Visibility of single layer MoS$_2$ for different dielectric layers on Si substrate

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Abstract. Molybdenum disulphide (MoS$_2$), the most widely studied two-dimensional transition metal dichalcogenides, has been investigated for many applications such as transistors, sensors and batteries. Understanding the visibility of single layer MoS$_2$ is of great importance to the research and development of the MoS$_2$-based devices. In this work, we thoroughly investigated the visibility of single layer MoS$_2$ for different dielectric layers (including hafnium dioxide, aluminum oxide and silicon oxide) on Si substrate using analytical calculations based on a Fresnel-law-based model. The analysis results provide not only guidance for selecting the right dielectric thickness, but also basis for choosing the appropriate light wavelength at a specific dielectric thickness.

1. Introduction

As a typical example from the layered semiconducting transition metal dichalcogenides family of materials, molybdenum disulphide (MoS$_2$) has been widely studied due to its excellent electrical, mechanical and optical properties [1-4]. Although there are many ways to produce thin-film MoS$_2$ samples, it is different to find small MoS$_2$ crystallites among copious thicker MoS$_2$ flakes. Many methods, such as atomic force microscopy, scanning electron microscopy and Raman microscopy, are capable of distinguishing MoS$_2$ monolayers [5-7]. However, these methods have not yet been automated to allow searching for MoS$_2$ crystallites because of their extremely low throughput at the absence of optical images of MoS$_2$ crystallites. Optical method has been widely used in MoS$_2$ research because it has no damage to the MoS$_2$ material and the recognition process is relatively simple. To get thin-film MoS$_2$ sample, the sample surface needs to be carefully scanned using an optical microscope. Thin film MoS$_2$ flakes can be searched by the contrast between the MoS$_2$ layers and the substrate. Moreover, the contrast decreases with reduction of the number of MoS$_2$ layers [8]. The MoS$_2$ layers’ number could be distinguished by the difference in color (i.e. the difference in contrast) between the MoS$_2$ layers and the substrate. Understanding the origin of this contrast is essential for optimizing the detection techniques and hence expediting the progress for MoS$_2$-based researches.

In this paper, we have thoroughly investigated the dependence of the contrast of single layer MoS$_2$ on dielectric layer thickness and light wavelength using analytical calculations based on a Fresnel-law-based model, wherein the dielectric layer comprises hafnium dioxide (HfO$_2$), aluminum oxide (Al$_2$O$_3$) and silicon oxide (SiO$_2$). It was noting that the contrast analysis results of SiO$_2$ layer are consistent with the measured results given in other paper [8]. The results of this work can be used to expedite MoS$_2$-related experiments by maximizing the contrast of single layer MoS$_2$ by choosing the optimized dielectric layer thickness and light wavelength.
2. Analytical calculations

The visibility of single layer MoS$_2$ is characterized in terms of the Michelson contrast [9]. Figure 1 shows a schematic of optical reflection and transmission for the layered thin-film system. The left part has three layers consisting of MoS$_2$, dielectric and Si, while the right part has two layers.

The contrast $C$ is defined as the relative intensity of reflected light without and with single layer MoS$_2$ [10],

$$ C = \frac{I(n_1 = n_0) - I(n_1)}{I(n_1 = n_0) + I(n_1)} $$  \hspace{1cm} (1)

Where, $I(n_1 = n_0)$ and $I(n_1)$ are the reflected light intensity without and with single layer MoS$_2$, respectively. In our calculation, the light is considered to be incident from air (refractive index $n_0 = 1$) and the substrate Si layer is assumed to be semi-infinite. The refractive index of single layer MoS$_2$, dielectric and Si layer are $n_1 (\lambda)$, $n_2 (\lambda)$ and $n_3 (\lambda)$, respectively. Using the described geometry, the reflected light intensity can be written as [11]:

$$ I(n_1) = \left( r_1 e^{i(\phi_1 + \phi_2)} + r_2 e^{-i(\phi_1 - \phi_2)} + r_3 e^{-i(\phi_2 + \phi_3)} + r_1 r_2 r_3 e^{i(\phi_1 - \phi_3)} \right) $$

$$ \times \left( e^{i(\phi_1 + \phi_3)} + r_1 r_2 e^{-i(\phi_1 - \phi_3)} + r_1 r_3 e^{-i(\phi_2 + \phi_3)} + r_2 r_3 e^{i(\phi_2 - \phi_3)} \right)^{-1} $$  \hspace{1cm} (2)

Where, $\phi_1 = \frac{2\pi n_1 d_1}{\lambda}$ and $\phi_2 = \frac{2\pi n_2 d_2}{\lambda}$ are the phase shifts due to the change in the optical path. $d_1$ and $d_2$ are the thicknesses of single layer MoS$_2$ and dielectric layer. $r_1$, $r_2$ and $r_3$ are the relative indices of refraction. Their expressions are defined as follows:
3. Results and discussion

The light source used in the microscope is generally a halogen lamp, and the wavelength range of light is about 400-760 nm, which is, the range of the incident light wavelength $\lambda$. The complex refractive index of highly crystalline single-layer MoS$_2$ is adopted from the literature [8] in which the high-quality single-layer MoS$_2$ is synthesized using a chemical vapor deposition method. The refractive index of HfO$_2$ and Al$_2$O$_3$ are obtained from Sopra Material Database. The refractive index of SiO$_2$ and Si layer are characterized by $\lambda$-dependent functions as suggested in [12-13]. The thickness of single layer MoS$_2$ is assumed to be about 0.65 nm [2], while the thickness of the dielectric material is set to be 0-450 nm, referring to the contrast distribution profile of single-layer MoS$_2$ on SiO$_2$ dielectric material [8]. By substituting different parameters, we can obtain the contrast of single-layer MoS$_2$ for different dielectric layers on Si substrate.

The three-dimensional (3D) and two-dimensional (2D) contrast distributions of single layer MoS$_2$ for HfO$_2$ dielectric layer on Si substrate are shown in Figure 2 (a) and (b). The highest contrast of single-layer MoS$_2$ for HfO$_2$ dielectric layer is 0.9994, which is very close to 1. As can be seen from Figure 2, the contrast exhibits a periodic fluctuation with the change in the thickness of the HfO$_2$ layer and the wavelength of the incident light. Generally, the contrast that the human eye can recognize is greater than 0.02. For HfO$_2$ dielectric on Si substrate, when the thickness of HfO$_2$ layer is below 18 nm, or within the 122-135 nm range, the human eye cannot observe a single layer of MoS$_2$. It means that by using filters, single layer MoS$_2$ can be visualized of any HfO$_2$ thickness except for 122-135 nm and below 18 nm.

![Figure 2. 3D (a) and 2D (b) contrast map as a function of wavelength and film thickness for HfO$_2$ layer on Si.](image)

The 3D and 2D contrast distributions of single layer MoS$_2$ for Al$_2$O$_3$ dielectric layer on Si substrate are plotted in Figure 3 (a) and (b), respectively. The contrast also exhibits a periodic fluctuation with the change in the thickness of the Al$_2$O$_3$ layer and the wavelength of the incident light. The highest contrast of single-layer MoS$_2$ for Al$_2$O$_3$ dielectric layer is 0.5682. From the calculation results, single

$$
R_1 = \frac{n_0 - n_i}{n_0 + n_i} \\
R_2 = \frac{n_i - n_2}{n_i + n_2} \\
R_3 = \frac{n_2 - n_3}{n_2 + n_3}
$$

(3)
layer MoS$_2$ can be visualized of any Al$_2$O$_3$ thickness except for the 106 nm, 133-146 nm and below 18 nm.

**Figure 3.** 3D (a) and 2D (b) contrast map as a function of wavelength and film thickness for Al$_2$O$_3$ layer on Si.

As shown in Figure 4 (a) and (b), the contrast exhibits a periodic fluctuation with the change in the thickness of the SiO$_2$ layer and the wavelength of the incident light. The highest contrast of single-layer MoS$_2$ for SiO$_2$ dielectric layer is 0.3266. From the calculation results, single layer MoS$_2$ can be visualized of any SiO$_2$ thickness except for 124-134 nm and below 17 nm. As an example, three monochromatic images of single layer MoS$_2$ are shown in Figure 4 (c) [8], where the SiO$_2$ layer is 262 nm in thickness. The calculated contrasts of single-layer MoS$_2$ under 445, 526 and 672-nm incident light are about -0.0498, 0.1629, and 0.0368, which are consistent with the monochromatic images in Figure 4 (c).

**Figure 4.** 3D (a) and 2D (b) contrast map as a function of wavelength and film thickness for SiO$_2$ layer on Si. (c) The monochromatic images of single layer MoS$_2$ under 445, 526 and 672-nm incident light, respectively.
To summarize, Figure 5 (a) compares the contrast distribution for three dielectric layers on Si substrate. The relationship between the refractive index of three dielectric layers and the incident light wavelength is shown in Figure 5 (b). It can be seen that the greater refractive index of the dielectric layer will lead to the higher contrast of single layer MoS$_2$. In order to more easily distinguish single-layer MoS$_2$ in practical experiments, a dielectric layer having a greater refractive index is suggested to be used.

4. Conclusions
We have investigated the visibility of single layer MoS$_2$ for three different dielectric layers (including HfO$_2$, Al$_2$O$_3$ and SiO$_2$) on Si substrate. The calculated results are validated and compared with the monochromatic images. It is found that the contrast depends on both the dielectric thickness and the light wavelength. The dielectric material with greater refractive index is revealed to be able to achieve higher contrast of single layer MoS$_2$. The results of this work can be used as an effective guidance to expedite MoS$_2$-related experiments.

Acknowledgments
This work was supported by the National Natural Science Foundation of China (Nos. 61474028, 61774042) and National S&T Project 02 (No. 2013ZX02303-004).

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