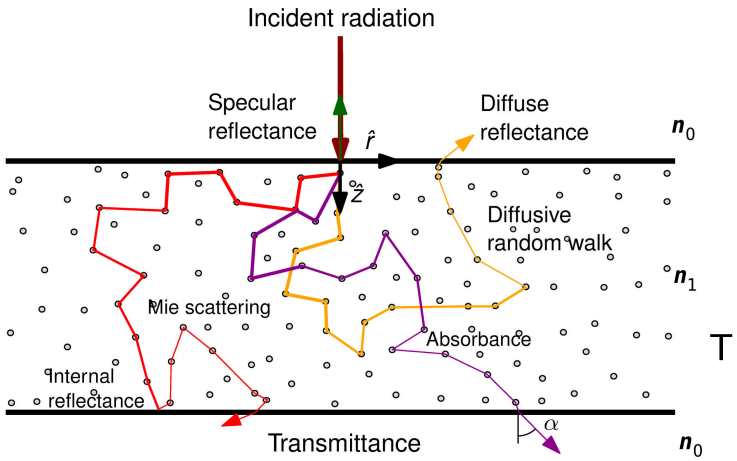
Highly reflective coatings for thermal radiation sensors

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 instaneously, 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 sharp surface scattering modes of semi-conductors reflect specific wavelengths and 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 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). 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.

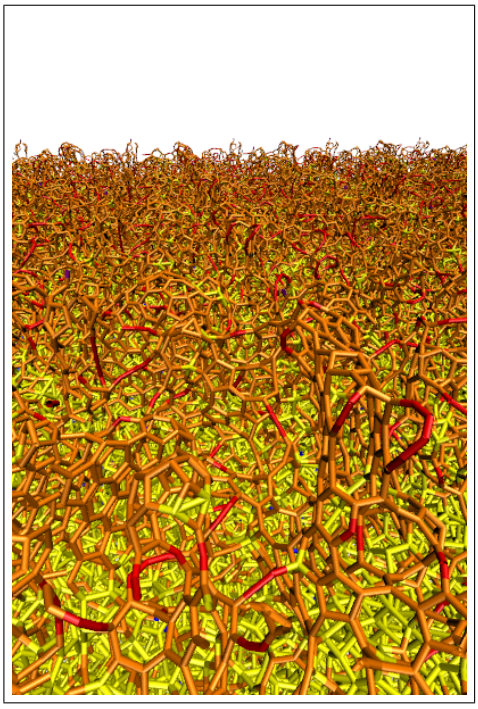

Figure 1: Tetrahedral amorphous carbon film grown by simulated deposition.

In this project, we will develop machine-learning-based potentials to study materials with important technological applications, for which reliable classical potentials do not exist. Initially, we will focus on elemental phosphorus and will use our new potential to study heat conductivity and other properties of 2-dimensional black phosphorus.

For further information and informal inquiries about the project, contact Miguel Caro (miguel.caro@aalto.fi).