# Using the compensating effect for Rayleigh anomalies to design a type of broadband mid-IR grating 

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We suggest and numerically demonstrate a specific design method of broadband mid-IR echelette grating. The method, which applies the compensating of the efficiency blaze in TM-plane polarization to Rayleigh anomalies, is called compensating effect method. This idea allows the grating designer to realize fully the considerable advantages of this type of echelette grating with an apex angle $90^{\circ}$ and a blaze angle $19.47^{\circ}$, especially, it can be fabricated easily with conventional (holographic and ruled) techniques. Its diffraction efficiency in unpolarized light has a minimum value of $40 \%$. The cases of Littrow mount and off-Littrow mount are both discussed.
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## References and links

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## 1. Introduction

The broadband spectrum is required in a infrared spectrophotometer, however, the spectrum of the commonly used grating is so limited that an instrument needs to be equipped with several gratings, for example, the IR-G type and IR-G type spectrophotometer [1]. The company of Hitachi further demonstrated a kind of plane dual-blaze grating [2] that can
achieve efficiency blaze both at $3 \mu \mathrm{~m}$ and $10 \mu \mathrm{~m}$. Its shape is similar to the convex dual-blaze grating in Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) that has two concentric panels, with each panel blazed at a different angle [3, 4]. Afterwards, we also fabricated a dual-angle blaze grating that is called the polygonal grating by PCGrate-SX software. It has an apex angle and two blaze angles that correspond to two blaze surfaces separately, Fig. 1 shows its scanning probe microscope scan at the dual-blaze boundary. Similarly, another polygonal grating (with a different profile consisting of a symmetry triangle groove $70.5^{\circ}$ apex angle and a flat region at the bottom) described by [5] can obtain high efficiency, but the spectral interval is not so broad.


Fig. 1. Atomic-force microscope scan of the polygonal grating
However, all these types are difficult or impossible to produce with conventional (holographic and ruled) techniques. Recently, on the base of integral theory of infinite conductivity gratings [6], after analyzing the characteristics of Rayleigh anomalies and blaze effect of efficiencies, we focus on the compensating effect of the blaze in TM-plane polarization to the Rayleigh anomalies. Utilizing the compensating effect that is not only applied in Littrow mount but in off-Littrow mount, a type of broadband, mid-IR, metallic, and echelette grating using in the range of $4 \sim 22 \mu \mathrm{~m}$ is designed. The grating is a single-panel, true blazed grating with an apex angle $90^{\circ}$, a blaze angle $19.47^{\circ}$ and a grating period $11 \mu \mathrm{~m}$. Obviously, it can be fabricated easily with conventional techniques.

## 2. The positions of Rayleigh anomalies

Rayleigh anomalies [7, 8] play a significant role in the efficiency of mid-IR grating, especially, the anomalies of TM-plane [9] do. Their positions can be derived by the grating equation

$$
\begin{equation*}
\sin \theta_{m}=\sin \theta_{i}+m \frac{\lambda}{d} \tag{1}
\end{equation*}
$$

where $\theta_{m}$ is the diffraction angle, $\theta_{i}$ is the incidence angle, $m$ is an integer, $\lambda$ is the wavelength and $d$ is the grating period. Using Eq. (1), the grating equation in Littrow mount becomes

$$
\begin{equation*}
2 \sin \theta_{i}=-m_{\varepsilon} \lambda / d \tag{2}
\end{equation*}
$$

where $m_{\varepsilon}$ is one of the Littrow order. Because a Rayleigh wavelength type is due to the emergence of a new spectral order at grazing angle, according to Eqs. (1) and (2), the positions of Rayleigh anomalies are determined by

$$
\begin{equation*}
\frac{\lambda_{R}^{m}}{d}= \pm \frac{2}{2 m-m_{\varepsilon}} \tag{3}
\end{equation*}
$$

where $\lambda_{R}^{m}$ is called Rayleigh wavelength, " + "corresponds $m \geq 0$, " - "corresponds $m<0$.

## 3. The blaze characteristics of diffraction efficiency

The blaze characteristics of diffracted wave vectors with different plane polarizations are different. Taking the $-1^{\text {st }}$ order Littrow mount for example, usually the perfectly metallic echelette gratings with an apex angle $\phi=90^{\circ}$ and a blaze angle $\alpha$ in TM polarization has three blaze wavelengths $\lambda_{b 1}, \lambda_{b 2}$ and $\lambda_{b 3}$. The equation $\lambda_{b 1}=2 d \sin \alpha$ can be derived from Maré chal-Stroke theorem [10]. The equation $\lambda_{b 2}=2 d \cos \alpha$ is a deduction of the reciprocity theorem [11]. According to numerical calculations, $\lambda_{b 3}$ is close to and slightly greater than $\lambda_{R}^{1}$. For the grating with blaze angle $\alpha=10^{\circ}$, its three blaze wavelengths of TM-plane are presented in the left-hand side of Fig. 2.

Unlike the TM-plane, the commonly used echelette grating (the groove depth is less than a wavelength) has only one blaze wavelength in TE-plane. Its position is not rigorous and located where is close to and slightly greater than $\lambda_{R}^{m} / d$. When Eq. (3) gets " + ", and Eq. (3) is equal to Eq. (2), we have

$$
\begin{equation*}
\sin \theta_{R}^{m}=\frac{-m_{\varepsilon}}{2 m-m_{\varepsilon}} \tag{4}
\end{equation*}
$$

where $\theta_{R}^{m}$ is a Rayleigh diffracted angle that corresponds Rayleigh anomaly. Adopting $m_{\varepsilon}=-1$ and $m>0$, the different values of $m$ correspond to different positions of Rayleigh diffracted angles and Rayleigh wavelengths. Based on the numerical calculations, the blaze wavelength in TE-plane is usually located where is slightly greater than $\lambda_{R}^{m+1} / d$ if the condition $\theta_{R}^{m}<\alpha<\theta_{R}^{m+1}$ is satisfied. The right-hand side of Fig. 2 shows that the locations of the blaze wavelengths in TE-plane when $\alpha$ varies from $5^{\circ}$ to $25^{\circ}$.


Fig. 2. The efficiencies of perfectly metallic echelette gratings show the efficiency blaze for both polarizations in $-1^{\text {st }}$ order Littrow mount. Left: the case of TM for the blaze angle $\alpha=10^{\circ}$, Right: the case of TE when $\alpha$ varies from $5^{\circ}$ to $25^{\circ}$.

## 4. The compensating effect of blaze wavelength to Rayleigh anomalies

It is an effective way of realizing broadband to find a method that can remove or weaken Rayleigh anomalies. Firstly, it is necessary to analysis Rayleigh anomalies qualitatively, so we define the name of the strength of Rayleigh anomalies, which is a percent denoted by the absolute value of difference between the efficiency peak and the efficiency valley in the vicinity of Rayleigh anomaly. Secondly, according to the former studies on the Rayleigh anomalies and efficiency characteristics, the numerical calculations represent that the strength
of Rayleigh anomalies are mainly affected by the distances between $\lambda_{b 1}$ and $\lambda_{R}^{m}$ in the axis of $\lambda / d$, i.e., the smaller the distances are, the smaller the strength are. For example, for the echelette grating with $\alpha=5^{\circ}, \phi=90^{\circ}$, Table.1.and the left-hand side of Fig. 3 show the strength of the first Rayleigh anomaly in TM-plane is the greatest, so it directly affects the spectrum performance. Fixing the apex angle $\phi=90^{\circ}$ and increasing of the blaze angle $\alpha$ from $5^{\circ}$ will make $\lambda_{b 1}$ shift to the direction of long wavelength and $\left|\lambda_{R}^{m}-\lambda_{b 1}\right| / d$ be smaller, which weakens the strength of Rayleigh anomalies [12]. Finally, when $\alpha$ is increased to a specific angle $19.47^{\circ}$, the first Rayleigh anomaly coincides with the first blaze wavelength in TM-plane, so it disappears at $\lambda / d \approx 0.667$. Meanwhile, the TM wave vector is still blazing and the blaze wavelength of TE is also close to it, so that the spectrum is broadened effectively. The broadened spectrum is shown by the right-hand side of Fig. 3, where "UN" denotes the efficiency of unpolarized light.

Table. 1. Strength of Rayleigh anomalies for the echelette grating ( $\alpha=5^{\circ}, \phi=90^{\circ}$ ).

| $\lambda_{b 1} / d=0.174$ | $m=3$ | $m=2$ | $m=1$ |
| :---: | :---: | :---: | :---: |
| $\lambda_{R}^{m} / d$ | 0.285 | 0.4 | 0.667 |
| $\left\|\lambda_{R}^{m}-\lambda_{b 1}\right\| / d$ | 0.111 | 0.226 | 0.493 |
| the strength | $5 \%$ | $20 \%$ | $80 \%$ |

Interestingly, the condition of removing the first Rayleigh anomaly and broadening spectrum is exactly the one that obtains the first blaze wavelength for TM polarization, so the phenomenon is called compensating effect of blaze wavelength to Rayleigh anomalies, furthermore, the corresponding design method is simply called compensating effect method.


Fig. 3. The efficiency curves show the influence of the distances between blaze wavelengths and Rayleigh anomalies to the strength of TM Rayleigh anomalies. Left: the case of strong
influence with $\alpha=5^{\circ}$, right: the case of weak one with $\alpha=19.47^{\circ}$.
According to the design example of broadband, mid-IR, metal, and echelette grating, the grating designed by compensating effect method is compared to the polygonal gratings. Keeping the grating period $d=11 \mu \mathrm{~m}$ and the wavelength needs to be greater than $4 \mu \mathrm{~m}$ for the infinite conductivity theory, so the broadest spectrum is $4 \sim 22 \mu \mathrm{~m}$.

There is no definite definition about the broadband, taking into account the application demands of grating in spectrum instruments, we give two definitions. First, the spectrum is called efficiency spectrum if the efficiency of unpolarized light remains above $40 \%$. Second,
the efficiency spectrum is called broadband if it covers the $90 \%$ of the broadest spectrum. For instance, the right-hand side of Fig. 3 shows that the curve shape of the "UN" efficiency looks like the letter " $M$ ". The spectrum of " $M$ " shape is broadband if the two conditions, the efficiencies of the three lowest points of the"M"all remain above $40 \%$ and the"M"covers $90 \%$ of the broadest spectrum, are satisfied. We use the definitions to judge if the spectrum is broad. The left-hand of Fig. 4 shows the compares of efficiencies computed by three design methods, method1 and method 2 for polygonal grating, method3 for echelette grating.


Fig. 4. The compares of efficiency curves in unpolarized light. Left: the compared curves computed by three design methods for echelette and polygonal gratings, right: The efficiency compare of the deep sinusoidal grooves (the ratio of groove depth to grating period is 0.36 ) and echelette grating designed by method 3 .

Method 1 is based on the grating equation that determines the two blaze angles $15.8^{\circ}$ and $72.7^{\circ}$ according to the two blaze wavelength $6 \mu \mathrm{~m}$ and $21 \mu \mathrm{~m}$, if we set 1.44 to 1 the ratio of lengths for the two blaze surfaces and $\phi=90^{\circ}$, the efficiency is so low that it can not be applied. In contrast, Method 2 that is based on the rigorous electromagnetic theory of gratings, optimizes 4 parameters including the two blaze angles $17.5^{\circ}$ and $24.5^{\circ}$, the 1.44 to1 ratio of lengths for the two blaze surfaces and $\phi=90^{\circ}$ (see also Fig. 1) by a mass of numerical calculations. However, though the grating designed by metohd2 can obtain broadband, it has two main defects: one is the complex design; the other one is the narrow span of the parameters due to the effects among the 4 independent parameters, which leads to the impossibility of realizing the theory design in technology. Method 3 that is highly recommended is compensating effect method. The shape of grating ( $\alpha=19.47^{\circ}, \phi=90^{\circ}$ ) designed by this method is not different from the commonly used grating but with the new design idea. Unlike the former methods, its advantages are not only to obtain the broadband, to design simply, but to be fabricated easily with conventional technologies. Obviously, it is superior to the former methods. Otherwise, it should be noted that the efficiency of the echelette grating designed by compensating effect method is not so high as the one of deep sinusoidal grooves grating with the same grating period $(11 \mu \mathrm{~m})$ and the ratio 0.36 of groove depth to grating period [12], however, its spectrum is broader. See the right-hand side of Fig. 4.

## 5. The compensating effect applied in off-Littrow mount

The separation angle $\delta$ between incidence wave vector and one diffracted wave vector is called deviation angle. It affects the efficiency directly, so it is necessary to discuss the effect. If $\delta, \quad \lambda$ and $d$ are all specified, according to Eq. (1) the positions of the Rayleigh anomalies in off-Littrow mount are

$$
\begin{equation*}
\frac{\lambda}{d}= \pm \frac{2 \cos ^{2}(\delta / 2)\left[-m_{\delta}+2 m-2 \sqrt{m\left(m-m_{\delta}\right)} \sin (\delta / 2)\right]}{4 m\left(m-m_{\sigma}\right) \cos ^{2}(\delta / 2)+m_{\delta}^{2}} \tag{5}
\end{equation*}
$$

where $m_{\delta}$ is the off-Littrow order, " + " corresponds to $m>0$ and "-" corresponds to $m<0$. Setting $m_{\delta}=-1$, the influence of $\delta$ to efficiency is reviewed when $\alpha$ is equal to $19.47^{\circ}$.
Figure 5 shows that the spectrum is still broadband as soon as $\delta$ is smaller than $20^{\circ}$ and $\phi$ is between $90^{\circ}$ and $95^{\circ}$, because the larger one will suppress the efficiency and narrow the spectrum [12]. Though Rayleigh wavelength shifts to long wavelength, the shift is basic in the blazing band, i.e. the compensating effect is still working on. In addition, the numerical calculations demonstrate that the efficiency curve will shift to short wavelength or long wavelength in terms of the different grating period, so the different grating with different groove density can be chosen in the light of using spectrum.


Fig. 5. The influence of deviation angle $\delta$ to "UN" efficiency in $-1^{\text {st }}$ order Littrow mount for the gratings with different apex angles but the same blaze angle ( $\alpha=19.47^{\circ}$ ). Left: the apex angle is $90^{\circ}$, right: the apex angle is $95^{\circ}$.

## 6. Conclusion

A design method for broadband mid-IR metal and echelette grating that makes use of the compensating effect of the first blaze wavelength in TM-plane to Rayleigh anomalies is given. Some conclusions about the method can be expressed as: Firstly, the strength of Rayleigh anomalies are mainly affected by the distances between the first blaze wavelength in TM polarization and Rayleigh anomalies. Secondly, the strength will reduce and the blaze wavelength will shift to the direction of the first Rayleigh anomaly if the blazed angle $\alpha$ is increased from $0^{\circ}$ to $19.47^{\circ}$. When the first Rayleigh anomaly coincides with the first blaze wavelength in TM-plane, it disappears and the other Rayleigh anomalies decrease. Thirdly, the compensating effect can be applied in Littrow mount and off-Littrow mount.

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