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Modeling the radiative properties of semitransparent wafers with rough surfaces and thin-film coatings

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Abstract

Semitransparent materials with rough surfaces and coatings have a wide range of applications. This work incorporates the thin-film optics formulation into the Monte Carlo ray-tracing method to predict the radiative properties of semitransparent wafers, considering the effect of surface roughness and a thin-film coating. Multiple reflections with interference inside the coating are included by assuming the uniform coating thickness. On the other hand, geometric optics is applied to trace the rays at the top and bottom surfaces of the wafer as well as inside the wafer. Instead of generating a random rough surface a priori, a weighted probability density function, based on the surface slope distribution and the projected area, is used to determine the microfacet orientation each time a ray hits the interface. The computational code has been validated against the conservation of energy and the reciprocity principle. The studied examples using Si wafers and either a SiO_2 or Au coating demonstrate the strong influence of roughness and coating on the bidirectional and directional—hemispherical radiative properties. This study helps gain a better understanding of the radiative properties of semitransparent wafers with rough surfaces and will have an impact on semiconductor processing.

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Keywords: Radiative properties; Bidirectional reflectance; Semitransparent; Thin-film coating; Rough surface

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1. Introduction

Silicon is a semiconductor that plays a vital role in integrated circuits and microtechnology [1]. Semitransparent crystalline silicon solar cells can improve the efficiency of solar power generation [2]. Accurate radiometric temperature measurements of silicon wafers and heat transfer analysis of rapid thermal processing furnaces require a thorough understanding of the bidirectional radiative properties of the silicon wafer, whose surface may be rough and coated with dielectric or absorbing films [3]. In fact, surface imperfection by roughness and modification by coatings can significantly affect the radiative properties of a material [4]. The radiative properties of layered structures with perfectly smooth surfaces can be accurately predicted by electromagnetic-wave theory [1,5]. However, the rigorous EM-wave theory has limited success in dealing with two-dimensional rough surfaces due to the unknown nature of surface statistics and the requirement of formidable computational resources [6]. Therefore, many approximation methods have been developed [7]. One of those is the geometric-optics approximation (GOA), which models a rough surface as an aggregate of small and mirror-like surfaces, called microfacets, upon which the incident rays are specularly reflected or refracted according to Snell's law [8]. The GOA can easily include multiple scattering and shadowing, but it cannot take into account the interference effects. For the GOA to be applicable, it is generally assumed that both the autocorrelation length (τ) and the root-mean-square (rms) roughness (σ) are greater than the wavelength (λ) of concern [6].

Although many researchers have studied the bidirectional radiative properties of rough surfaces, very few studies dealt with thin-film coatings on the rough surfaces. Tang et al. [9] used the Monte Carlo method to study the effect of thin-film coatings on the bidirectional reflectance of rough surfaces. They treated the coating with thin-film optics and the scattering from rough surfaces with the GOA. Good agreement was obtained between the predicted and measured bidirectional reflectance. However, the substrate was assumed to be semi-infinite [9]. The studies of semitransparent materials with rough surfaces are even rarer. Zhou and Zhang [10] developed a model to trace the rays between the surfaces of a semitransparent wafer by statistically determining the microfacet orientation each time a ray hits the interface, without generating a two-dimensional random rough surface a priori. This procedure can be integrated into the Monte Carlo method to compute the bidirectional reflectance and transmittance, the directional–hemispherical reflectance and transmittance, and the directional emittance of a semitransparent wafer. The effect of a thin-film coating, however, was not included. Furthermore, without considering the influence of the projected area on the probability of microfacet slope generation, previously calculated results [10] deviated from the reciprocity principle, which states that the bidirectional reflectance remains the same when the incidence and reflection directions are interchanged [5]. Prokhorov and Hanssen [11] used a similar method to study the heat transfer between rough surfaces. However, their predicted bidirectional reflectance also failed to observe the reciprocity principle.

The present study extends the previous works [9,10] by including thin-film coatings on semitransparent wafers with rough surfaces. In order to ensure the reciprocity of the calculated bidirectional reflectance and transmittance, a weighted probability density function that takes into account the projected area of the microfacet is introduced for the determination of the microfacet orientation.