THERMAL CONDUCTIVITY OF INTERFACES IN GRAPHENE – METAL COMPOSITES

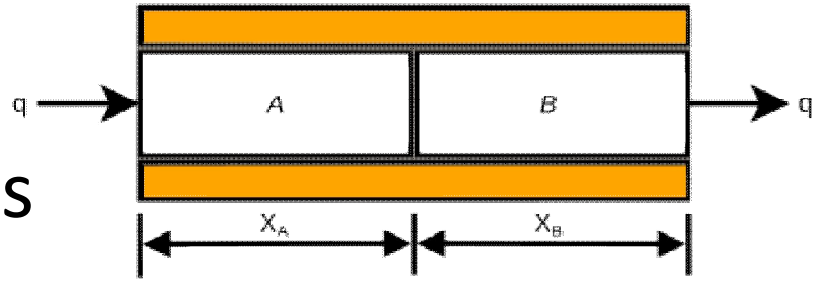
Mateusz GRYBCZUK*, M. Wasiluk, T. Wejrzanowski and K. J. Kurzydlowski

Warsaw University of Technology, Faculty of Materials Science and Engineering
Woloska 141, 02-507 Warsaw, Poland

*mateusz.grybczuk@inmat.pw.edu.pl

Introduction

- What - simulation of heat transfer through metal – graphene interfaces
- Why
- How - molecular dynamics
- Results
- Discussion



http://commons.wikimedia.org/wiki/File:Contact_conductance.svg

Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY

SiC MAT

EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND

Motivation

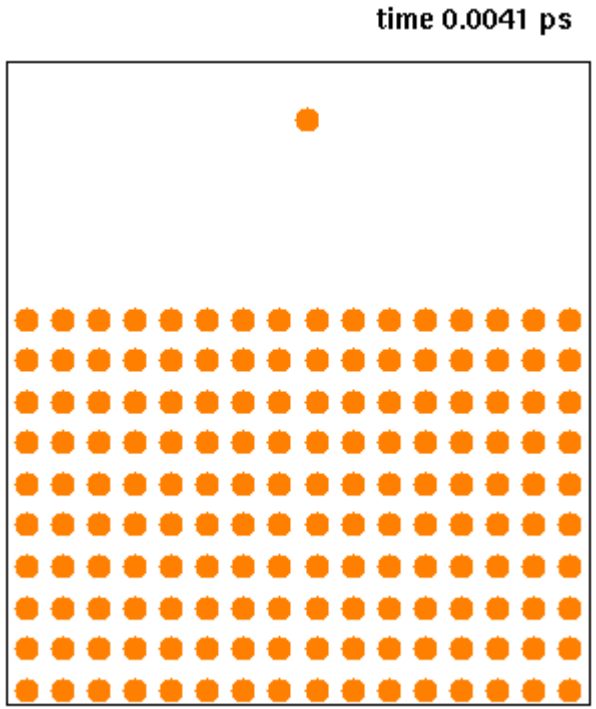
- Replicating results
- Using new potentials
- Prediciton of metal – graphene composites heat conductivity
- Creating multiscale model

Chang S.W., Nair A.K., Buehler M.J., *Geometry and temperature effects of the interfacial thermal conductance in copper- and nickel-graphene nanocomposites.* J Phys Condens Matter. 2012 Jun 20,24(24), 245301.

Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

Molecular dynamics

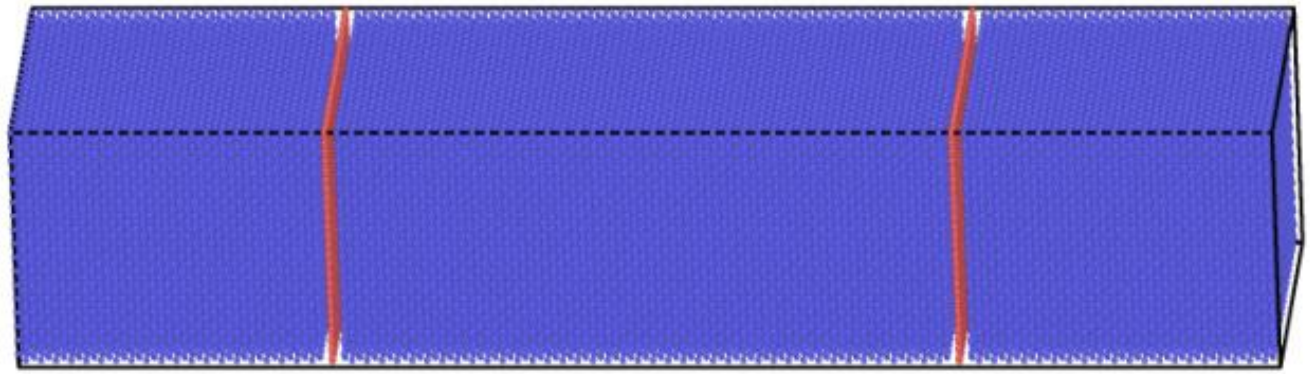
- Atomic scale
- Interaction – Newtonian equations
- Forces based on ‘potentials’
- Disregard for quantum effects
  - Correct under certain circumstances

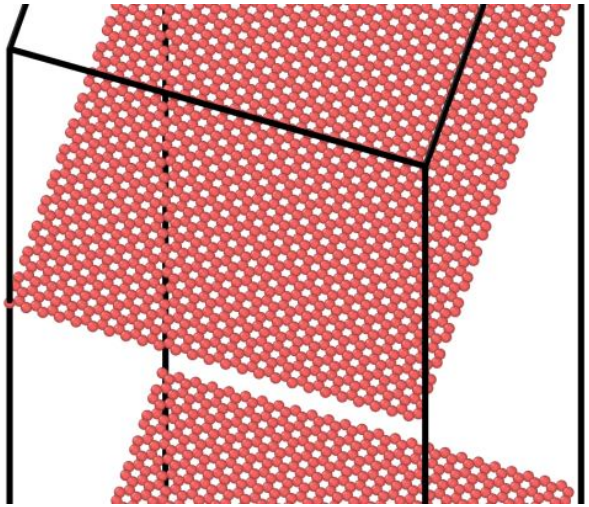


Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

Methodology – simulation domain

{100}





Periodic Boundary conditions
Atom count: 114240
Box dimensions: 62x72x303 Å
Time: ~150 ps

Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

Methodology – code and potentials

S. J. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, J Comp Phys, 117, 1-19 (1995)

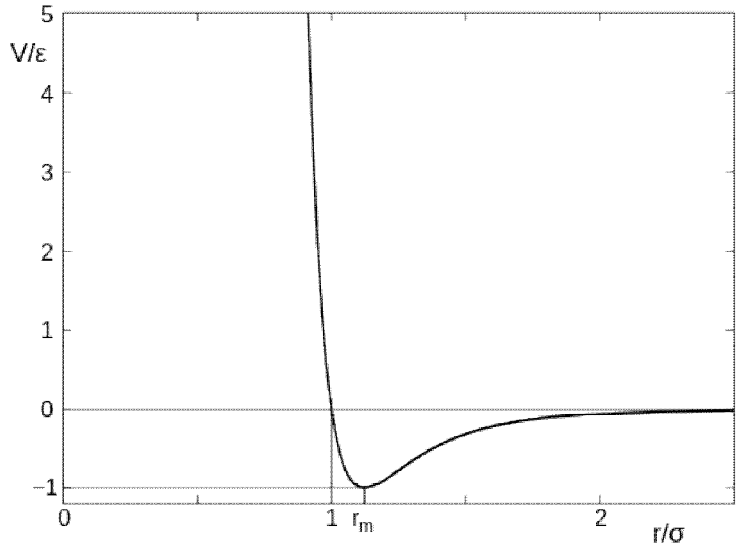
LAMMPS + Potentials

-Airebo

-EAM

-Lenard-Jonnes

Interaction	d[Å]	E_b[meV]
Cu-graphene	3.58	38
Au-graphene	3.55	33



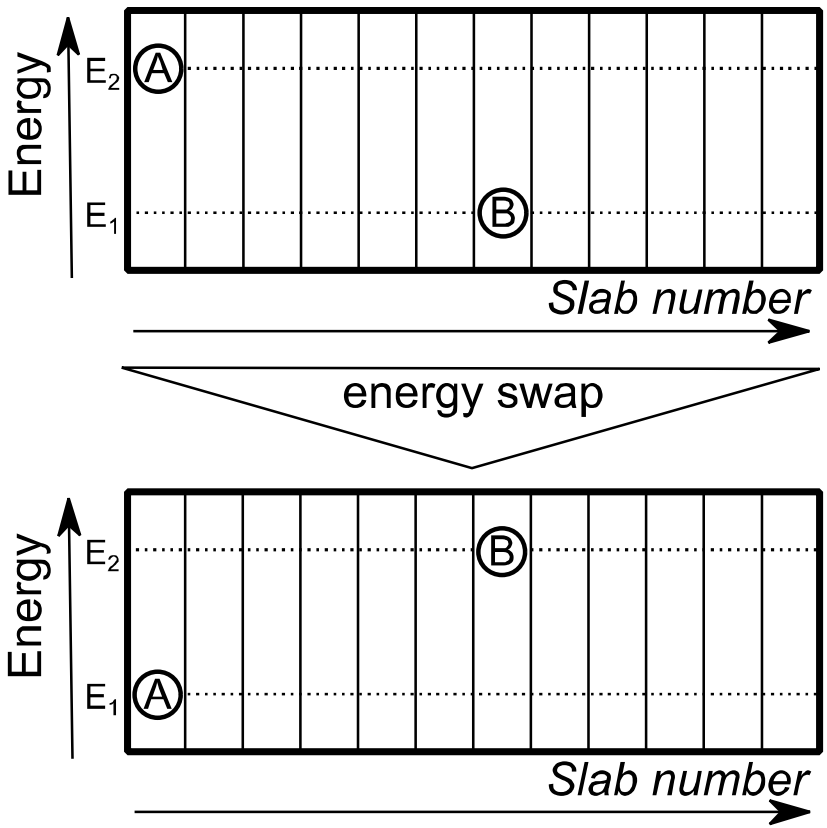
http://commons.wikimedia.org/wiki/File:12-6-Lennard-Jones-Potential.svg

Vanin M., Mortensen J.J., Kelkkanen A.K., Garcia-Lastra J.M., Thygesen K.S., Jacobsen K.W., *Graphene on metals: A van der waals density functional study.* Phys.Rev.B. 2010 Feb,81(8), 081408.

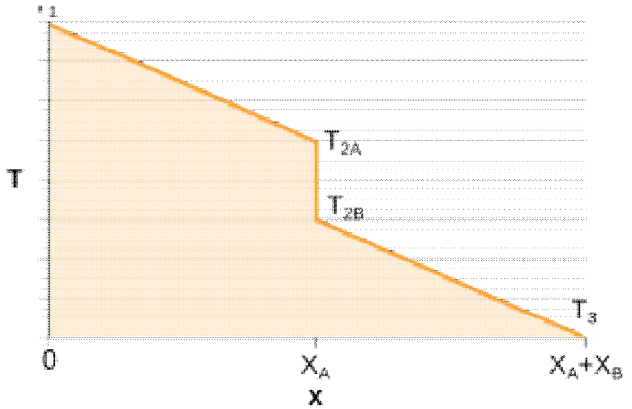
Stuart S.J., Tutein A.B., Harrison J.A., *A reactive potential for hydrocarbons with intermolecular interactions.* J Chem Phys. 2000,112(14), 6472-86

Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

Methodology – thermal conductivity



$$R_{th} = \frac{1}{Ah_c}\left[\frac{K}{W}\right]$$



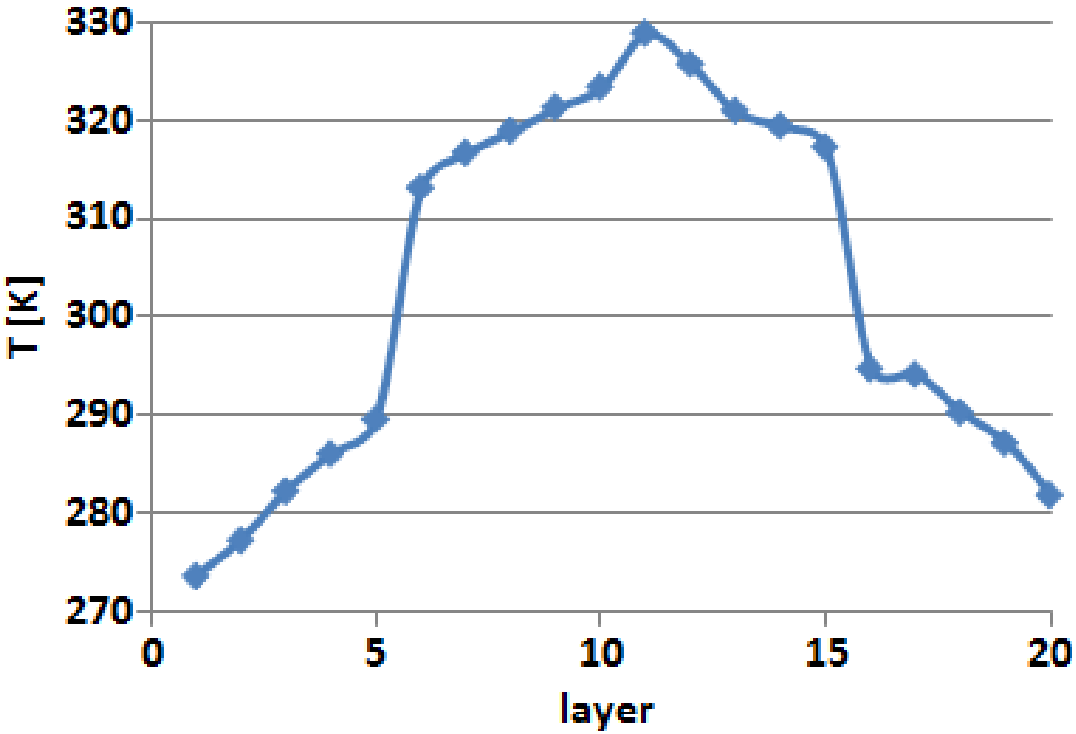
Müller-Plathe F., *A simple nonequilibrium molecular dynamics method for calculating the thermal conductivity.* J Chem Phys. 1997,106(14), 6082-5

http://commons.wikimedia.org/wiki/File:Contact_conductance.svg

Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

Results: silver - monolayer graphene

κ = 6,35e8 [W/m²K]



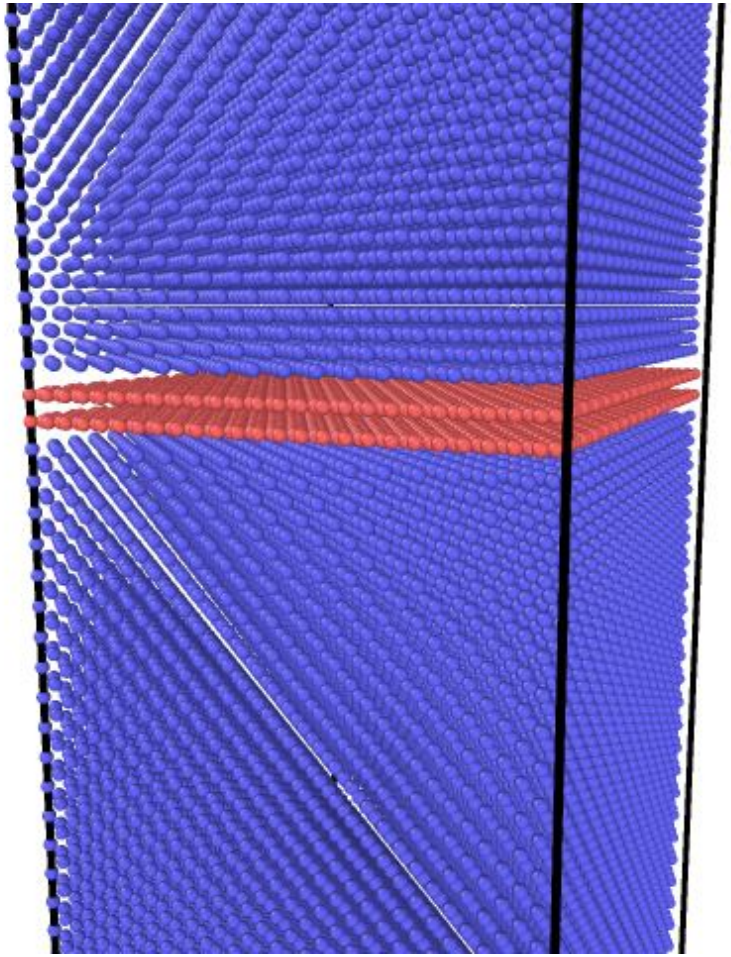
Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY

SiC MAT

EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND

Double layer graphene

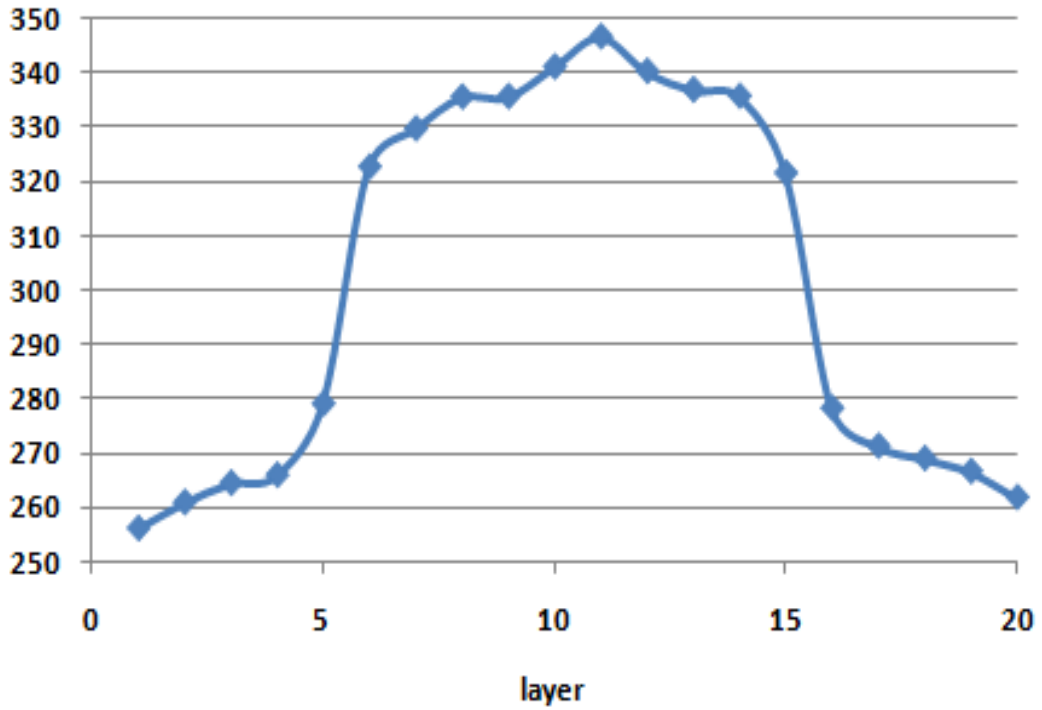


3,35 [A]

Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

Results: silver – double layer graphene

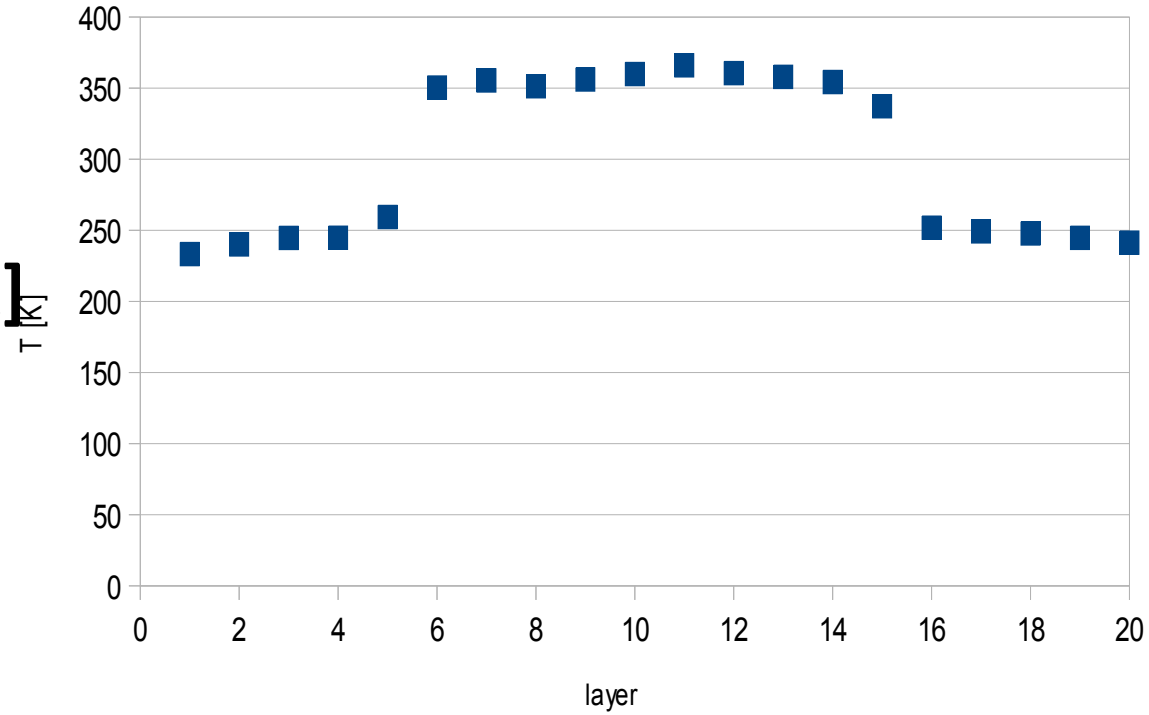
κ = 2,79e8 [W/m²K]



Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

Results: copper – monolayer graphene

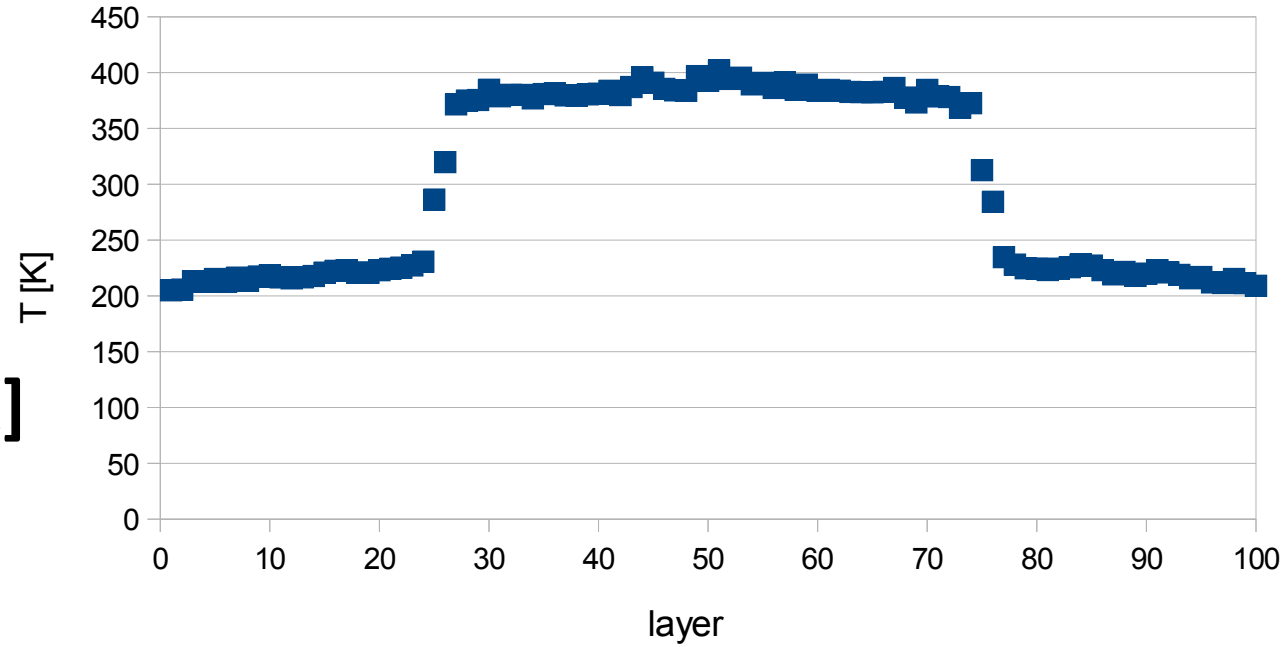
$\kappa = 4{,}18e8[W/m^2K]$



Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

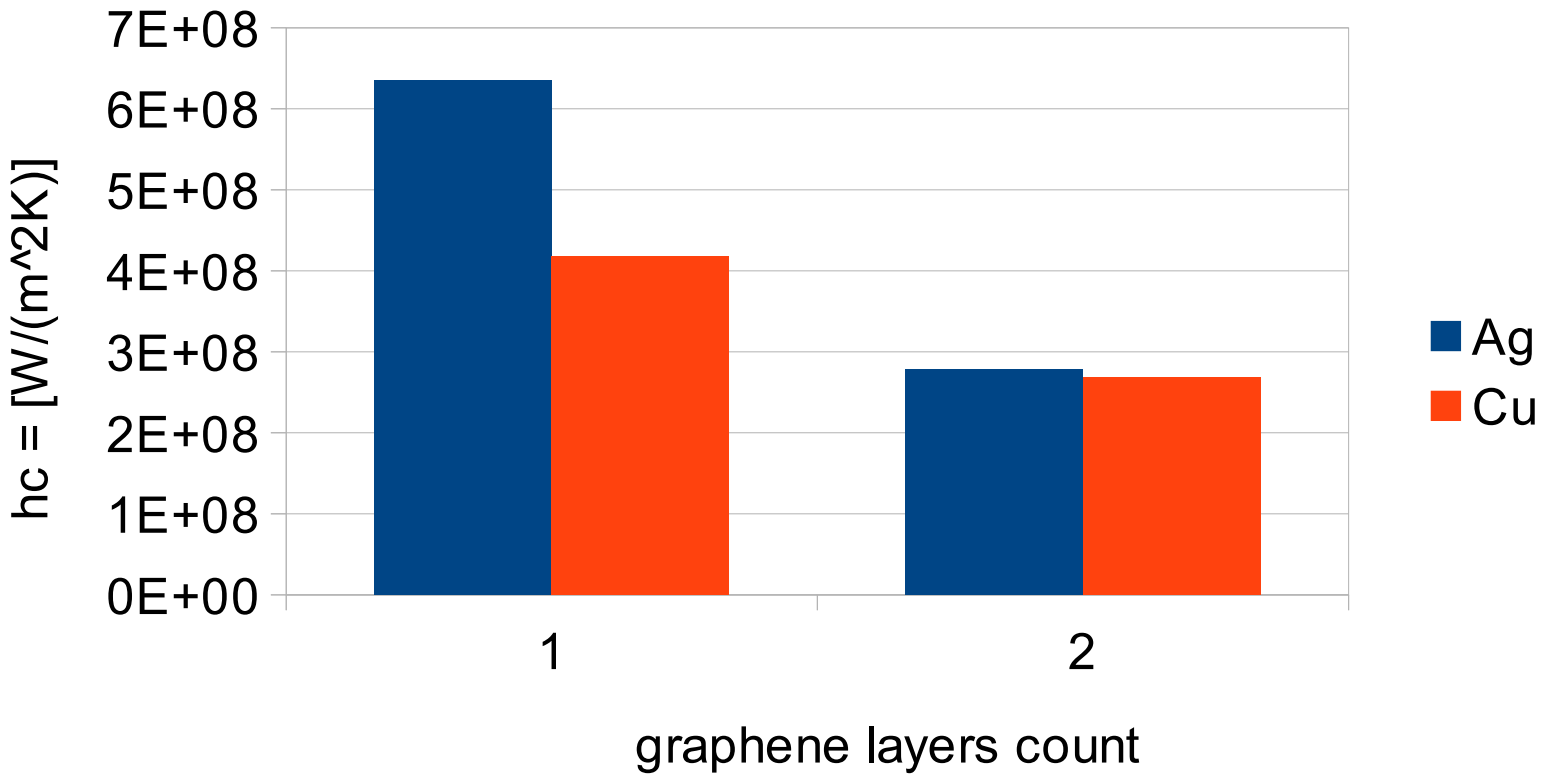
Results: copper – monolayer graphene

$\kappa = 2{,}68e8[W/m^2K]$



Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

Number of graphene layers and interfacial heat conducitivity



Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

Comparisons

- to experimental data
  - Measurements of composite and calculations from EMA (1,2-2,2e9 [W/m^{2}K], DMM and AMM (4,7-5,3e8 [W/m2K]) (Jagannadham K., *Thermal conductivity of copper-graphene composite films synthesized by electrochemical deposition with exfoliated graphene platelets.* Metallurgical and Materials Transactions B. 2012 04/01,43(2), 316-24.)
  - Au/Ti/graphene/SiO_2 interfacial thermal conductivity changes only slightly with temperature and has value of 2,5e8 [W/m^{2}K], (Koh Y.K., Bae M.H., Cahill D.G., Pop E., *Heat conduction across monolayer and few-layer graphenes.* Nano Lett. 2010 Nov 10,10(11), 4363-8.)
- to interfaces in macroscale
  - Four orders of magnitude higher than real life macro scale interfaces. (Lienhard ,Heat transfer textbook, 3rd edition p. 66)

Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy

INNOVATIVE ECONOMY
NATIONAL COHESION STRATEGY

SiC MAT

EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND

Summary

- Presented models are probably not including every aspect of investigatedphenomena
- Atomistic models can be used for calculation of thermal conductivity of graphene – metal interfaces
- Obtained results are consistent with other simulation and experimental data
- Results can be used in higher scale models

Project co-financed by the European Regional Development Fund under the Operational Programme Innovative Economy