HORIZON 2020

ALL-SCALE PREDICTIVE DESIGN OF HEAT MANAGEMENT MATERIAL STRUCTURES WITH APPLICATIONS IN POWER ELECTRONICS

Berichterstattung

Projektinformationen

ALMA

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Periodic Reporting for period 2 - ALMA (ALL-SCALE PREDICTIVE DESIGN OF HEAT MANAGEMENT MATERIAL STRUCTURES WITH APPLICATIONS IN POWER ELECTRONICS)

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Zusammenfassung vom Kontext und den Gesamtzielen des Projekts

In semiconductors and insulators heat transport is mainly mediated by phonons. Although for many decades most semiconductor modeling efforts have concentrated on electronic transport, in recent years phonon thermal transport modeling has become an increasingly growing priority. In many technologies, the problem of heat dissipation stands on the way to further progress. The spectrum of areas affected by heat management is very diverse. Also, in all cases, our ability to solve the challenge relies on being able to understand and predict heat flow in non-trivial systems, often involving micro and nanostructures.

In power electronic devices, such as LEDs or High Electron Mobility Transistors (HEMT), the choice of substrate is crucial for the lifetime of the device. For example, lowering the temperature of the active region in a HEMT by 50 degrees increases the device lifetime by one order of magnitude. Thus, various generations of multi-layer structured substrates have been evolving in recent times in order to increase heat flow, while also satisfying other constraints such as structural integrity and cost. The difficulty in this design process is that modeling thermal transport in these structures is a much more complex problem than for macroscopic systems. The problem in hand may contain simultaneous ballistic and diffusive flow of phonons, which are scattered by complex defect types such as vacancies, dislocations, interfaces, or nanoinclusions, and it may involve novel materials which have not yet been thoroughly explored.

The originally stated objectives of the project are:
O1. Model extension to mesoscale (TRL 3)
This objective was to solve the phonon Boltzmann equation for spatially inhomogeneous systems in a totally ab-initio fashion. Target metrics for the achievement of this objective were predictive accuracy with less than 20% error.
O2. Integration into a modelling software (TRL 4)
This objective aims at integrating the model into a new software that can be used by industry to help in the computer design of new substrates for power electronics, capable of predicting heat flow in layered multiscale structures comprising novel materials, and including ballistic and wave-like effects that are not present in standard TCAD modeling software.
O3. Design of new generation substrates for GaN-based power electronics (TRL 5).
The 3rd objective was to use our model and software to design a new generation of substrates for power electronics, enabling the operation of new power transistors under highly demanding conditions.

CONCLUSIONS OF THE ACTION
We have achieved all the objectives. The project has resulted in:

1) A first-class software: almaBTE is the first open-source software to deal with multiscale thermal modeling predictively, with fundamental and industrial applications, hundreds of users, and interfaced with TCAD.

2) A thoroughly validated approach, checked against dozens of experiments, with agreement better than 15% in most cases, pioneering experiments and novel methods.
3) A new design tool for electronics, directly used in R+D to design HEMT substrates, finFETs, and LEDs.

Arbeit, die ab Beginn des Projekts bis zum Ende des durch den Bericht erfassten Berichtszeitraums geleistet wurde, und die wichtigsten bis dahin erzielten Ergebnisse

Overview of the main results pertaining to each of the stated objectives:

1) Model extension to mesoscale:
The model extension (WP1-2) was attained during the first 18 months. Experimental validation of the model (WP5) was done on thin films, two- and three-dimensional materials with defects, and superlattices, and industrial systems, focusing on SiC and GaN materials and devices. The model fulfills our accuracy target, achieving less than 20% error.

The validation results have been disseminated in 30 published articles, including high profile journals (PRL, PRX, Adv. Mat., Nature Materials), presented in 38 conferences, including the Gordon Conference, the MRS, IMAPS, or the EMRS, and led to 10 invited talks.

2) Integration into a modelling software:
This objective targeted a professional level software package, user interface, and documentation. These three targets have been attained within WP3 and WP4. A database of ab-initio materials input files has been made available online, containing the most relevant semiconductors used in the electronics industry.

The almaBTE software has been disseminated in many ways, including a press release, dedicated website, user forum, published review of the method, 5 software releases, mailing list announcements reaching ~4000 people, a training course and a webinar.

3) Design of new generation substrates for GaN-based power electronics:
WP6 demonstrated the use of AlmaBTE in an industrial environment. The TCAD team of ST-microelectronics employed almaBTE to conceive new layered substrates for GaN based power electronics devices. Aixtron assessed process feasibility for the substrate fabrication. The conception process also permitted to address practical user issues and improve the CAD interface.

The conception of new substrates enabled by almaBTE has been disseminated in four conferences, and two plenary presentations at LETI (France) and IMEC (Belgium).

Production of high power electronics and LEDs are key markets for AIXTRON products. Both markets will significantly profit from increased device lifetime and reliability due to improved thermal behavior of the devices. Therefore AIXTRON uses trade shows, conferences and direct customer contacts to disseminate and exploit the new almaBTE substrate concepts. The results obtained within the ALMA project are encouraging and make rise the expectation on the duration of the device lifetime: possibly 15% longer lifetime for devices on Si substrates; perhaps 30% longer lifetime for devices on SiC substrates, opening exploitation opportunities for ST microelectronics.

Fortschritte, die über den aktuellen Stand der Technik hinausgehen und voraussichtliche potenzielle Auswirkungen (einschließlich der bis dato erzielten sozioökonomischen Auswirkungen und weiter gefassten gesellschaftlichen Auswirkungen des Projekts)

AlmaBTE is the first public software of its kind, capable of predicting heat flow ab-initio in layered multiscale structures comprising novel materials, and including ballistic and wave-like effects that are not present in standard TCAD modeling software. AlmaBTE can accelerate the design and development of new devices in technologies were thermal dissipation constitutes a bottleneck, like power electronic devices.

We have validated the model onto which AlmaBTE is based, by modeling various systems with first principles BTE for the first time and comparing them with experimental measurements, including many industrially relevant systems.

The results obtained regarding new substrate design are encouraging and make rise the expectation on the duration of the device lifetime: possibly 15% longer lifetime for devices on Si substrates; perhaps 30% longer lifetime for devices on SiC substrates. Performances and reliability are two factors essential in the automotive application field. Adding an extended lifetime can make electric and hybrid vehicles more cost effective and have a big impact on the environment given that the electronic equipment and battery disposal process shall be reduced.
The ALMA project enables the industrial community to introduce thermal modeling in their designs at a higher level of sohistication and accuracy than the previous state of the art. This is not just impacting the electronics industry, but also increasing a collective societal awareness of the importance of heat dissipation for new green technologies, and the enhanced role that modeling is playing in this respect.

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