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Antireflection coating for sapphire with consideration of mechanical properties

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ABSTRACT

A theoretical model based on the model of elasticity is used to simulate the stress field of several simplified single- and multilayer coatings under indentation load. Based on these results the stresses relevant for the failure of the coating are identified. The influence of different coating parameters like thickness, material choice and layer arrangement is examined. The results of this analysis are considered when designing an antireflective coating with optimized mechanical resilience. A modified coating is deposited and the scratch resistance is compared to an established coating. As indicated by the simulation the optimized coating shows an enhanced scratch resistance.

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1. Introduction

The daily usage of optical surfaces exposes them to mechanical stresses that eventually might damage the coating. Usually the optical and mechanical properties of thin films have been examined separately. There are extensive amounts of literature regarding tribological coatings without optical function [1–3]. Biomaterials like nacre, a nanocomposite of calcium carbonate and different proteins, are known for their exceptional fracture toughness. The mechanical properties of the composites may significantly exceed those of its constituents [4]. So far these aspects have not been regarded in the design of optical interference coatings. Basically there are multiple solutions to create an interference coating with a specified optical performance [5]. Therefore it should be possible to realize different coatings with varying mechanical resilience even for a given set of coating materials.

Optical coatings always pose a weak spot for the mechanical very resilient substrate material sapphire. On the other hand the excellent scratch and abrasion resistance of sapphire should be preserved when applying optical coatings such as antireflective (AR) coatings. In this study the mechanical behavior of thin film coatings is simulated to gain additional information that can be used during the design stage to optimize the mechanical resilience of antireflective coatings on sapphire. Key parameters are the total thickness of the multilayer stack and a reasonable arrangement of the layers that has to realize the optical function as well. The simulations are based on the theory of elasticity [6]. They examine the elastic deformation of a multilayered system under a defined load caused by spherical particles. The software allows it to calculate the complete elastic field of a complex multilayer and to evaluate it with a spatial resolution of single nanometers [7]. Input values for the simulation are the mechanical parameters, especially Young's modulus (E) and yield strength (Y), of the layer materials SiO_2 and HfO_2. HfO_2 had been determined experimentally as the most promising high-refractive material for a durable antireflective coating [8]. Silica is the only possible durable low-index material for AR-coatings.

2. Experimental

Single layer coatings with a thickness of 240 nm have been prepared to determine the mechanical properties of the layer materials SiO_2 and HfO_2. Several multilayer AR coatings were produced to compare the optical and mechanical properties of the different designs. All coatings were prepared on a Leybold APS-904 boxed coater using plasma-ion-assisted deposition (PIAD) [9]. This coating chamber is equipped with an advanced plasma source (APS) and two electron beam guns for evaporation. During the deposition process the growing film is densified by bombardment with argon ions emitted from the plasma source. To ensure dense layers the APS-bias voltage was kept in a high energy range (130–140 V) and a slow deposition rate (0.2 and 0.5 nm/s) was chosen.

To characterize the mechanical properties of the used materials several indentation measurements were performed using a UNAT nanoindenter (ASMEC GmbH). Since the sapphire substrates comply with the assumption of a homogenous elastic half space, static indentation with a conventional Oliver-Pharr-Analysis (OP-Method) was sufficient to determine the Young's modulus [10].

To simulate the mechanical behavior of thin film coatings and to determine the mechanical constants of the coating materials the FilmDoctor software suite was used [7]. For the simulation a contact situation is defined by choosing an indenter shape and material and the load the indenter applies to the coating. Based on this information

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the pressure distribution that acts on the coating is calculated. The coating is defined using thickness, Young's modulus and Poisson's ratio of the individual layers and the substrate. Now the complete elastic field (stresses, strains and deformations) for the loaded coating is calculated. This model uses the concept of the effective indenter [11] and an extension of the Hertzian approach [12] to create an analytically solvable pressure distribution for indenters with arbitrary symmetry of revolution. Some methods from the potential theory are used to generalize the calculations from an isotropic elastic half space to a layered elastic half space [6,13].

The Optilayer software package was used for the design of the different optical coatings [14]. It provides the necessary tools to determine the optical constants of a coating material from the spectra of a single layer coating and to calculate the optical performance of a given multilayer stack. Furthermore it offers several synthesis and optimization algorithms to modify a starting multilayer so that the optical performance matches a desired target function. It is possible to limit the thickness variation of certain layers within defined bounds.

The scratch resistance of the coatings was characterized using a scanning scratch tester (Shimadzu SST 101). This device uses a diamond needle with a spherical tip of 10 μm diameter to scratch the surface of the sample. An increasing normal load in the range of 0 to 1000 mN is applied. The critical load is defined by the failure of the coating.

Transmission and reflectance of the samples were measured using a spectral photometer (Perkin Elmer, Lambda 900). The samples were characterized for wavelengths between 300 and 900 nm with a spectral resolution of 2 nm. The accuracy for the measured intensity was better than 0.2 %.

3. Results and discussion

3.1. Simulation

Single layers of SiO_2 and HfO_2 have been deposited on sapphire by PIAD. These samples were used to determine the Young's modulus and the yield strength of the materials. As these samples form a layered half-space instead of a homogenous one the OP-Method would not give the correct results. Instead the “Oliver & Pharr for Coatings” module of the FilmDoctor software is used. It accounts for the known mechanical parameters of the sapphire substrate when calculating the moduli of the films. The values are given in Table 1.

Scratches on coated glass mostly result of hard particles the size of a few microns that happen to be in the loaded area, for example when cleaning with a piece of cloth. Therefore the simulated contact situation uses a spherical diamond indenter ($E = 1141$ GPa) of 10 μm radius and a load of up to 25 mN. This research focuses on the influence of external stresses as source of coating damage. To achieve comparable results all coatings are regarded as free of intrinsic stresses for the calculations.

As the simulation software is limited to the elastic deformation one has to be aware of the limits of elasticity. Usually the yield strength gives the stress limit for a uniaxial stress that can be tolerated without plastic deformation. The indention of a multilayered system will not cause a uniaxial stress, but a stress tensor composed of multiple normal and tensile stresses. Therefore the *von Mises* stress is used to indicate a coating failure. The *von Mises* stress σ_{vM} is a scalar equivalent stress that is calculated from the stress tensor. While the *von Mises* stress stays below the yield strength of the layer material, the occurring deformation is considered elastic. It is reversible and after the unloading no residual deformation will remain. When the *von Mises* stress surpasses the yield strength, plastic deformation will occur. This implies a failure of the coating. Therefore a coating material with high yield strength is more resilient to plastic deformation. The FilmDoctor software allows it to calculate the stresses within a multilayer system with consideration of the used materials and the layer arrangement. This model is not suited to describe the formation of fractures which depends on the surface geometry, superficial defects and the materials fracture toughness. Once a fracture appears the stress distribution within the multilayer system changes drastically. Therefor this study will be restricted to the case of plastic deformations.

Table 1
Comparison of Young's moduli (E), Yield strengths (Y) and Poisson's ratios (ν) for the substrate and the layer materials.

Material	E (GPa)	Y (GPa)	ν
Sapphire	445	27.7	0.235
SiO_2	56	5.1	0.25
HfO_2	134	7.2	0.235

At first simplified models for the materials and single layers under load are considered. Fig. 1 shows the distribution of the *von Mises* stress along the axis of rotational symmetry below the indenter. The different materials are regarded as bulk materials. The higher the Young's modulus of the material, the lower is the elastic deformation of the substrate and the higher are the occurring *von Mises* stresses. Furthermore the maximum of the *von Mises* stresses lies deeper below the substrate surface as the Young's modulus of the material decreases. For this example with a load of 25 mN the maximum of the *von Mises* stress is below the yield strength of each material. Consequently no plastic deformations are expected.

Using the example of single layers, the influence of layer thickness on the stress distribution shall be analyzed. For this purpose SiO_2 films of varying thickness on a sapphire substrate are investigated for an indentation load of 25 mN. Fig. 2 shows the stress distribution along the axis of rotational symmetry below the indenter for three films of 50 nm, 200 nm and 1000 nm thickness. The horizontal line marks the yield strength of SiO_2 (5.1 GPa), the vertical lines accent the depth of the film-substrate-interface. For films thinner than 1000 nm the *von Mises* stresses surpass the yield strength of the SiO_2. The higher stiffness of the sapphire substrate forces higher *von Mises* stresses into the film. Only for SiO_2 layers of more than 1000 nm the elastic deformation of the film can compensate the rigidity of the substrate. In general, an increase in film thickness will reduce the *von Mises* stresses for films that have lower Young's moduli than the substrate.

Since real optical systems consist of at least two different layer materials the interfaces between those are also of interest. According to the common nomenclature in thin film optics, S denotes the substrate (sapphire), L the low index material (SiO_2), H the high index medium and A the ambient medium (air). A number gives the geometrical thickness in nm. A simple 3-layer model is used to illustrate the situation in

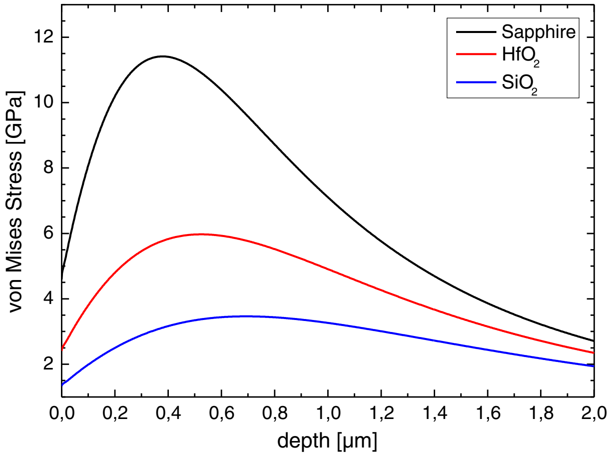

Fig. 1. *Von Mises* stress along the axis of rotational symmetry below the indenter for different materials (simulation parameters: spherical diamond, 10 μm radius, 25 mN).

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