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Coupled electrical and heat transfer modelling of hexagonal boron nitride encapsulated graphene

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Abstract

Calibration drift of temperature sensors is a well-known problem which adversely affects process measurement and control, particularly at high temperatures. New approaches to overcome this problem are currently being developed, but degradation of the resistive sensor elements on which they rely is hard to prevent. To overcome this, graphene, which has desirable electrical properties such as a relatively high, tunable resistance, has been encapsulated in hexagonal boron nitride to protect it from oxidation and contamination. This van der Waals heterostructure stack involves nanofabrication on a silicon wafer. Electrodes connect the graphene to external bonding pads to enable resistance measurement. The resistance measurement requires the application of a current, which causes Joule heating; this must be well understood. A coupled electrical and thermal model is implemented in COMSOL; the high aspect ratio (several millimetres across for the silicon wafer and tens of nanometres thick for the stack) causes some challenges with the modelling which can be overcome using domain partitioning and swept meshing. For the application of a (typical) 10 μA current, a temperature rise of a few mK is predicted by the model, which is comparable to that of conventional industrial resistance thermometers.

Keywords: Temperature measurement; driftless thermometry; graphene; heat transfer; electric currents

Introduction

Calibration drift of temperature sensors is a well-known problem which adversely affects process measurement and control, particularly at high temperatures, and causes a degradation in product assurance. Some new approaches are being developed to overcome this problem, including inherently driftless devices such as a practical Johnson noise thermometer [1,2], and alternative designs of industrial resistance thermometers, but degradation of the resistive sensor elements on which they rely is problematic and difficult to prevent.

To overcome this, graphene[1], which has desirable electrical properties such as a relatively high, tunable resistance, has been encapsulated in hexagonal boron nitride (hBN) to protect it from contamination, and from oxidation at temperatures above approximately 400 °C [3-6]. This involves nanofabrication of the hBN/graphene/hBN van der Waals heterostructure stack on a Si/SiO_2 wafer [6]. Platinum (Pt) electrodes[2] connect the graphene to external bonding pads to enable resistance measurement. The electrode-graphene junction is created by etching the stack, while ensuring the graphene layer remains fully encapsulated.

Resistance measurement requires the application of a current, which causes Joule heating; this self-heating is associated with any resistance thermometer [7] and must be well understood. It results in overreading of temperature, and considerable effort has been devoted to optimizing correction techniques for self-heating effects.

A coupled transient electrical and thermal model is implemented in COMSOL to quantify this Joule heating. The high aspect ratio of the geometry (several millimetres across for the silicon wafer and tens of nanometres thick for the stack) causes some challenges with the modelling which can be overcome using domain partitioning and swept meshing.

In this paper the device is described, and how its geometry and the associated physics is represented in COMSOL. The model is then used, with some representative parameters, to characterize the temperature distribution which results from Joule heating of the resistive graphene sensor element as

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[1] Graphene is a single layer of carbon atoms arranged in a two-dimensional honeycomb lattice, renowned for its exceptional electrical, thermal, and mechanical properties.

[2] Tens of nanometres thick gold tracks are too mechanically unstable at temperatures above approximately 400 °C, and, in any case, they melt at 1064 °C, restricting the upper temperature.

a function of time. Finally, the model and results are briefly summarized.

Simulation

An optical microscope image of the hBN/graphene/hBN stack on a Si/SiO$_2$ wafer and the corresponding COMSOL geometry are shown in Figure 1. This comprises the sensor element. Transient (i.e. time-dependent) coupled 'Electric Currents' and 'Heat Transfer in Solids' interfaces are used to apply a current across the electrodes (necessary to determine the resistance). The resulting Joule heating causes a temperature rise, which is the aspect of interest here due to its influence on the use of graphene as a temperature sensor.

It can be seen in Figure 1 that the Si wafer surface is approximately square with a length of approximately 2 mm, while the nanofabricated structure on it has a depth of a few tens of nanometres. This high aspect ratio, combined with the complex layered geometry, could not be modelled with COMSOL using the default meshing approaches.

A swept mesh is used to handle the high aspect ratio geometries, with the use of a distribution node to ensure at least two elements along the thickness. This is complicated by the number of different crossovers between the layers. The solution is to partition the domains so that the geometry is more suitable for swept meshing. To manage the complexity, only two of the 10 electrodes are modelled, which provides enough information for the simulation to be useful.

To simulate the behavior of the sensor element when mounted within a probe assembly inside a protective outer sheath, a convective heat transfer boundary condition is applied on all external surfaces. This means that the temperature rise on application of an electric current depends on the convective heat transfer coefficient. As, in use, the device will be enclosed in a protective sheath, a coefficient[3] of 5 m^{-2} K^{-1} is used. The ambient temperature is taken to be 20 °C.

Physical, thermophysical and electrical properties were taken from the materials library of COMSOL, except those of graphene, for which customized values were used[4].

A current of I = 10 µA is applied at a time, t, of 5 s and kept constant thereafter; a sigmoid function is used to smooth the rise from 0 µA to 10 µA:

$$I(t) = \frac{I_0}{1 + e^{-k(t-t_0)}}$$

where t_0 = 5 s is the time at which the rise is centered and k = 1 s^{-1} is the steepness (i.e. the inverse of the rise time).

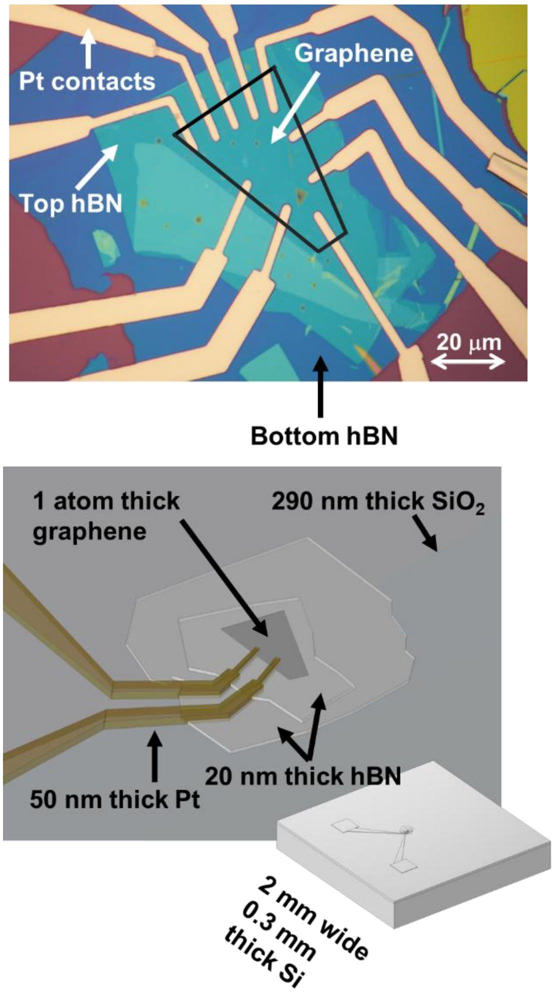

Figure 1. Geometry and dimensions of the hBN-encapsulated graphene stack. Top: optical microscope image of the real system. Bottom: COMSOL geometry (dimensions perpendicular to the plane are exaggerated to show the components). Only two electrodes are modelled, due to the complexity of the domain partitioning required for the swept mesh. The graphene is modelled as a 5 nm layer.

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[3] Values between 0.5 W m^{-2} K^{-1} and 10 W m^{-2} K^{-1} are expected [8,9].

[4] Electric conductivity 1 x 10^5 S m^{-1}, relative permittivity 2.8, heat capacity at constant pressure 700 J kg^{-1} K^{-1}, density 2267 kg m^{-3}, thermal conductivity 4000 W m^{-1} K^{-1}.

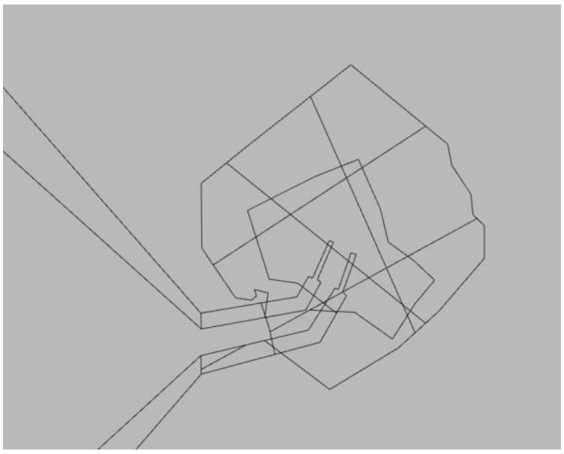

Figure 2. Domain partitions, arranged to simplify swept meshing.

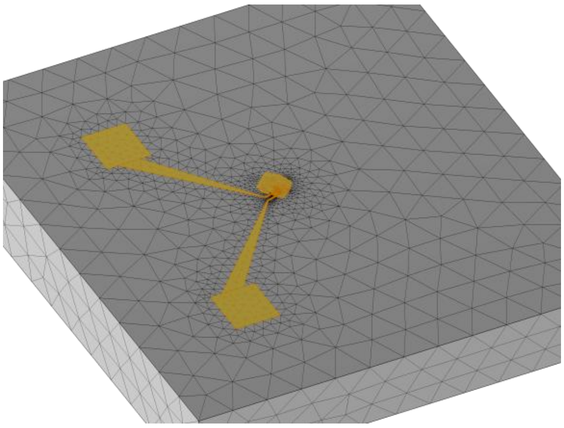

Figure 3. The mesh. The highlighted region is the separate swept mesh (with partitioned domains) for the nanofabricated components on the Si wafer. The larger Si wafer also has a swept mesh.

Due to the high aspect ratio of the geometry, a swept mesh is required, with a distribution node to ensure fewer elements in the direction perpendicular to the plane, keeping the model computationally feasible. Because of the complicated geometry of the various layers which are not conveniently aligned vertically, it was not possible to make a swept mesh using the default mesh settings. To overcome this, the domains were partitioned so that a swept mesh could be generated in each set of stacked domains. The domain partitions are shown in Figure 2. The mesh is shown in Figure 3; the highlighted region represents the swept mesh associated with the nanofabricated components on the Si/SiO$_2$ wafer.

Simulation Results

The temperature distribution at a time of 100 s (i.e. 95 s after application of the current, which was done at 5 s) which approximates the steady state for applied current of 10 μA and convective heat transfer coefficient of 5 W m^{-2} K^{-1} on the external surfaces is shown in Figure 4. The heating of the graphene is highly localized in the vicinity of the electrodes, thanks to the nanometre scale dimensions and high aspect ratio of the stack, which means that the underlying Si wafer acts as a very effective heat sink.

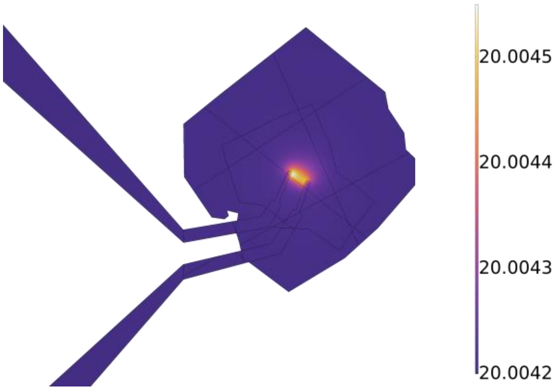

Figure 4. Temperature distribution in the hBN/graphite/hBN stack (current 10 μA, convective heat transfer coefficient on all external surfaces 5 W m^{-2} K^{-1}), showing localized heating of the graphene in the vicinity of the electrodes, and the slightly smaller temperature rise over the wider wafer. The electrodes can be seen leading away to the left. The Si wafer is omitted for clarity. Legend shows temperature in °C.

The temperature of the graphene between the electrodes as a function of time following application of the measuring current is shown in Figure 5, for several typical convective heat transfer coefficients. This is comparable to conventional industrial platinum resistance thermometers. While the temperature rise appears localized, there is in fact an appreciable temperature rise of the Si wafer too, because it rapidly absorbs the heat generated within the graphene and can only release that heat to the environment at a rate governed by the convective heat transfer on the external surfaces. The temperature rise amounts to a few mK for the applied current of 10 μA, which is, broadly speaking, comparable to that of a conventional industrial resistance thermometer.

This means that no particular difficulties are expected with respect to correction of the measured temperature for self-heating effects.

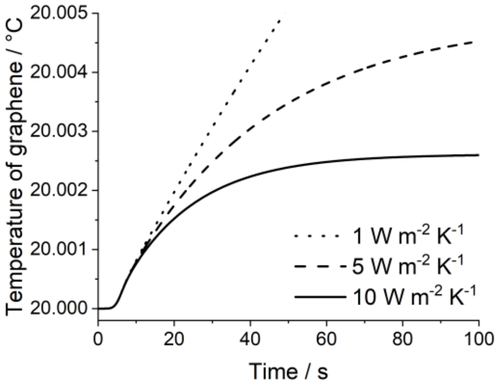

Figure 5. Temperature of the graphene as a function of time when instantaneous application of a 10 μA measuring current is made at 5 s and kept constant thereafter. Representative heat transfer coefficients (typical of this kind of device) on all outer surfaces are employed, as indicated in the legend.

Conclusions

Transient coupled Electric Currents and Heat Transfer in Solids interfaces are used to simulate the Joule heating of a resistive graphene element sandwiched between two layers of hBN, mounted on a Si substrate. Pt electrodes are used to apply the electric current. The resulting Joule heating causes a temperature rise, which is the aspect of interest here due to its influence on the use of graphene as a temperature sensor.

The geometry of the sensor has been presented, and techniques for domain partitioning and swept meshing described, which overcome the difficulty associated with the high aspect of this geometry (a few millimetres wide and a few tens of nanometers thick).

Some initial results have been presented, namely the temperature rise on application of typical measuring current and typical thermal environmental conditions; for the application of a 10 μA current, a temperature rise of a few mK is predicted by the model, which is comparable to that of conventional industrial resistance thermometers.

The model will be employed to examine both the stationary and transient ‘self-heating’ characteristics of the device, and the findings will be used to optimize its geometry. It is also of interest to extend the modelling to examine varying temperatures and larger currents.

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