# ALMA: All-scale predictive design of heat management material structures

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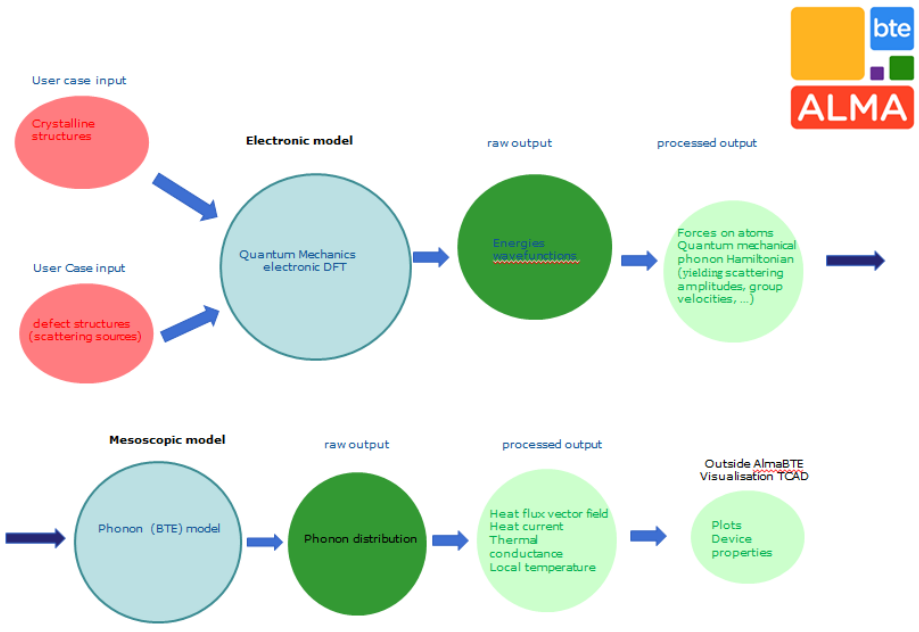
**Purpose of this document:**
Definition of a data organisation that is applicable to ALL materials modelling simulations. The fiche should contain all elements that are needed to describe a simulation. This information spans from the end-user (manufacturer) information to the computational modelling details.

| THE SIMULATION GENERAL DESCRIPTION | | | |
|---|---|---|---|
| 1 | USER CASE | The user wants to analyse the time and space evolution of the temperature distribution in a device, including effects beyond the reach of Fourier's law, such as ballistic and sub-ballistic transport, and frequency-dependent boundary effects. | |
| 2 | CHAIN OF MODELS | MODEL 1 | Electronic model: Electronic Density Functional Theory |
| | | MODEL 2 | Atomistic phonon model: Monte Carlo solution of the Boltzmann Transport Equation in the relaxation time approximation |
| 3 | PUBLICATION | • W. Li, J. Carrete, N. A. Katcho & N. Mingo, Comp. Phys. Comm. 185 (2014) 1747<br>• J.-P. M. Péraud, C. D. Landon & N.G. Hadjiconstantinou, Annual Rev. Heat Transfer, 17 (2014) 205 | |
| 4 | ACCESS CONDITIONS | A variety of DFT packages are available under either commercial or open-source licenses. The BTE part is implemented in AlmaBTE, an Apache-licensed (open-source) software package developed and owned by the ALMA development team (J. Carrete, G. Madsen, N. Mingo, B. Vermeersch & T. Wang). Web site: http://www.almabte.eu | |

## Workflow

The BTE model will be applied to the complete semiconductor device. The Hamiltonian expresses the forces on the atoms and these are calculated with a DFT model for each layer of the device.



## Model 1

| 1 | Aspect of the User Case/System to be Simulated | |
|---|---|---|
| 1.1 | Aspect of the User Case to be simulated and its role in the workflow | Forces on each atom in a part of a semiconductor device consisting of atoms whose species and positions are known. |
| 1.2 | Material | A crystalline semiconductor |
| 1.3 | Geometry | Bravais lattice + atomic motif |
| 1.4 | Time Lapse | Zero: static setting |
| 1.5 | Manufacturing process or in-service conditions | Zero pressure, zero temperature |
| 1.6 | Publication | R. Martin, Electronic Structure: Basic Theory and Practical Methods (Cambridge University Press, 2004), ISBN 0521782856 |

| 2 | Generic Physics Of The Model Equation | | |
|---|---|---|---|
| 2.0 | Model type and name | Electronic model: Quantum Density Functional Theory | |
| 2.1 | Model entity | Electrons | |
| 2.2 | Model Physics/ Chemistry equation PE's | **Equations** | Kohn – Sham DFT |
| | | **Physical quantities for each equation** | Spatial coordinates, Bloch wave vector, Kohn – Sham wave functions, Hamiltonian, electronic charge density |
| Materials relations | | **Equations** | 1. Exchange and correlation functional<br>2. Projected-augmented wave dataset |
| | | **Physical quantities/ descriptors for each MR** | 1. Exchange energy, correlation energy, electronic charge density<br>2. Kinetic energy, all-electron charge densities, pseudo electron core densities, all-electron partial waves, pseudo partial waves, projector functions, matching radii |
| 2.3 | Publication on this simulation | | |

*This part is similar to the description on input files to simulation software and requires understanding of the underlying architecture of the data in certain class of solvers for the models.*

| 3 | Specific Computational Modelling Metadata | | |
|---|---|---|---|
| 3.1 | Numerical Solver | Self-Consistent Field (SCF) procedure | |
| 3.2 | Software tool | VASP, https://www.vasp.at/ | |
| 3.4 | Time step | Stationary state solution | |
| 3.5 | Computational Representation *Refers to how your* | Physics Equation | The DFT equations are applied to the set of valence electrons defined by the constituent atoms in the semiconductor. Nuclei are represented by points. The wave functions of electrons are defined over a parallelepipedic unit cell. One-electron orbitals, the electronic charge density, and the local |

| | | | |
|---|---|---|---|
| | *computational solver represents the material, properties, equation variables,* | | potential are expressed in plane wave basis sets. |
| | | **MATERIAL RELATIONS** | The exchange and correlation functionals are hardcoded. |
| | | **MATERIAL** | The PAW datasets characterizing each kind of atom are expressed in terms of spherical harmonics and radial grids |
| | | **BOUNDARY CONDITIONS** | The calculations are done on a representative parallelepipedic unit cell with periodic boundary conditions |
| | | **ADDITIONAL SOLVER PARAMETERS** | 1. Plane wave energy cutoff<br>2. Number of Bloch wave vectors<br>3. Tolerance for the convergence of the SCF method |
| **3.6** | **PUBLICATION** | | |

## Post processing

The “raw output” calculated by the model for the model entities is contained in the metadata above. This output is processed by a post processor in order to calculate values for physics variable for larger entities.
When this post-processed output is used in a next model, a pre-processor might be used.

| **4** | **POST PROCESSING** | |
|---|---|---|
| **4.1** | **THE PROCESSED OUTPUT IS CALCULATED FOR** | Forces on atoms, Quantum mechanical phonon Hamiltonian (yielding scattering amplitudes, group velocities, …) for atoms |
| **4.2** | **METHODOLOGIES** | The Hellmann-Feynman theorem is used to compute the forces on atoms in a set of configurations. A quantum mechanical phonon Hamiltonian is built from finite differences between these forces. |
| **4.3** | **MARGIN OF ERROR** | Margin of error: typically within 10%, mostly due to the error in the material relations (exchange and correlation functionals). |

## Model 2

| 1 | Aspect of the User Case/System to be Simulated | |
|---|---|---|
| 1.1 | Aspect of the User Case to be simulated and its role in the workflow | Distribution of temperature vs. space and time, the thermal conductivities , and so on in a system made up of crystalline materials with or without explicit defects |
| 1.2 | Material | Crystalline semiconductors with various distributions of defects (vacancies, dislocations…) |
| 1.3 | Geometry | Arbitrary geometries in scales ranging from nm to mm. The geometry is defined by an external boundary plus a set of atomistically described interfaces. |
| 1.4 | Time Lapse | From ps to ms |
| 1.5 | Manufacturing process or in-service conditions | Isothermal or diffusive walls (interfaces between parts of the system) |
| 1.6 | Publication | Unpublished work |

| 2 | Generic Physics Of The Model Equation | | |
|---|---|---|---|
| 2.0 | Model type and name | Atomistic phonon model: Boltzmann Transport Equation and atomistic quantum-mechanics for electromagnetics scattering | |
| 2.1 | Model entity | Atoms | |
| 2.2 | Model Physics/ Chemistry equation PE's | **Equations** | 1. Peierls-Boltzmann transport equation<br>2. Lippmann–Schwinger equation |
| | | **Physical quantities for each equation** | 1. Time, spatial coordinates, phonon frequencies, phonon group velocities, phonon occupation numbers, scattering rates<br>2. Green's function, phonon wave functions, perturbation matrix, t matrix |
| Materials relations | | **Equations** | 1. Phonon dispersion relations<br>2. Anharmonic force constants<br>3. Perturbation matrix |
| | | **Physical quantities/ descriptors for each MR** | 1. Phonon wave vectors, phonon frequencies, phonon group velocities<br>2. Phonon wave vectors, phonon branch indices, anharmonic force constants<br>3. Perturbation to the phonon Hamiltonian in real or mixed real / reciprocal space |
| 2.3 | Simulated Input | A quantum mechanical phonon Hamiltonian calculated with DFT to simulate phonon dynamics. | |
| 2.4 | Publication | | |

*This part is similar to the description on input files to simulation software and requires understanding of the underlying architecture of the data in certain class of models.*

| 3 | SPECIFIC COMPUTATIONAL MODELLING METADATA | | |
|---|---|---|---|
| 3.1 | NUMERICAL SOLVER | Monte Carlo | |
| 3.2 | SOFTWARE TOOL | AlmaBTE, http://www.almabte.eu, Apache license | |
| 3.4 | TIME STEP | Time is not discretized | |
| 3.5 | COMPUTATIONAL REPRESENTATION *Refers to how your computational solver represents the material, properties, equation variables,* | PHYSICS EQUATION | Phonon-related quantities are defined over phonon wave vectors and over phonon branches. Real space dependences are explicitly considered |
| | | MATERIAL RELATIONS | Anharmonic force constants are defined over atoms in real space. General perturbation matrices are defined in N real space dimensions and M reciprocal space dimensions, with N+M=3. |
| | | MATERIAL | Materials are characterized by<br>by an computationally described geometry of the atoms and the properties <which> for each type of atoms stored in HDF5 files |
| | | BOUNDARY CONDITIONS | Isothermal walls (phonon reservoirs in thermal equilibrium), periodic boundaries, diffusive walls (with elastic but otherwise random scattering of phonons) and atomistically described internal interfaces. |
| | | ADDITIONAL SOLVER PARAMETERS | 1. Density of the wave vector grid<br>2. Broadening of the phonon modes |
| 3.6 | PUBLICATION | | |

## Post processing

The “raw output” calculated by the model for the model entities is contained in the metadata above. This output is processed by a post processor in order to calculate values for physics variable for larger entities.
When this post-processed output is used in a next model, a pre-processor might be used.

| 4 | POST PROCESSING | |
|---|---|---|
| 4.1 | THE PROCESSED OUTPUT IS CALCULATED FOR | Finite volumes |
| 4.2 | METHODOLOGIES | Temperatures, thermal currents and thermal conductivities and functions of space and time are computed by integrating the results of the BTE solver over wave vectors and frequencies |
| 4.3 | MARGIN OF ERROR | For most semiconductors, errors within 10% are achievable, and come mostly from imprecisions inherited from DFT. For some high-conductivity materials, systematic errors of 20-30% come from the relaxation time approximation. |