Highly reflective coatings for thermal radiation sensors

Introduction

Fires and explosions are a threat to life, property, and environment. About one-third of the thermal energy in fires is released as thermal radiation, i.e. electromagnetic radiation in the IR range. New gradient heat flux sensor technology allows small, non-intrusive detectors to measure the heat flux directly and instantaneously, unlike in detectors which measure the consequences of fire (heat convection or smoke).

To distinguish between radiation from fire and other heat sources, these sensors are embedded with semi-conductors designed to reflect unwanted wavelengths using localized surface plasmons.

Project description

In this project, we will design highly reflective, spectrally sensitive coatings for thermal radiation detectors using semi-conductor micro-inclusions. The surface plasmons of semi-conductors are highly tunable by adjusting the size, geometry, and dielectric environment. The spectral response of composites with spherical inclusions has been simulated with multiscale modelling methods. In this project, these methods will be extended to non-spherical, anisotropic particles (cubes, rods, etc.) using surface integral equations and Monte Carlo simulations.

These coatings will be manufactured by the Fire Safety Engineering group at Aalto University, and this is an opportunity to make practical connections between computational results and applications. Some experience with programming and code development is useful.

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Development of machine-learning-based interatomic potentials and models to study nanoscale systems

Nanotechnology and miniaturization are paving the way towards a more energy-efficient and sustainable future for humanity. Nanostructures are commonly employed for commercial electronics such as computer chips, solar cells and electromechanical devices. Nanoengineered materials, such as carbon nanotubes, are also finding their uses for structural and chemical applications, for instance drug delivery and in vivo molecular detection. Understanding interatomic interactions is a crucial step along the path to controlling and engineering nanoscale systems. Because of reduced dimensionality, these interactions are difficult to study directly using experimental techniques, and much of the knowledge that we possess about the nature of atomic-scale processes has been gathered from theory and simulation.

Simulating a nanoscale system at the quantum level is very computationally demanding, and so the computational physics community is hard at work on developing effective interatomic potentials (also known as “force fields”) which can reproduce quantum-mechanical potential energy surfaces. Unfortunately, “classical” potentials, based on closed analytical forms, fail at accurately reproducing many phenomena, such as bond breaking/formation, defect formation energies, etc. A promising route, and one that provides a compromise between accuracy and CPU cost, is machine-learning-based interatomic potentials. We have used such potentials to explain for the first time the growth mechanism and origin of the high degree of diamond likeness observed in tetrahedral amorphous carbon (Fig. 1) [1]. Within the same methodological framework, we have also shown that machine learning is a powerful tool to predict general interatomic interactions, for instance chemical reactivity of material surfaces [2]. Understanding the chemistry that drives interfacial reactions between a solid surface and an atmosphere or an electrolyte holds the key for future applications in energy harvesting, including more efficient solar cells and carbon sequestration.

Ultimately, our objective is to run computational experiments which will expedite and reduce the cost of developing new nanomaterials and nanostructures, by allowing experimentalists to avoid the trial-and-error approach currently employed.

In this project, we will develop 1) machine-learning-based potentials to study materials with important technological applications, for which reliable classical potentials do not exist and 2) faster and more accurate algorithms and computer codes to run machine-learning based atomistic simulations. Specific topics include, but are not limited to, elemental phosphorus for 2D applications, nanostructured carbon, free energy estimates from machine-learning-based molecular dynamics, machine learning of van der Waals interactions, development of new models for computational X-ray spectroscopy, and new improved algorithms to compute many-body descriptors. The candidate student is welcome to inquire about the specific projects and to choose the one that best fits their interests. For further information and informal inquiries about the project, contact Miguel Caro (miguel.caro@aalto.fi).


Correlations in thermodynamics of open quantum systems

Thermodynamics is one of the most successful theories to describe macroscopic systems. In contrast, quantum mechanics successfully describes nature in microscopic level. Revisiting thermodynamics as a theory emerging from quantum mechanics (without resorting to extra assumptions such as ergodicity and equipartitions) has recently attracted much attention. Introducing quantum versions of thermodynamic concepts such as heat, work, free energy, temperature, and so on, are still open for investigation in quantum thermodynamics. Analyzing the laws of thermodynamics and investigating their validity in quantum regime [1], and employing quantum features such as superposition and entanglement to enhance quantum heat engines to work beyond their classical limits are among other subjects of interest in quantum thermodynamics.

In the heart of quantum thermodynamics lies open quantum system theory, since thermodynamics usually involve a system in interaction with some heat baths—hence, the system is open. Studying the role of quantum correlations in energy exchanges between the system and the heat baths as well as their function in thermalization and equilibration are among the most important questions in this field. This can also help better understand fundamental phenomenon of quantum-classical transition. In addition, we will employ techniques and concepts in open quantum system theory in order to engineer suitable heat baths or environment for specific applications. This will be used to control thermodynamic properties of the system such as heat flow or to realize quantum heat engines with higher efficiency, and thermodynamic simulation of quantum dynamics.

The specific project that we are going to follow is to study the role of quantum correlations in thermodynamic properties of open quantum systems. To this end, we use our recently developed dynamical equation for open quantum systems, in which system-bath correlations are explicitly present [2]. Using this equation, we analyze energy exchange between the system and the heat bath as well as conditions for equilibration and thermalization. Our focus will be on unambiguously understanding the role of correlations in these thermodynamics processes. We will use the acquired insight to design a quantum heat engine which uses correlations to enhance its power beyond its classical limits. Figure 1 shows a typical quantum heat engine, with isothermal strokes I and III, and thermalizing strokes II and IV where the system thermalizes with the hot and cold heat baths, respectively. Employing and controlling quantum correlations to speed up thermalization and to increase the extracted work will lead to power maximization of the heat engine.

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