# Mid-infrared High-resolution Spectrograph for SPICA

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## ABSTRACT

We present a preliminary optical design and layout for the mid-infrared (4-18 $\mu$m) high-resolution spectrograph for SPICA, Japanese next-generation space IR observatory with 3.5 m telescope. MIR high-resolution spectroscopy is a powerful probe to study gas-phase molecules/atoms in a variety of astronomical objects. Space observation provides a great opportunity to study many molecular lines especially in between the atmospheric windows. SPICA gives us a chance to realize MIR high-resolution spectroscopy from space with the large telescope aperture. The major technical challenge is the size of the spectrograph, which tends to be too large for space. We hope to overcome this problem with a novel MIR immersion grating, which can make the instrument smaller by a factor of the refractive index of the grating material. We plan to fabricate a large pitch ZnSe ($n = 2.4$) immersion grating with the fly-cutting technique at LLNL (see Poster paper 7018-183 by Ikeda et al.[1] and 7018-181 by Kuzmenko et al.[2] in the proceedings of this conference). We show our preliminary spectrograph designs with a spectral resolution of ~30,000 in 4-8 $\mu$m (short mode) and 12-18 $\mu$m (long mode). The instrument size can be as small as 200 × 400 mm thanks to the MIR immersion gratings. With unprecedented spectral resolution in space, which is 10-times higher than ISO-SWS, the high-resolution spectrograph for SPICA (SPICA-HIRES) could be a unique instrument that can provide most sensitive and clear spectra of this kind.

**Keywords:** SPICA, space telescope, infrared, astronomy, molecular spectroscopy, extra-terrestrial life, high-resolution spectroscopy, optical device, immersion grating

## 1. INTRODUCTION

### 1.1 Scientific Objective

There is a growing needs for astronomical MIR ($3-30\,\mu$m) high-resolution spectroscopy because of the numerous rotational-vibration bands of interstellar molecules in this wavelength range (see e.g., a concise review by Richter et al.[3]). While the rotational lines in the mm/sub-mm wavelengths are spread over the wide wavelength range, MIR ro-vibrational lines are packed in relatively much narrower wavelength range. Also, many important organic molecules, such as $CH_4$ and $H_2$, do not have rotational dipole transitions in mm/sub-mm while they have many vibrational transitions in MIR. Therefore, MIR spectroscopy has advantages to be able to get the spectra of many excitation levels simultaneously compared to mm/sub-mm spectroscopy, resulting in fruitful information on physical/chemical conditions of the interstellar medium (ISM). Table 1 summarizes major target molecular lines. Besides major astronomical molecules, such as CO or $H_2$, many organic molecules that could be bio-marker show up in the MIR region. Although not listed, there are also many other atomic lines (mostly forbidden lines), which are critical for the study of physics/chemistry and kinematics of star formations and galaxies.

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Space Telescopes and Instrumentation 2008: Optical, Infrared, and Millimeter,
edited by Jacobus M. Oschmann, Jr., Mattheus W. M. de Graauw, Howard A. MacEwen,
Proc. of SPIE Vol. 7010, 701032, (2008) · 0277-786X/08/$18 · doi: 10.1117/12.799423

Table 1. **Major molecular lines for MIR high-resolution spectroscopy**

| Molecule | | Band wavelength | Polarity[†] | Good probe for |
|---|---|---|---|---|
| carbon dioxide | $CO_2$ | 4.2 $\mu$m | | biomarker? |
| carbon monoxide | CO | 4.6 $\mu$m | | ISM kinematics |
| methane | $CH_4$ | 7.7 $\mu$m | NO | biomarker? |
| silicon monoxide | SiO | 8.1 $\mu$m | | |
| ammonia | $NH_3$ | 10.0 $\mu$m | | |
| ethane | $C_2H_6$ | 12.2 $\mu$m | | biomarker? |
| acetylene | $C_2H_2$ | 13.7 $\mu$m | NO | biomarker? |
| hydrogen cyanide | HCN | 14.0 $\mu$m | | |
| carbon dioxide | $CO_2$ | 15.2 $\mu$m | | biomarker? |
| hydrogen molecule | $H_2$ 0–0 S(1) | 17.03 $\mu$m | NO | ISM kinematics |

[†] Because those non-polarized molecules (w/NO) cannot be observed in mm/sub-mm wavelengths, they are important targets for MIR high-resolution spectroscopy.

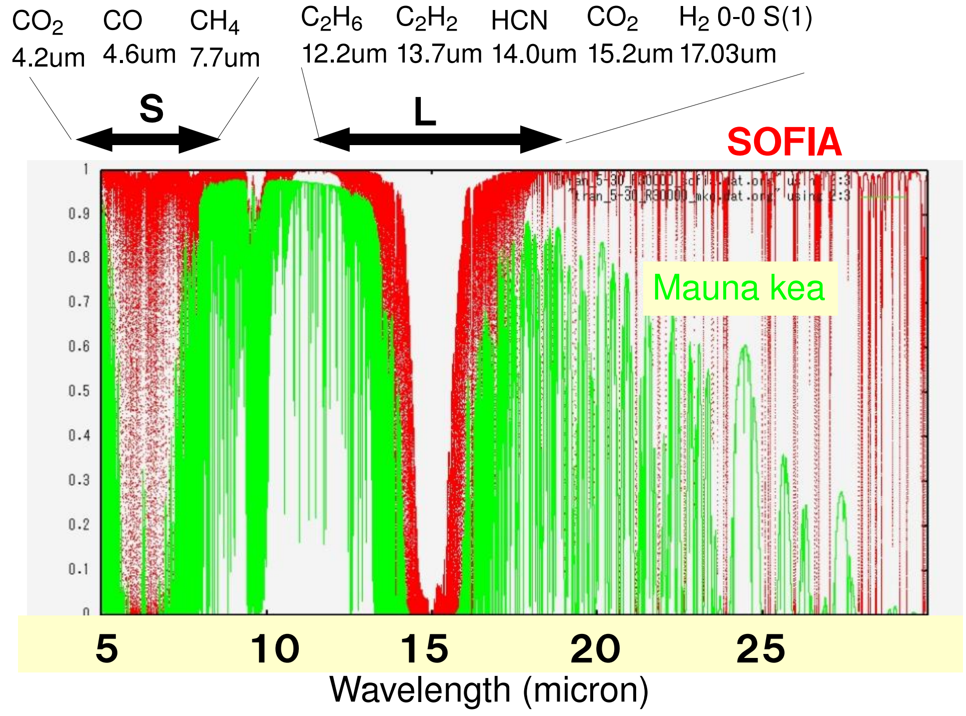

Figure 1. **Atmospheric transmission in the MIR** The transmission was calculated with ATRAN software (Lord 1992, NASA Technical Memorandum 103957) for ground-base (Mauna Kea, 4200m) and airborne (SOFIA, 12000 m) altitudes. Note even at the SOFIA altitude, strong atmospheric absorption bands still remain at around 6 and 15 $\mu$m, where many important molecules have absorption bands. The proposed SPICA-HIRES covers those two absorption bands with Short-mode (4-8 $\mu$m) and Long-mode (12-18 $\mu$m) spectrographs. Space observations can avoid many strong atmospheric absorption lines even in the good atmospheric windows.

### 1.2 MIR High-resolution Spectroscopy from Ground and Space

Because of the needs for a large telescope aperture, MIR high-resolution spectroscopy has been pursued from ground-based observatories with cutting-edge instruments such as TEXES[4,5] at IRTF/Gemini by Texas group and MICHELLE[6] at UKIRT/Gemini, and VISIR at ESO-VLT.[7] MIR high-resolution spectroscopy will become one of the most important targets for the next generation extremely large ground-based telescopes, such as TMT (Thirty Meter Telescope) 30 m telescope and E-ELT (European Extremely Large Telescope) 50-100 m telescope. For the TMT project, a large instrument, MIRES,[8, 9] is proposed for $R = 100,000$ spectroscopy in MIR. However, systematic observations have been hampered by the strong atmospheric extinction, which limits the observable wavelength range (Fig.1), and also the large amount of thermal background, which reduces the sensitivity in most cases. Therefore high-resolution spectroscopy from space has been awaited for exploiting this exciting field.

EXES on board SOFIA[10–13] will be the first instrument of this kind, which explores the wavelength regions that cannot be observed from the ground. Because even cleaner wavelength coverage without any atmospheric absorption with less thermal background is expected from space (Fig.1), space observation offers an excellent opportunity to explore the wavelength region with systematic MIR high-resolution spectroscopy. Although the only drawback is the limited telescope aperture in space, next generation spaceborne observatories, such as JWST (6.5 m) or SPICA (3.5 m), can realize highly sensitive MIR high-resolution spectroscopy from space even compared to the ground-based large aperture telescope.

SPICA (Space Infrared Telescope for Cosmology and Astrophysics) is a next-generation infrared astronomical mission in space with a cooled 3.5 m telescope. The overview of the mission concepts, current status of the project are described in Nakagawa (2008, in this volume).[14] Here we present a detailed optical design of the space MIR high-resolution (R$\equiv \lambda/\Delta\lambda \sim 20,000-30,000$) spectrograph proposed for SPICA as one of the MIR focal plane instruments.[15] Because such high-resolution instrument is uniquely proposed only for SPICA, it would become one of the most unique MIR space instruments.

## 2. SPECIFICATIONS AND OPTICAL DESIGN

### 2.1 Specifications

In this preliminary study, we focused on two wavelength ranges, $4-8\,\mu$m (Short-wavelength mode, hereafter S-mode) and $12-18\,\mu$m (Long-wavelength mode, hereafter L-mode), which are difficult to access from ground and even from the airborne altitude (see Fig.1). These wavelength ranges are also determined to cover the molecular lines shown in Table 1 as much as possible. The specifications of our initial design are summarized in Table 2. Two independent spectrographs for S-mode and L-mode are considered at the moment.

### 2.2 Optical Design

Our initial optical designs based on the above specifications are shown in Figs.2 and 3. All the collimator/camera optics are transmissive to realize 1) compact size of the spectrograph, 2) easy fabrication/alignment. Especially 1) is essential as space instrument. Because of the use of the immersion grating and the transmissive optics, very compact design of 200mm(L) × 200mm(W) × 100mm(H) (S-mode) and 350mm(L) × 350mm(W) × 200mm(H) (L-mode) can be achieved with the high-resolution ($\lambda/\Delta\lambda_{max} = 30,000$). Immersion grating material was selected to maximize the spectral resolution and the throughput for each wavelength range. The wavelength

| | Short(S)-mode | Long(L)-mode |
|---|---|---|
| Wavelengths | $4-8\,\mu$m | $12-18\,\mu$m |
| Spectral resolution($\lambda/\Delta\lambda$) | 30,000 | 20,000 $\sim$ 30,000 |
| Slit width($''$) | $0.72''$ | $1.20''$ |
| Slit length($''$) | $3.5''$ | $6.0''$ |
| Spectrometer type | white pupil-type | white pupil-type |
| Size | 200mm(L) × 200mm(W) × 100mm(H) | 350mm(L) × 350mm(W) × 200mm(H) |
| Magnification | ×0.82 | ×1.40 |
| Dispersion element | ZnSe immersion grating | KRS5 immersion grating |
| X-disperser | reflective | reflective |
| Detector | Si:As 1024 × 1024 | Si:As 1024 × 1024 |

Table 2. **Specifications of SPICA-HIRES** The telescope diameter and the f-ratio are assumed to be 3.5 m and f/5.2.

coverage for each mode was set to be roughly one octave to enable the required wide-band AR coating of the transmissive optics.

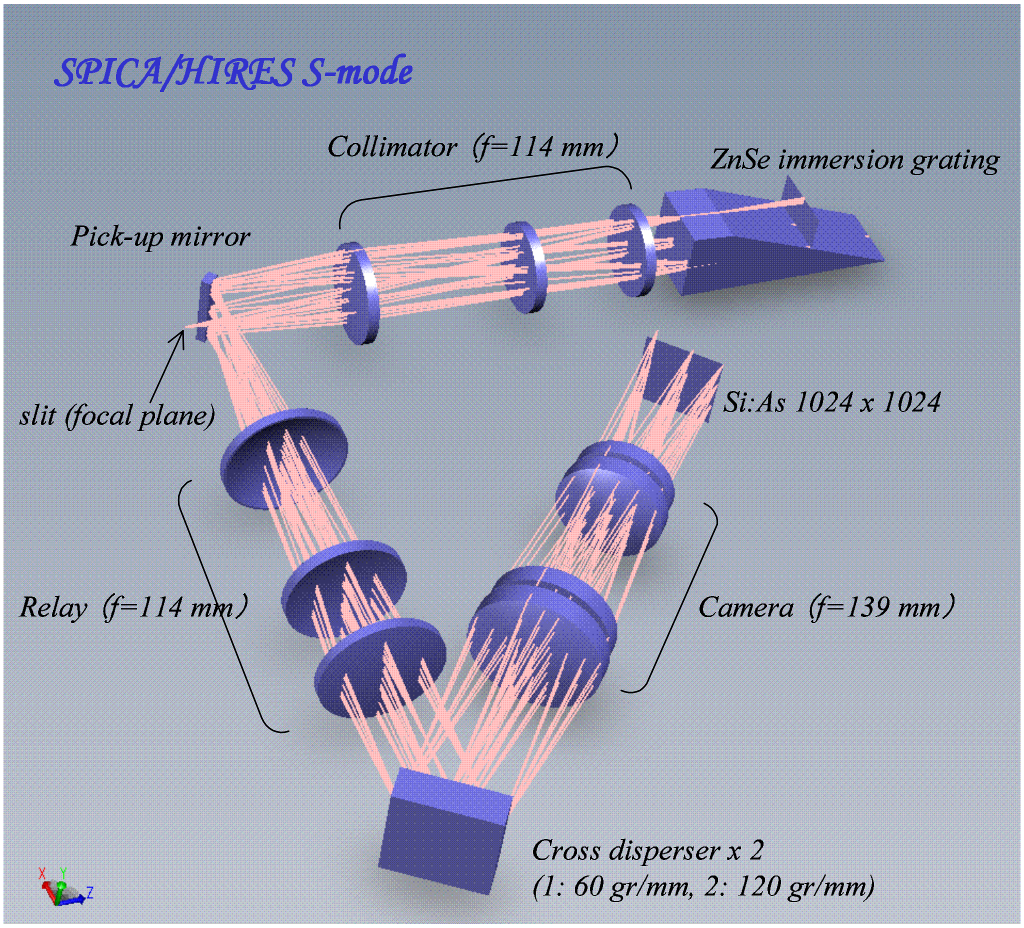

Figure 2. **Optical layout of SPICA-HIRES/S-mode** The light from the slit enters to the immersion grating through the collimator lenses. The dispersed light goes through the collimator lenses again, then collimated by the relay optics. This relay optics makes a pupil image on the cross-disperser, resulting in the small size of the entire optical system. S-mode requires two cross-dispersers to cover the entire $4 - 8\,\mu$m range. The cross-dispersed light enters to the detector through the camera optics. The size of the entire optical system is about 200mm(L)×200mm(WW)× 100mm(H).

Figs.4,5 and 6 show the point-spread-function (PSF) on the detectors for the spectrographs of S-mode w/short wavelength cross-disperser, S-mode w/long wavelength cross-disperser, and L-mode. Strehl ratio of $> 0.88$ is achieved for all the wavelengths and through the entire array.

## 3. IMMERSION GRATING

### 3.1 Immersion Grating for Spaceborne Instrument

Unlike ground-based spectrometers, whose spectral resolution is determined by the slit-width (or, seeing size of the image), the spectral resolution of spaceborne spectrometer is directly determined by the theoretical resolution of the grating ($\lambda/\Delta\lambda = Nm$). The large collimator beam required to achieve higher spectral resolution could be a serious problem for space instrument, for which the available space in the focal plane is quite limited. Immersion grating (Fig.7) is a vital solution for this problem because the required collimator beam size can be reduced by a factor of the refractive index ($n$) of the material (see more detail in Ikeda et al.[1] and Kuzmenko et al.[2]).

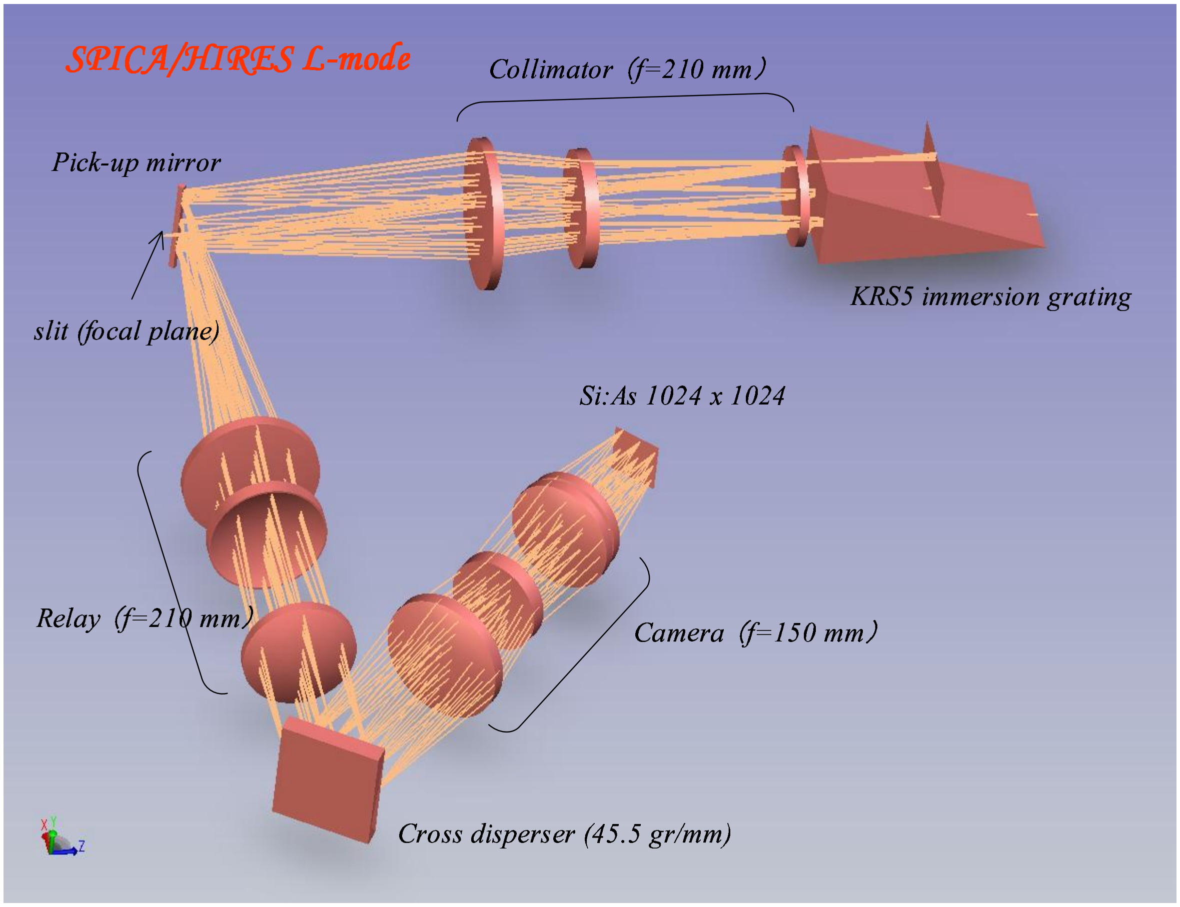

Figure 3. **Optical layout of SPICA-HIRES/L-mode** Similar optical layout as for S-mode (Fig.2). Only one cross-disperser is required to cover the entire wavelength range ($12 - 18\,\mu$m). The size of the entire optical system is about 350mm(L)×350mm(W)×200mm(H).

## 3.2 Material for Immersion Grating

Infrared semiconducting materials generally have high refractive index $n$ and are suitable for immersion grating. However, the required large bulk material may have significant degradation of transmission due to internal extinction. Fig.8 shows the transmission of various infrared materials that are suitable for immersion grating in MIR. Although polycrystalline CdTe is the best material that shows high transmittance and high refractive index ($n = 2.6$), it is still difficult to find an optical-quality block that is large enough for the required immersion grating. Therefore, polycrystalline ZnSe ($n = 2.4$) is our first choice for the S-mode because it is known to have good optical homogeneity and fabrication method of large ZnSe block is well established. Note that Germanium is not as good material as usually thought for MIR immersion grating because of the large absorption for thick bulk material.

Because ZnSe is not transparent at $\lambda > 15\,\mu$m, we are temporarily considering KRS-5 as a candidate material for the immersion grating for L-mode. A large KRS-5 bulk material is available and grating grooves can be made with ruling for this soft material.[16,17] It is also space-qualified IR material. Although it is known to have relatively large inhomogeneity, it should not be a problem for longer wavelengths at $\lambda > 10\,\mu$m since it is successfully used in $3\,\mu$m band.[16,17] Table 3 summarizes the immersion gratings for SPICA-HIRES.

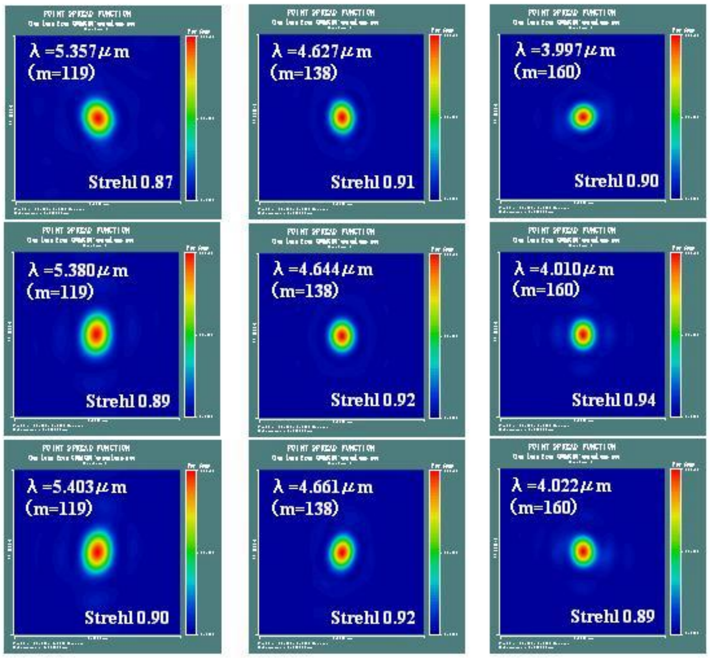

Figure 4. **PSF of spectra on the array: S-mode (w/short wavelength X-disperser)** The columns from left to right show the PSF of spectra in $m = 119, 138, 160$, respectively. The rows from top to bottom show the PSF for the longest wavelength, center wavelength, and the shortest wavelength in the echelle order, respectively.

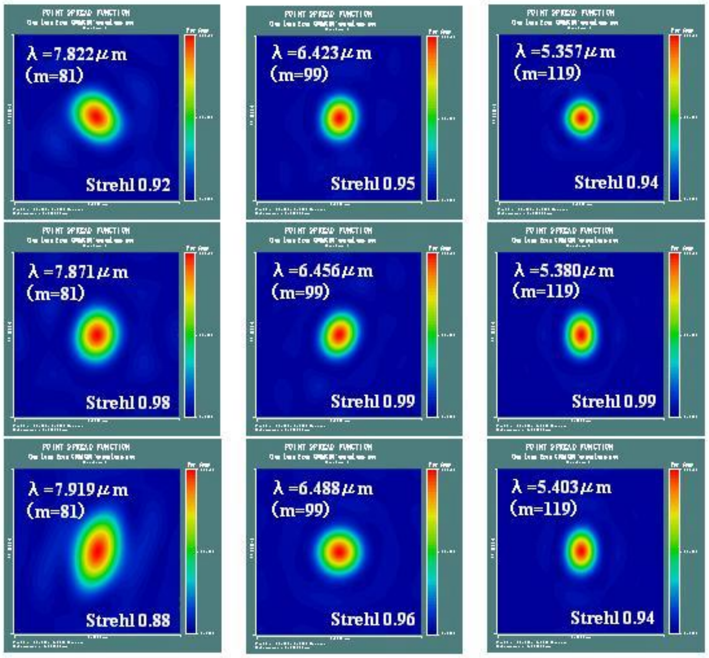

Figure 5. **PSF of spectra on the array: S-mode (w/long wavelength X-disperser)** Similar to Fig.4. The columns from left to right show the PSF of spectra in $m = 81, 99, 119$, respectively.

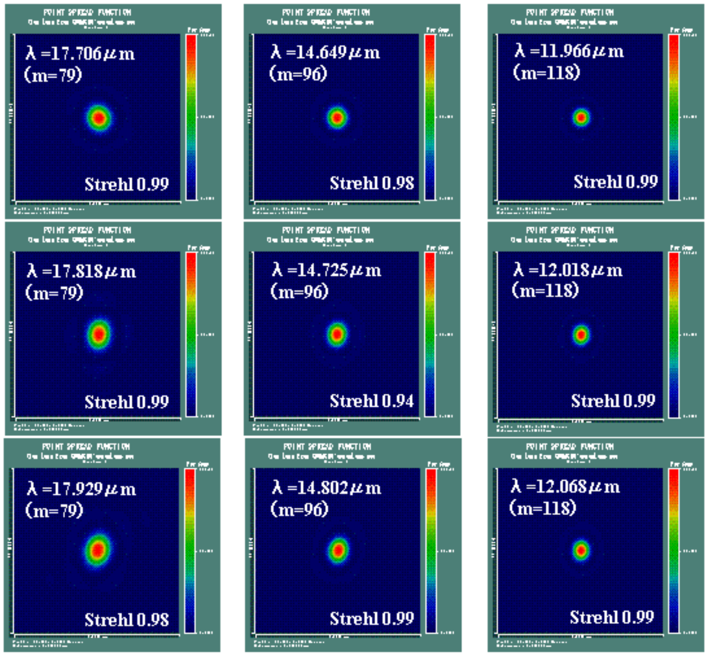

Figure 6. **PSF of spectra on the array: L-mode** Similar to Fig.4. The columns from left to right show the PSF of spectra in $m = 76, 96, 118$, respectively.

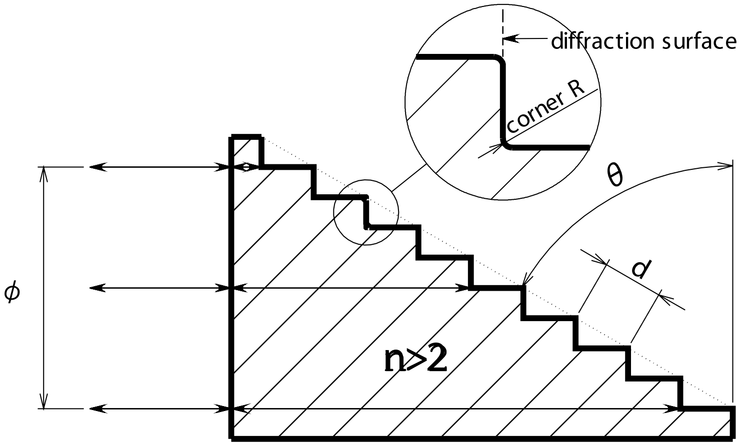

Figure 7. **Immersion grating parameters** $n$: refractive index, $\theta$: braze angle, $\phi$: collimator beam size, $d$: groove pitch.

### 3.3 Development of Immersion Grating

We have been studying the fabrication method of ZnSe immersion grating. First we tried a grinding method that was developed by RIKEN in Japan and was successfully used for a fabrication of a large Ge immersion grating.[18] However, required good surface roughness and small corner R could not be achieved with this technique for ZnSe, which is brittle material (see Ikeda et al.[19]). Since Kuzmenko et al.[20–22] have successfully fabricated high-quality Ge grating with a closed-loop controlled fly-cutting technique at Lawrence Livermore National Laboratory (LLNL), we applied this technique to ZnSe.[1, 2]

We made two samples of A) braze pitch $d = 30\,\mu$m and braze angle $\theta_B = 65°$, B) $d = 150\,\mu$m and $\theta_B = 70°$. Sample A was made for application to shorter wavelengths (see Ikeda et al.[1]) and was good as a first step to

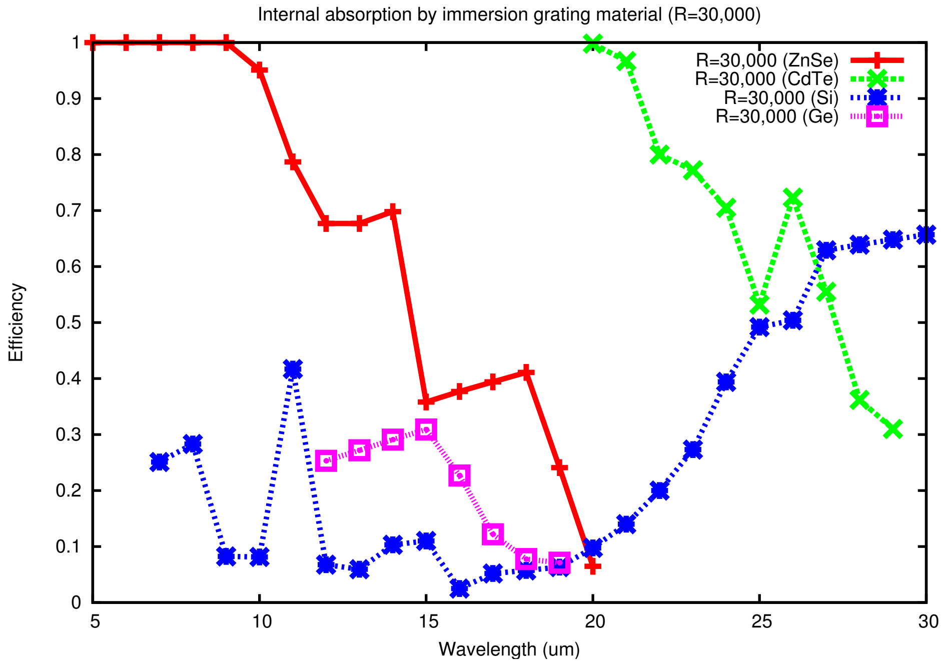

Figure 8. **MIR transmission of candidate bulk materials for SPICA immersion grating** The size of the immersion grating was set to achieve $\lambda/\Delta\lambda = 30,000$ for SPICA. Only absorption (no scattering) is considered for the extinction. The complex refractive indices are from the theoretical calculations by Hawkins(1998). The ambient temperature is assumed to be 50K. ZnSe and CdTe show good transmittance at $\lambda < 15\,\mu$m and $< 25\,\mu$m, respectively, while Si and Ge show significant absorption in this wavelength range.

check the basic performance of this method because tighter specifications are required for shorter wavelengths. Sample B was made for application to longer wavelengths specifically for SPICA HIRES.

To evaluate the optical performances, we put a HeNe laser beam with a diameter of 1 mm to the sample grating B from the air side with the Littrow condition, and carefully observed the diffracted spectrum focused on a CCD camera. Fig.9 shows the obtained spectrum around the strongest orders, which is normalized using the two strongest orders and a blaze function given in Shroeder's book[23]

$$I(\Delta\theta) = \gamma \frac{\sin^2\left[\frac{\pi d\cos\theta}{\lambda}\left\{\sin(\beta-\theta_\mathrm{B})+\sin(\alpha-\theta_\mathrm{B})\right\}\right]}{\left[\frac{\pi d\cos\theta}{\lambda}\left\{\sin(\beta-\theta_\mathrm{B})+\sin(\alpha-\theta_\mathrm{B})\right\}\right]^2}, \tag{1}$$

where $\alpha$ and $\beta$ are the incidence and diffraction angles, $\Delta\theta$ is the diffraction angle measured from the optical axis corresponding to $\beta - \theta_\mathrm{B}$, $\gamma$ is the vignetting factor due to the shadowing effect[24] presented by

$$\gamma = \begin{cases} 1, & \text{for } \alpha \geq \beta \\ \frac{\cos\beta}{\cos\alpha}, & \text{for } \alpha < \beta. \end{cases} \tag{2}$$

In Fig.9, the intensities of the side-lobe orders ($m = 213$, 216, and 217) well agree with the blaze function curve, which indicates that the diffraction light strongly concentrates on the main order, showing the high diffraction

| | S-mode ($4-8\,\mu$m) | L-mode ($12-18\,\mu$m) |
|---|---|---|
| Material | ZnSe(polycrystalline) | KRS5 |
| Groove pitch | $140.3\,\mu$m | $318.3\,\mu$m |
| Blaze | 70 deg. | 70 deg. |
| Clear aperture | $\phi$ 25mm | $\phi$ 42mm |

Table 3. **Specifications of SPICA-HIRES immersion gratings**

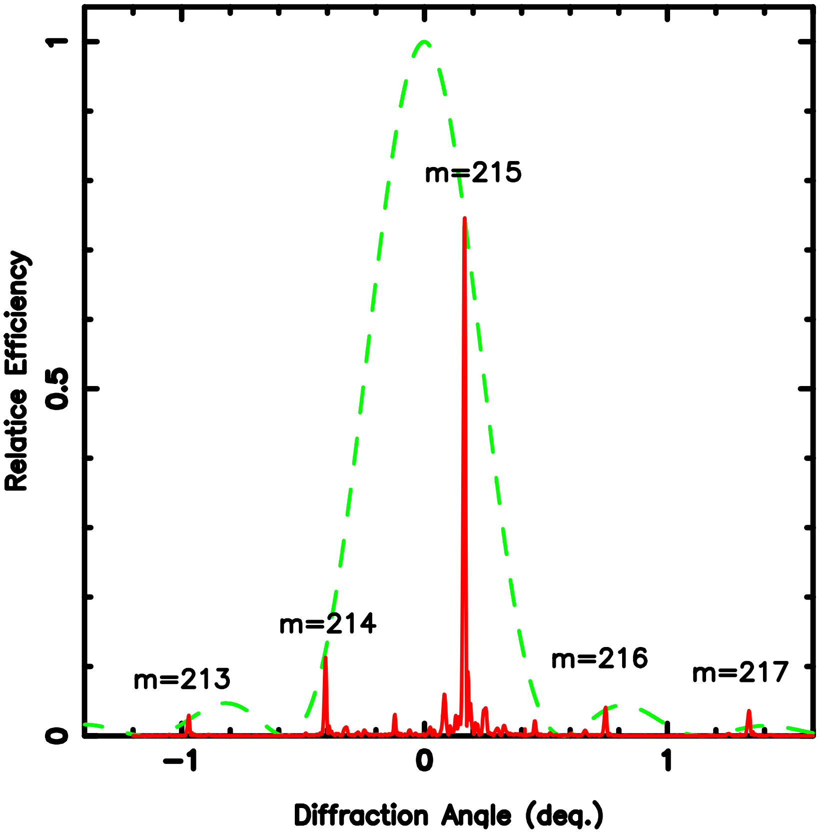

Figure 9. **Diffraction spectrum by test ZnSe grating (Sample B)** Obtained spectra with He-Ne (633 nm) laser beam. The dashed line presents the blaze function defined as Eq.(1).

efficiency of this sample grating. This is consistent with the sharp groove corner with the radius of $< 0.2\ \mu$m shown in Fig.5 of Ikeda et al.[1]

The integrated background scattered light seen between the main orders is found to be $I_{\rm bk}/\sum I \simeq 4.3$ % where $\sum I$ is the total intensity of the diffracted light. In principle, the scattered light is primarily produced by the surface roughness $\sigma_{\rm H}$ and the random groove pitch error $\sigma_{\rm d}$ (see Ikeda et al.[1] for more details). We have measured the surface roughness to be 7.2 nm (rms) with a Vecco optical profirometer, which is equivalent with the scattered light of 2.1 %. Therefore, the scattered light due to the random pitch error is estimated to be $\sim 2.2$ % ($= 4.3\% - 2.1\%$), resulting in the equivalent random pitch error of 8.0 nm (rms).

Many ghost-like patterns are visible between the orders in Fig.9. Although these patterns should include the diffraction ripple pattern caused by the use of the collimated beam of a small diameter as mentioned in Ikeda et al.,[1] the integral intensity of the ghost-like patters is up to 25.3% of the total diffraction light which cannot be explained only by the diffraction ripple pattern (according to scalar diffraction theory, the total intensity of the diffraction ripple pattern should be less than 10%). This ghost-like pattern might be related to the dust on the groove surface and/or the chipping of the groove edge, because its intensity varies across the position of the laser beam exposure and it becomes stronger at the position where prominent chippings are clearly seen.

The maximum diffraction efficiency at $m = 215$ is theoretically determined by $I_{215}/\sum I_k = 0.95$, where $I_k$ is the intensity of $k$-th order, calculated by Eq.(1). Assuming the energy loss due to the scattered light (4.3%) and ghost-like pattern ($\leq 25.3\%$), the relative diffraction efficiency is conservatively estimated to be $\geq 70.4\% \times 0.95 = 67.1\%$ at $\lambda = 0.633\,$nm. When used as an immersion grating at $\lambda = 5\,\mu$m, the relative diffraction efficiency is estimated to be $\geq 71\%$ since the scattered light is magnified by $(n/\lambda)^2$ (see Ikeda et al.[1]).

| | Specification | As built (grinding) | As built (fly-cutting: sampleB) |
|---|---|---|---|
| Surface roughness | $< 16.5$ nm (rms) | 25 nm (rms) | 7.2 nm (rms) |
| Periodic pitch error$^\dagger$ | $< 12$ nm | – | $< 15$ nm |
| Random pitch error | $< 13.5$ nm (rms) | – | 8.0 nm (rms) |
| Corner R | $< 1\mu$m | $> 15\mu$m | $< 0.2\mu$m |
| Surface figure | $< 0.4\lambda$ @633nm | – | $< 0.2\lambda$ @633nm |

Table 4. **Performance of ZnSe test gratings** The specifications are for the shortest wavelength ($\lambda = 5\,\mu$m), where the requirement is tightest. ($^\dagger$Shown as an amplitude)

The absolute diffraction efficiency can be also estimated to be $\geq 66\%$ at $5\,\mu$m, assuming (i) the imperfection of BBAR (Broad-Band Anti-Reflection) coating on the entrance/exit surface of the immersion grating to be $\leq 1\%$ per each surface, (ii) the absorption of metal coating on the diffraction surface to be $\leq 5\%$.

The resultant measured performances of the test ZnSe gratings by two fabrication methods (grinding and fly-cutting) are summarized in Table 4. The LLNL fly-cutting satisfies almost all the specifications, showing that the SPICA ZnSe immersion grating for S-mode can be fabricated with currently existing technique. We plan to continue further R&D by fabricating ZnSe immersion grating on ZnSe prism (see Ikeda et al.[1]) to test its performance with IR beam.

## ACKNOWLEDGMENTS

We would like to thank SPICA team at ISAS/JAXA for providing the interesting opportunity to work on the space instrument development. We truly thank Paul Kuzmenko at LLNL for his dedicated support on the immersion grating development. It became successful thanks to the cutting-edge technique and wonderful staffs at LLNL. A portion of optical measurements were carried out using equipments at the Advanced Technology Center (= ATC), National Astronomical Observatory of Japan. We feel most grateful to all the staffs at ATC, who maintain the easy-to-use equipments in good shapes. This program was financially supported by the Grant for Basic Developments for Space Instruments (FY2006, FY2007, FY2008) by ISAS. This study was also financially supported by KAKENHI(16684001) Grant-in-Aid for Young Scientists (A) and KAKENHI(20340042) Grant-in-Aid for Scientific Research (B) by Japan Society for the Promotion of Science.

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