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Published in:
Proceedings of European Optical Society Annual Meeting (EOSAM 2016)

Publication date:
2016

Document Version
Publisher's PDF, also known as Version of record

A two-stage model of rough-interface scattering for embedded nano-structures

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Summary

We decompose scattering by nanostructures on rough substrates into two surface transfer functions: one heuristic, computed for the bare substrate from experimental BRDF data, and the other sparse and constructed for nanostructures on smooth surfaces. We explore numerically the performance and the commutativity of this approach.

Introduction

Fast and accurate scatterometric characterisation of nano-structures embedded in rough substrates is challenging; the inverse scheme has to deal with the unknown roughness or contamination of the substrate, while retaining the mathematical and computational simplicity of the forward model. Common scattering models for rough surfaces [1] tend to complicate and slow down forward field solvers, at least when included naïvely. We here [2, 3] model the scattering by the product of two transfer functions: a heuristic surface transfer function H_{rough} that accounts for the roughness and the contamination, and a synthetic transfer function H_{nanostr}, computed numerically for the nano-structure embedded in a smooth substrate. This keeps the problem geometry simple and allows the use of the efficient Method of Fundamental Solutions (MFS) solver with complex images [3] to compute H_{nanostr}.

Heuristic and synthetic surface transfer functions

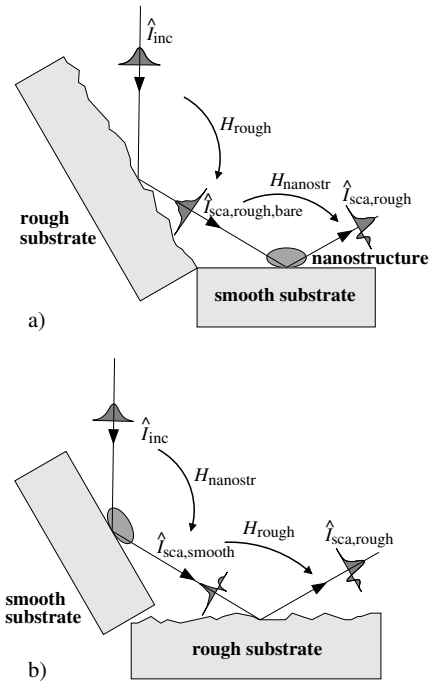

Fig 1. Two ways of multiplying the heuristic and the synthetic surface transfer function.

Figure 1 illustrates how we decompose the scattering process. The Fourier transforms $\widehat{I}_{\text{inc}}$ and $\widehat{I}_{\text{sca,rough}}$ of the incident and the scattered power pattern, respectively, are related via a surface transfer function H via $\widehat{I}_{\text{sca,rough}} = H\widehat{I}_{\text{inc}}$, where $H \approx H_{\text{nanostr}}H_{\text{rough}}$ (Figure 1a) or $H \approx H_{\text{rough}}H_{\text{nanostr}}$ (Figure 1b). While the product of the two transfer functions is itself commutative, the different orders in which the functions are multiplied result in different numerical implementations. To compute the transfer function H_{rough}, we measure the BRDF for the bare rough contaminated substrate, denoise the corresponding scattered power pattern $I_{\text{sca,rough,bare}}$ by Gaussian fitting, and find $H_{\text{rough}} = \widehat{I}_{\text{sca,rough,bare}}/\widehat{I}_{\text{inc}}$. The transfer function H_{nanostr} is realised by a numerical scheme based on the MFS with complex images [3]. This scheme is sparse and fast,

and, crucially, it can here be used in its original, simple form involving half-space Green's functions because our decomposition ensures the substrate-air interface is smooth and planar in the computation of H_{nanostr}. Consequently, our forward computation, and any inverse scheme using it, is only negligibly slower compared to the roughness-free MFS forward computation.

Numerical results and discussion

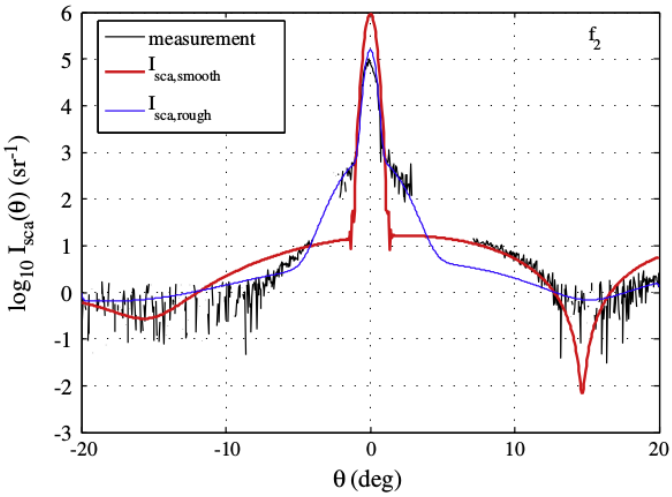

Fig 2. Measured and simulated angular-resolved scattered power for a Pt submicron wire on a rough contaminated Si substrate.

Figure 2 shows a representative result of the inclusion of our heuristic surface transfer function in the scattering model in terms of the product $H \approx H_{\text{rough}} H_{\text{nanostr}}$. The improvement in the predicted scattered power pattern, compared to a roughness-free forward model, is especially noticeable in the angular interval between specular reflection and wide-angle scatter, $3^\circ < |\theta| < 5^\circ$. The root mean square error over the whole angular interval $[-20^\circ, 20^\circ]$ is 0.3754 for our forward model and 0.6386 for the roughness-free MFS forward computation. Our numerical investigation showed that the decomposition $H \approx H_{\text{rough}} H_{\text{nanostr}}$ generally yields better-quality results than the decomposition $H \approx H_{\text{nanostr}} H_{\text{rough}}$.

Conclusion and perspective

For nano-structures embedded in rough material interfaces, it is possible to incorporate the surface roughness and contamination into the scattering model without compromising the mathematical simplicity of the model, or the accuracy and speed of the computation. We achieved this by a formal decomposition of the scattering process into two distinct and different subprocesses, de-coupling roughness effects from the interaction of the nano-structure with the material interface. With the heuristic approach to finding the surface transfer function H_{rough} presented here, we expect our decomposition strategy to be especially advantageous in the characterisation of complicated structures such as rough, contaminated multi-layered structures with embedded nano-particles. It will also be of interest to investigate how this decomposition performs when the surface transfer functions H_{rough} and H_{nanostr} are obtained differently than presented here – for example, H_{rough} can be expressed using an effective medium layer description, or a statistical description of the surface roughness.

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