Modeling Complex Atomic Structures with the Surface Integral Equation Method

P. Mavrikakis[1], **N. Brosseau-Habert**[2], **M. Devel**[2], **and O. J. F. Martin**[1]

[1]École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland
[2]FEMTO-ST Institute, 25000 Besançon, France

Abstract— The simulation of electromagnetic interactions in extremely small-scale and complex structures is crucial for advancing our understanding in various scientific and engineering fields such as photonics, chemistry, biology, and nanotechnology. Surface integral equations (SIEs) provide a robust framework for modeling these interactions, including complex atomistic geometries where volumetric methods may become computationally prohibitive. This is illustrated in Fig. 1, where we show the scattering cross section (SCS) and the near-field distribution for a soot particle built from 2753 Carbon atoms. In this work, in order to model such intricate geometries, we resort to the SIE method, which is based on the integral form of Maxwell's equations. A finite element approach is used to discretize the equations and the T-PMCHWT (Poggio, Miller, Chang, Harrington, Wu, and Tsai) formulation is considered [1]. We emphasize the method's accuracy and computational efficiency while showcasing its versatility in capturing both near-field and far-field electromagnetic responses of diverse atomic configurations. Using multipoles expansions obtained from the full-field electromagnetic calculations, we demonstrate the far-field response of complex atomistic geometries. Furthermore, by applying Green's function singularity subtraction, we accurately resolve near-field patterns, emphasizing the influence of geometric smoothness on the electromagnetic response of ideal and intricate atomic structures. Another significant aspect of this work is the extension of the SIE framework to stratified media, enabling the modeling of small-scale scattering bodies situated in layered backgrounds. Stratified media are common in natural and engineered systems, such as biological tissues, nanophotonic devices, and multilayer coatings, where the electromagnetic properties vary across layers. We detail the incorporation of Green's function for stratified media into the SIE formalism, highlighting its role in accurately capturing the interaction between the scatterer and its surrounding layers. The presence of layered media usually exerts a significant influence on scattering and absorption characteristics, necessitating specialized adaptations in the integral equation framework to accurately account for these interactions, while preserving the computational efficiency by maintaining the number of unknowns constant.

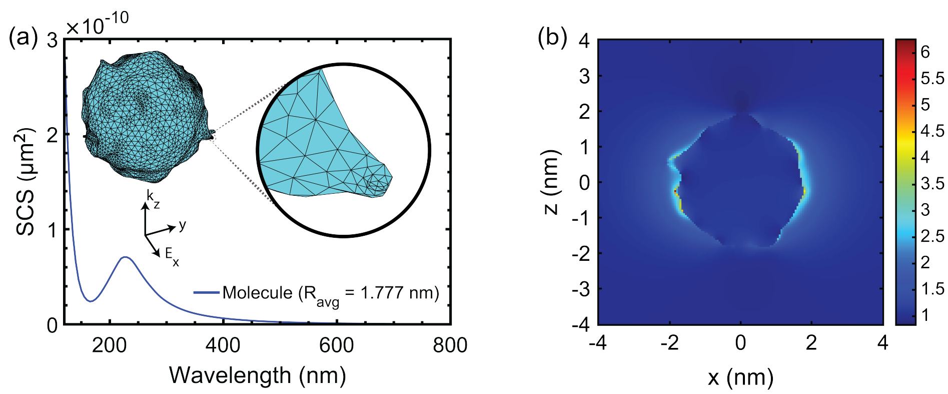

Figure 1: Atomic soot structure with average radius $R_{avg} = 1.777\,\text{nm}$ (a) scattering cross-section, and (b) near-field intensity $|\mathbf{E}|^2$ pattern ($\lambda = 225\,\text{nm}$) for a x-polarized incident plane wave propagating towards z.

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