Development of wideband spectral dispersers for exoplanetary science: comparative study of material, design, and fabrication

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ABSTRACT

We present the development of wideband spectral dispersers of which the primary scientific objective is the characterization of the atmospheres of exoplanets, including the challenge of detecting biomarkers. A disperser comprising a prism with a grating pattern on its surface provides simultaneous wideband coverage with low spectral resolution ($R \geq 300$). The optics is simple, compact, and contains no moving parts. A comparative study of 21 materials for the disperser was carried out for use in the optical, near-infrared, and mid-infrared wavelength regions. KRS-5, CdZnTe, ZnS LiF, Sapphire, and S-TIH11 were selected, and designs of the optics for single-channel wideband spectrometers using the selected six materials were considered. Then, trial designs of the multi-channel spectrometers were carried out taking the properties of the detectors into consideration. The 3-channel design covers the wavelength region of ~0.2−23 μm using a CCD detector, an InSb detector, and a Si:As detector. The 2-channel design covers ~0.4−23 μm using a HgCdTe detector and a Si:As detector. A fabricated ZnS disperser is shown together with a CsI sub-prism which compensates for the optical axis. The application of defocusing, high dispersion spectroscopy, extension to the UV wavelength region, and the combination of the disperser with future space telescopes are discussed.

Keywords: spectrometer, wideband, simultaneous, exoplanet, transit, fabrication, ZnS, space telescope

1. INTRODUCTION

An important issue in space science is characterization of the atmospheres of exoplanets, including the challenging task of detecting biomarkers. The atmospheres of exoplanets have important molecular absorption features in the optical and infrared wavelength regions, e.g., H_2O (0.51, 0.57, 0.65, 0.72, 0.82, 0.94, 1.13, 1.38, 1.9, 2.69, 6.2 μm), CO_2 (1.21, 1.57, 1.6, 2.03, 4.25, 15.0 μm), CH_4 (0.48, 0.57, 0.6, 0.7, 0.79, 0.86, 1.65, 2.2, 2.31, 2.37, 3.3, 6.5, 7.7 μm), NH_3 (0.55, 0.65, 0.93, 1.5, 2.0, 2.25, 2.9, 3.0, 6.1, 10.5 μm), and especially O_3 (4.7, 9.1, 9.6, 14.3 μm), O_2 (0.58, 0.69, 0.76, 1.27 μm) [1]. The temporary differential observation of exoplanets, including monitoring of transits and secondary eclipses of exoplanets, is one of the promising methods used to analyze their atmospheres. For the temporary differential observation of exoplanets, the stability of the observation is a critical issue, and simultaneous wavelength coverage with high efficiency is important. Thus, space-borne telescopes carrying wideband spectrometers are invaluable for this challenging task.

We previously introduced the concept of a wideband spectrometer for use in exoplanetary science, and presented various designs specifically for the temporary differential observation of exoplanets [2-6]. In this paper, first, a systematic comparison of many candidate materials for the spectral disperser is undertaken. Next, the designs of single-channel spectrometers using the selected materials are presented. Based on the single-channel designs, we then designed multi-channel spectrometers to realize wide wavelength coverage with high efficiency. Finally, the fabrication of a disperser and discussion are described.

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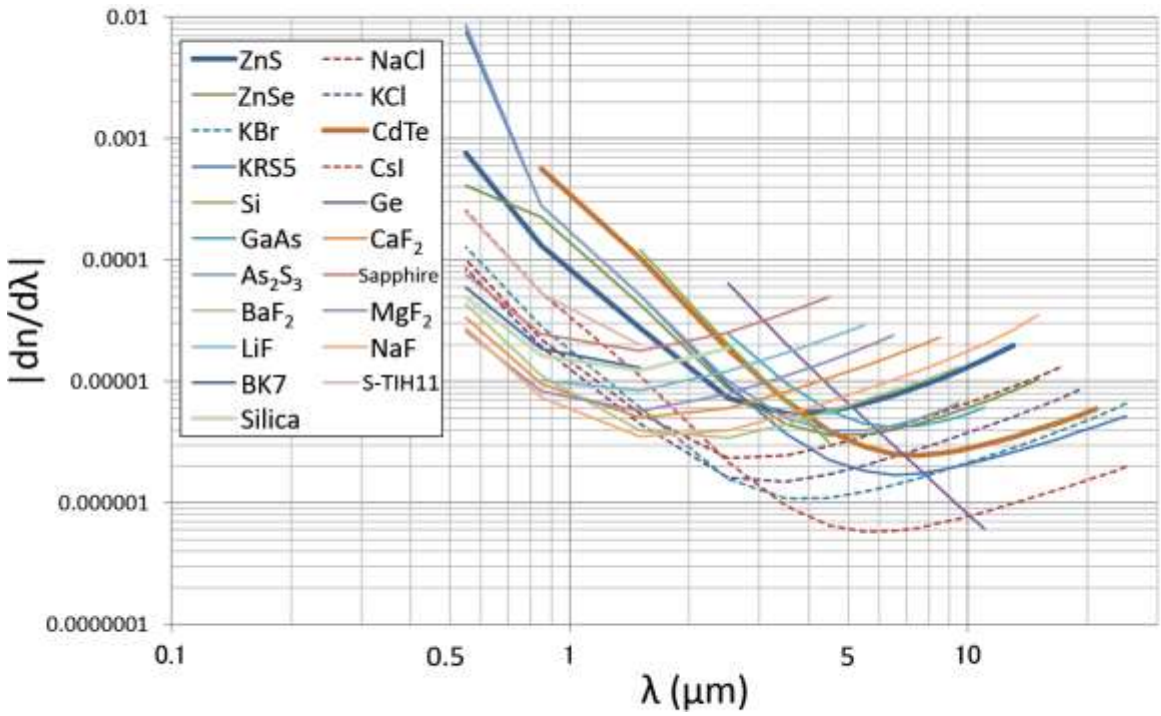

Figure 1. |*dn/dλ*| of candidate materials for wideband spectral dispersers.

2. COMPARISON OF MATERIALS

The wideband spectrometers presented here include a prism with a grating manufactured on one surface. Direction of the spectral dispersion power of the prism and the grating is crossed each other. The power of the prism separates the orders of spectrum, and the grating produces spectral resolution in the each orders. As a result, simultaneous wide wavelength coverage is realized by simple, compact, and highly stable optics without using a mechanical changer.

For this method, in this work, a comparison of candidate materials was carried out. Figure 1 shows |*dn/dλ*| of the materials as a function of *λ* in the optical, near-infrared, and mid-infrared wavelength regions, in which *n* and *λ* are the refractive index and wavelength, respectively. The plots are for 21 materials; ZnS, ZnSe, KBr, KRS5, Si, GaAs, As_2S_3, BaF_2, LiF, BK7, Silica, NaCl, KCl, CdTe, CsI, Ge, CaF_2, sapphire, MgF_2, NaF, and S-TIH11. The data is based on that found in the literature [7]. In Figure 1, those materials with larger |*dn/dλ*| perform better in separating the spectral orders.

3. DESIGN OF SINGLE-CHANNEL SPECTROMETERS

Based on the above comparison, six materials, KRS-5, CdZnTe, ZnS LiF, Sapphire, and S-TIH11, were selected. The manufacturability of each material for the prism was also considered together with its optical properties. Figure 2 shows some simple designs for single-channel spectrometers using these materials, the primary purpose of which is to demonstrate the optical performance of dispersers made of these materials. An ideal lens is supposed. The spectral resolving power, *R*, is designed to be > 300, for which the limiting factor is simply the diffraction limited spot size. It is possible to realize more various values for *R* by a combination of the design of the disperser, the aberration due to the optics, and the pixel scale of the detector array. The pitch of the grating was constrained to be larger than the longest wavelength by a factor of 5 to satisfy the scalar approximation. Consequently, the size of dispersers for longer wavelength regions tends to be larger.

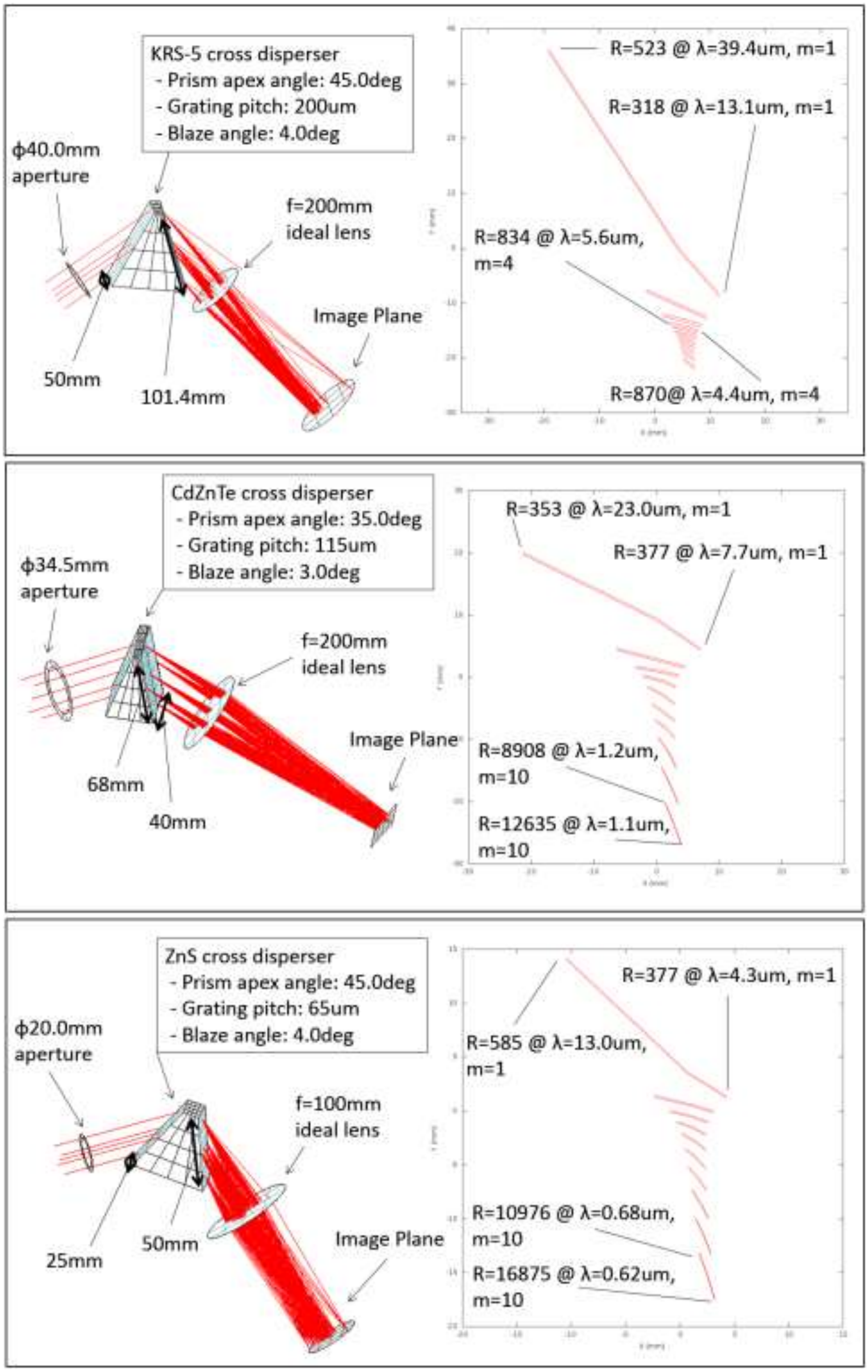

Figure 2. Optical designs of spectrometers with cross dispersers made of KRS-5, CdZnTe, and ZnS.

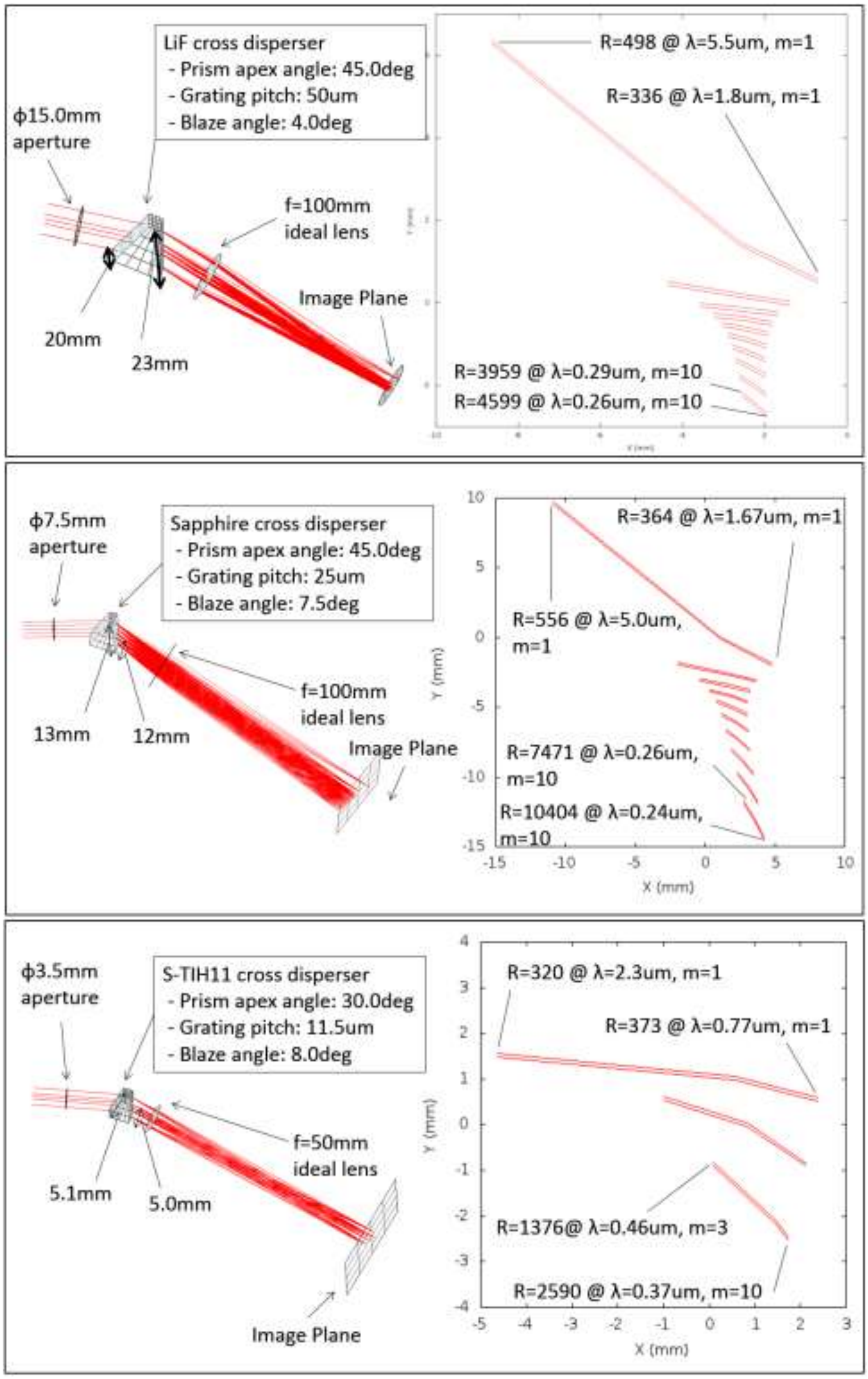

Figure 2. (Continued) Optical designs of spectrometers with cross dispersers made of LiF, Sapphire, and S-TIH11.

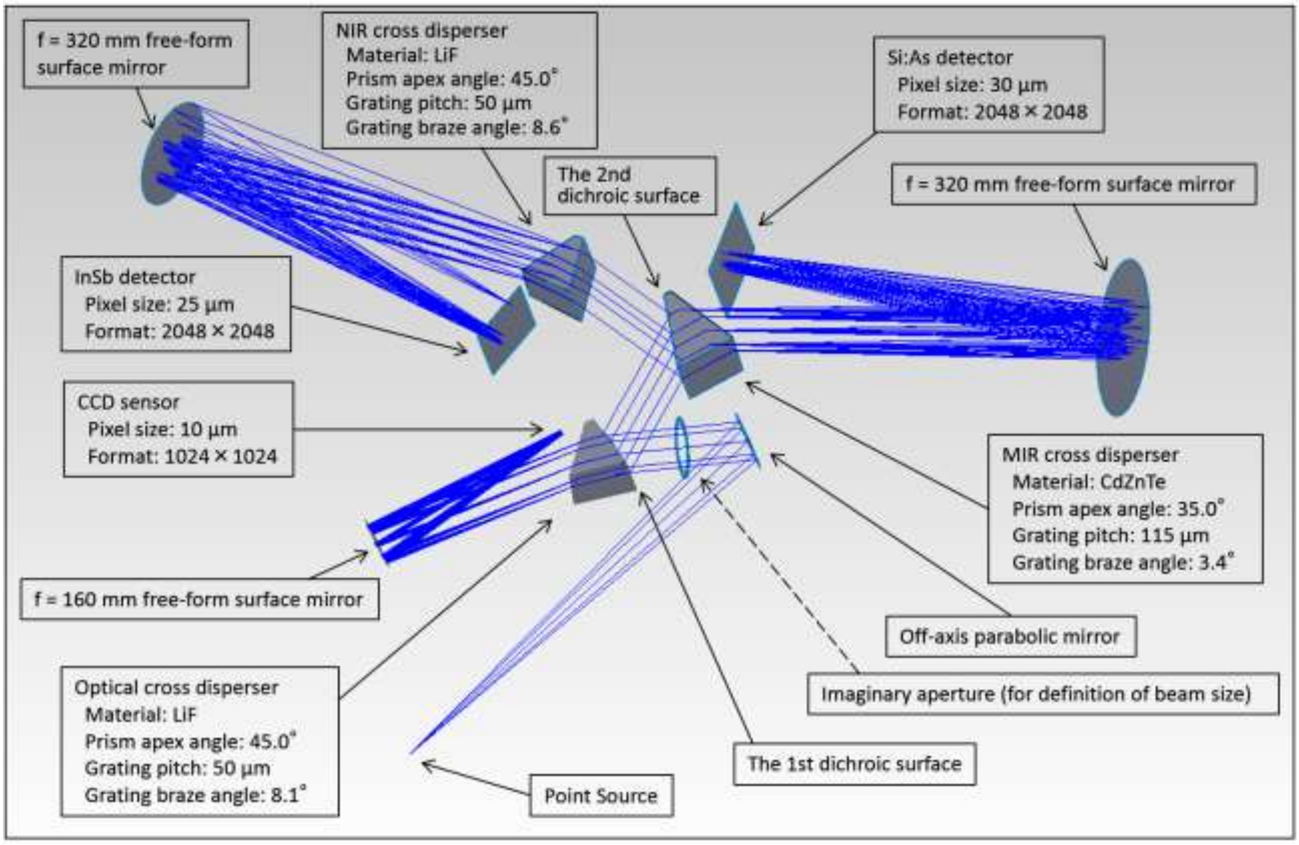

Figure 3. Optical design consisting of three channels.

It should be noted that the plots in the echellograms in Figure 2 are limited to just 10 spectral orders because of the constraints of the optical software. The wavelength coverage of these materials, which is determined by the transmission of the material and the separation power of the spectral orders, are 4.4−39.4 μm for KRS-5, 1.0−23.0 μm for CdZnTe, 0.6−13.0 μm for ZnS, 0.1−5.5 μm for LiF, 0.2−5.5 μm for Sapphire, and 0.37−2.3 μm for S-TIH11. The actual wavelength coverage of optical devices of these materials is also limited by the surface roughness achievable in fabrication. Moreover, the design using sapphire should be done carefully because of birefringence.

4. DESIGNS OF MULTI-CHANNEL SPECTROMETERS

As described in the section above and our previous papers, even simple, compact single-channel spectrometers provide significantly wider wavelength coverage than normal spectrometers. On the other hand, the important molecular features of exoplanetary atmospheres are widely distributed in the optical, near-infrared (NIR), and mid-infrared (MIR) regions, and different types of detectors are necessary to cover these wavelength regions with the best efficiency. Therefore, a multi-channel spectrometer is worth consideration. A design which has 3-channels is presented in Figure 3. In this design, the optical (λ < 1 μm), NIR (1 < λ < 5 μm), and MIR (λ > 5 μm) channels use a CCD detector, an InSb detector, and a Si:As detector, respectively. A dichroic coating on the surface of the disperser distributes the light from the object to each channel. So no additional optical device is necessary for the dichroic function. A free-formed mirror is used for focusing in each channel. No moving mechanism is used. As a result, the spectrometer is simple, compact, efficient, and

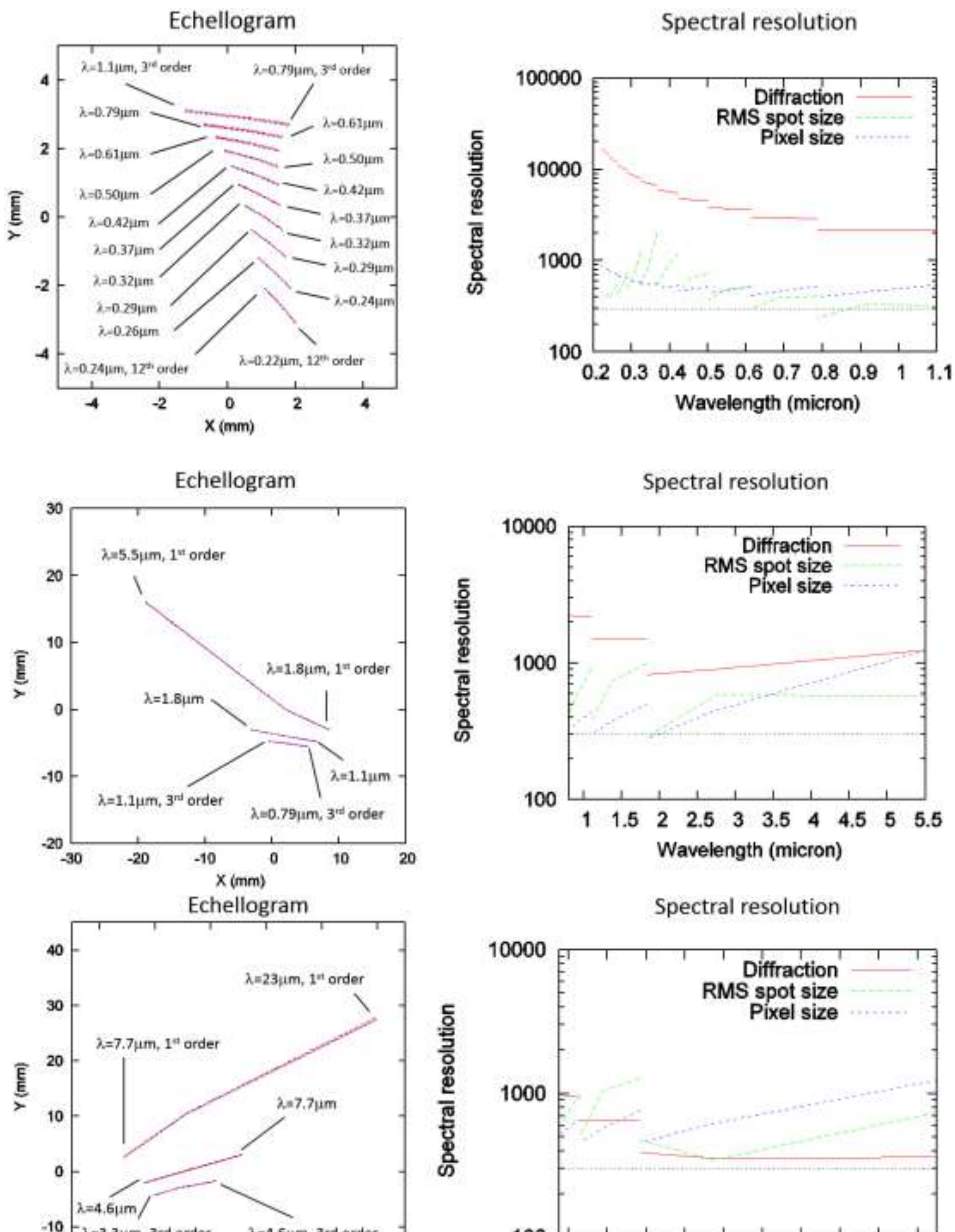

Figure 4. Echellograms and the spectral resolution of each channel in the three channel optical design shown in Figure 3.

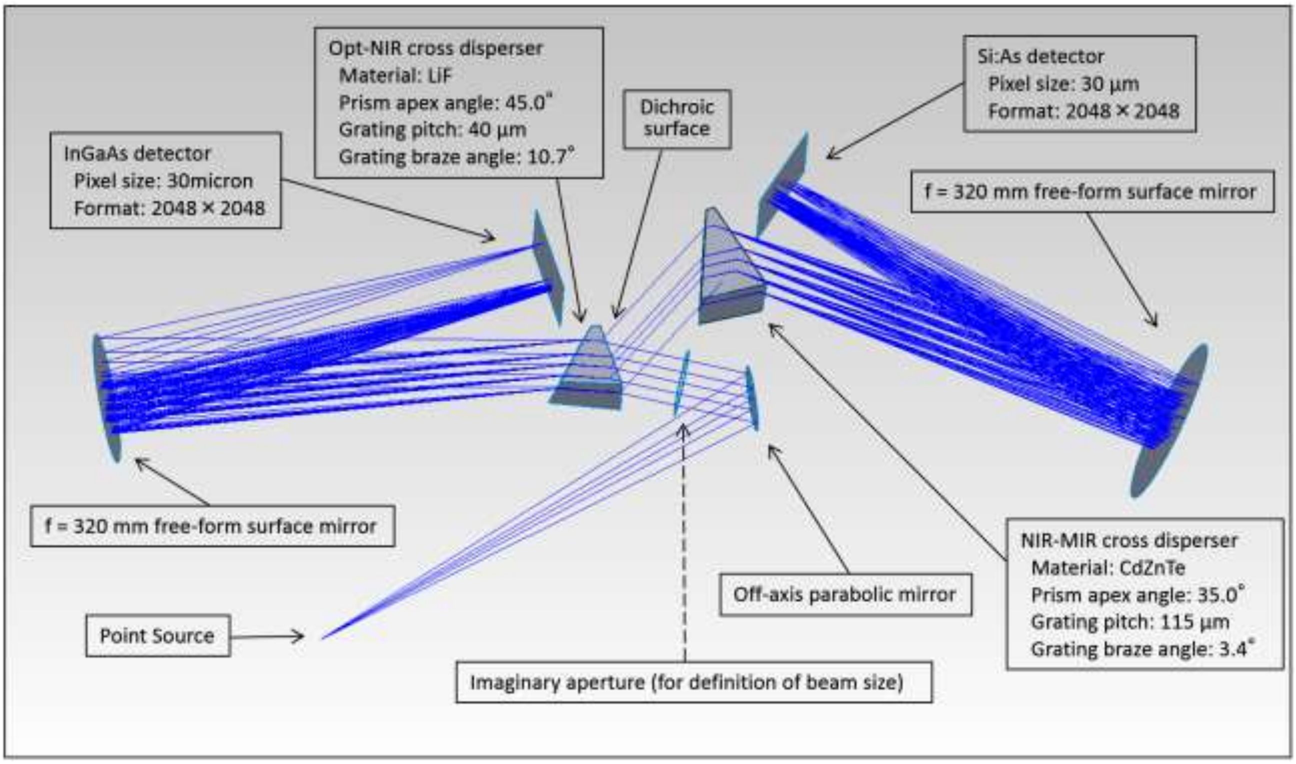

Figure 5. Optical design consisting of two channels.

highly stable. The longest and shortest observable wavelengths with this optical system are limited by the material properties of CdZnTe and the sensitivity of the CCD detector, respectively. As the cut-off of the sensitivity of the detector is not ideally sharp, we assume the short wavelength to be 0.2 µm. R is designed to be > 300, for which the limiting factor is the diffraction limited spot size, the RMS spot size, or the pixel sizes of the detectors.

Figure 4 shows the echellograms and the spectral resolution of the three channels. The echellograms are plotted showing the spectral orders containing the transition wavelengths (1 µm for the optical-NIR channels and 5 µm for the NIR-MIR channels) in each channel. The performance of the actual dichroic coating is not perfectly sharp. So it is reasonable to have the channels overlapping at the transition wavelength. The specification of the dichroic function should be optimized together with the design of the whole spectrometer. A dichroic coating presented recently is a promising option for the first dichroic surface separating the optical and wide infrared wavelength regions [8].

A design solution adopting 2-channels is presented in Figure 5. In this design, the optical-NIR (λ < 2.4 µm) and NIR-MIR (2.4 < λ < 23 µm) channels use a HgCdTe detector and a Si:As detector, respectively. While the performance of the 2-channel design is not as high as the 3-channel design, the 2-channel design is simpler, more compact, and the resource requirements from the satellite system are more modest. Figure 6 shows the echellograms and the spectral resolution of the two channels. The longest and the shortest observable wavelengths with this optical system are limited by the material properties of CdZnTe and the sensitivity of the HgCdTe detector, respectively. We assume the short wavelength to be 0.4 µm. R is designed to be > 300 as for the case of the 3-channel design.

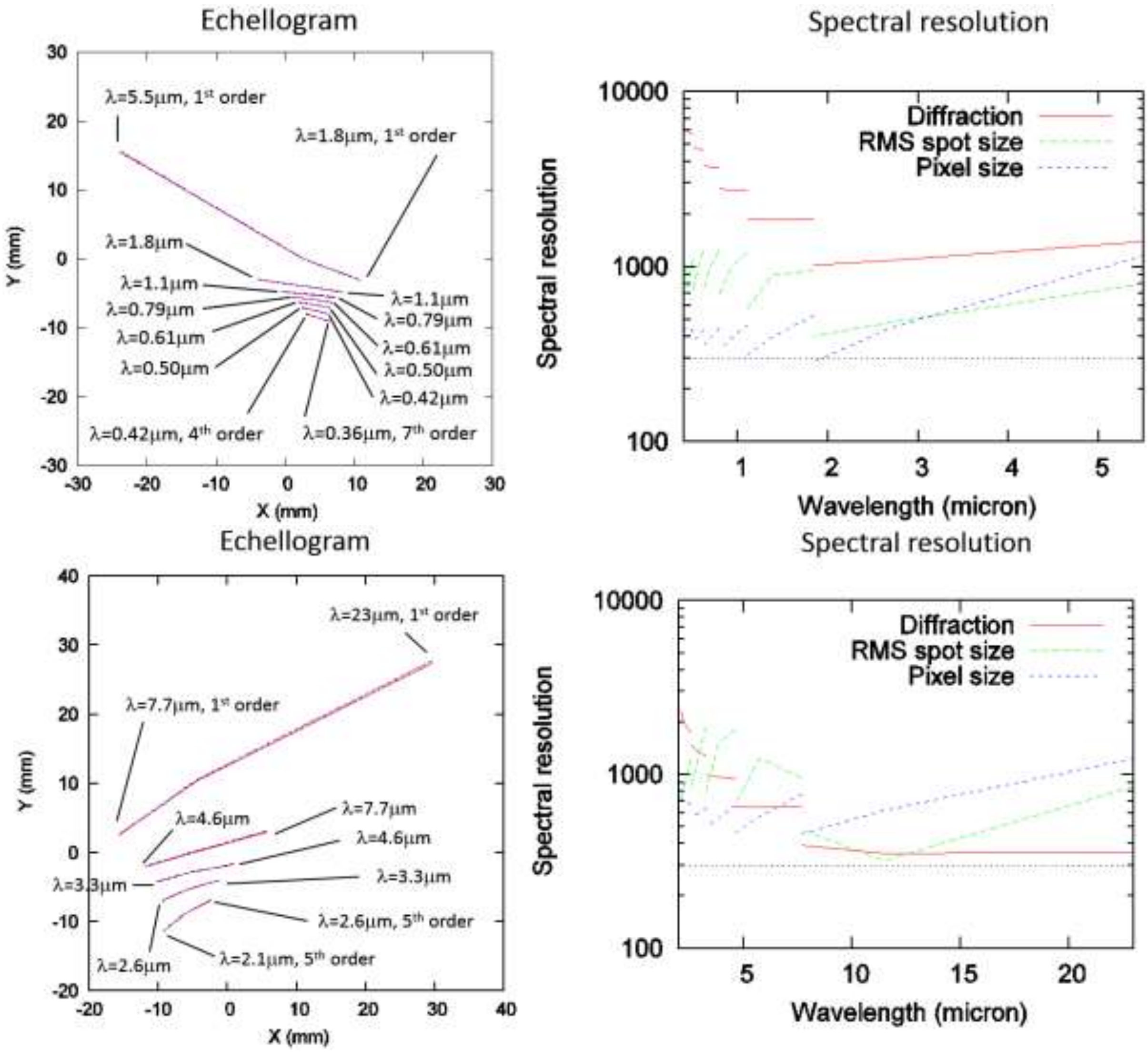

Figure 6. Echellogram and spectral resolution for each channel of the optical design with two channels shown in Figure 5.

5. FABRICATION

From among the various candidate materials for the disperser, we selected ZnS as the material for our first trial fabrication because a single-channel spectrometer made of ZnS provides suitable wavelength coverage (as shown in Figure 2) for O_3 (9.6 μm) and other important molecular features in exoplanetary atmospheres [2]. The feasibility of fabrication, cost, and availability are also reasons for the selection. The design of this cross disperser is shown in Figure 7, and a photograph of the fabricated cross disperser is presented in Figure 8. As shown in previous papers, it is possible to compensate for the optical axis by an additional sub-prism. This combination enables application of wideband cross dispersion not only for spectrometers but also various other optical imaging systems. It should be noted that this method was also utilized for JWST/NIRISS [9]. In this work, we fabricated a sub-prism of CsI. The design and a photograph of the fabricated sub-prism are shown in Figures 7 and 8, respectively. The ZnS cross disperser and the CsI sub-prism presented in this work were fabricated by Tsuboi Seisakusyo Inc., and Crystal Optics Inc., respectively. Basic checks on these fabricated devices are ongoing.

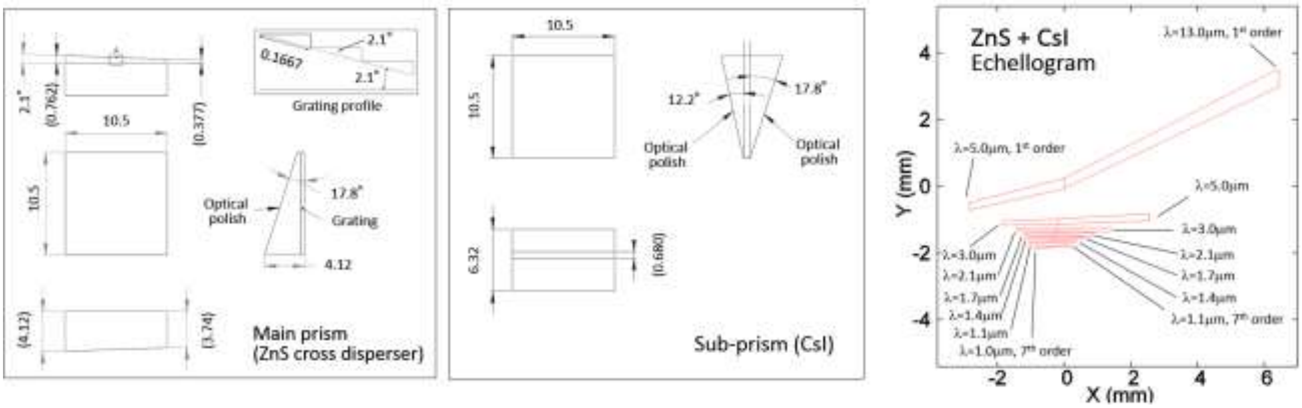

Figure 7. Design of a ZnS cross disperser and a CsI sub-prism for trial fabrication.

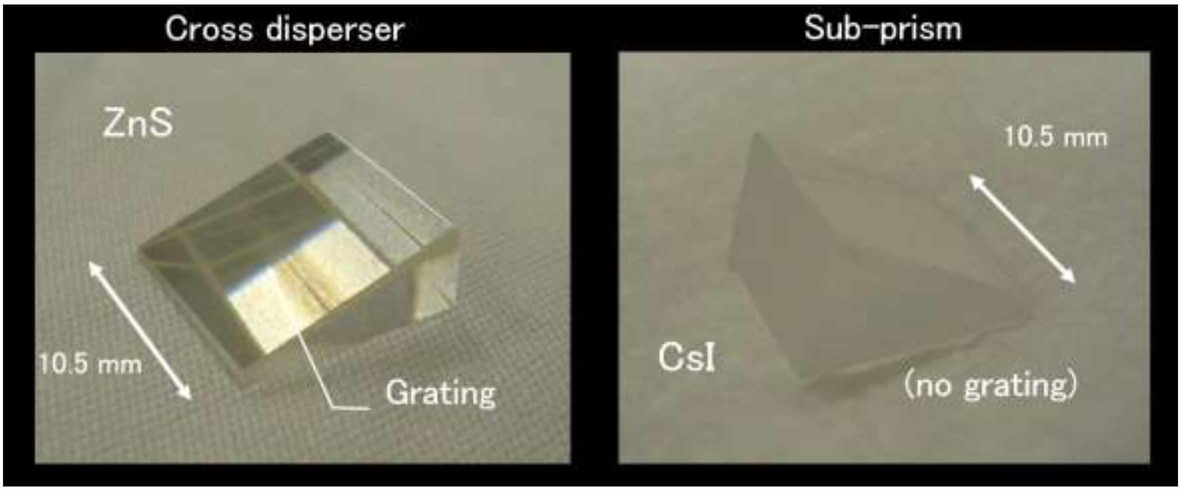

Figure 8. (Left) Fabricated ZnS cross disperser. The grating is machined onto the surface. (Right) Fabricated CsI sub-prism.

6. DISCUSSION

This work is primarily focused on a comparative study of the optical performance of various materials, and therefore *R* is simply assumed to be >300 and “defocusing” (intentionally introduced aberration) is not applied to the optical designs. However, there is freedom for tuning the value of *R* and varying the defocusing.

Temporary differential observations to study exoplanetary atmospheres measure the extremely small variabilities of very bright point sources. So it is extremely important to make highly stable observations and to avoid saturation of the detectors. Defocusing is a promising solution for both of these. Another advantage of defocusing is that it makes the spot size roughly uniform over a very wide wavelength region. Defocusing reduces *R*, which limits some of the scientific objectives. Nevertheless, one of the critical scientific objectives, the detection of the molecular composition of exoplanetary atmospheres, is possible with *R* less than 300.

High resolution spectroscopy brings us more details about the science of exoplanetary atmospheres, and is another solution for the saturation problem. Moreover, in photon-limited observations, use of high resolution spectroscopy improves the signal to noise ratio of absorption molecules in the exoplanetary atmosphere because the resolved lines are observed as fine and deep features. Combination of defocusing and the use of high resolution spectroscopy are also possible. It is encouraging that work on the fabrication of high resolution immersion grating devices made of important materials exists, e.g., CdZnTe, KRS-5, ZnS, and ZnSe [10-13]. On the other hand, high resolution spectroscopy needs larger telescope apertures than low resolution spectroscopy to realize photon-limited observations.

Fortunately, the temporary differential observation of exoplanets does not require the extremely high quality wavefront to the telescope as coronagraphic observations do. Moreover, wavefront correction by additional small deformable mirrors and/or fixed wavefront correction mirrors enables us to relax the requirements on the telescope [14, 15]. We consider this solution increases the potential for realizing a large telescope. A latchable deformable mirror is especially useful for space telescope missions [15].

It is enough to design not an actively cooled space telescope (like SPICA) but just a passively cooled space telescope (like JWST) for the observation of molecular features in the atmospheres of exoplanets. On the other hand, the operating temperature of the detector depends on the type of detector. For instance, a Si:As detector requires ~5 K and a CCD detector should be operated at much warmer temperatures in the 3-channel design. It is an issue of the thermal design to realize coexisting detector stages with quite different temperature constraints with the limited resources of a satellite. Therefore, reducing the number of channels, modifying the specifications of the detectors, and/or limiting the wavelength coverage of the observations can help from the point of view of the thermal design of the satellite. Optimization depends on the scientific case and the objective of each mission.

In both the 2-channel and 3-channel designs, the short side of the wavelength coverage is limited by the CCD detector. For a science mission requiring the shorter wavelength region [16], a possible solution is to extend the sensitivity to the shorter wavelength region by modifying the specification of the CCD or having an additional UV channel.

The spectrometer presented in this paper, which is simple, compact and highly stable, enables simultaneous wide wavelength coverage for exoplanetary science, including studies of biomarkers. Ideally, it is needed to realize a space telescope mission dedicated for these challenging scientific goals (e.g., ECHO [1], THESIS, FINESSE [17, 18]). On the other hand, there are many opportunities to participate in ongoing or proposed telescope missions that have various wavelength coverage and the telescope aperture size can take us a considerable way along the paths to reach these goals step by step. Indeed, last year, we proposed a wideband infrared spectrometer and dedicated exoplanetary science using it to SPICA again.

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