polymer interface. In Figure S1b, the temperature distribution is shown colored in dark red (initial temperature) to white (hot regions) at 40 µs after laser pulse shot which is about 10 times shorter than the laser pulse duration itself. The picture shows that the temperature distribution over fiber gets uniform immediately during the pulse duration, while it only starts to increase at the bottom of the surrounding polymer. The heat from the fiber also starts to propagate through the interface to the surrounding matrix with the rate, depending on the thermal resistivity of the interface. It is important to note that the detector cannot follow the 2D variation of the temperature field, but measures the average temperature over the sample surface.

Representative diagrams of dynamics of the average temperature evolution at the top surface are shown in Figure 5 [1].

References

1. Vorobyeva, E.A.; Chechenin, N.G.; Makarenko, I.V.; Kepman, A.V. Heat propagation in anisotropic heterogeneous polymer-CNT composites. *J. Compos. Sci*. **2017**, *1*, 5.