Wavelength calibration of the JWST Near Infrared Spectrograph (NIRSpec)

Stephan M. Birkmann^a, Torsten Böker^a, Pierre Ferruit^a, Giovanna Giardino^a, Peter Jakobsen^a, Guido De Marchi^a, Marco Sirianni^a, Maurice B. J. te Plate^a, Jean-Christophe Salvignol^a, Xavier Gnata^b, Thomas Wettemann^b, Bernhard Dorner^c, Giovanni Cresci^d, Fabiàn Rosales-Ortega^e, Martin Stuhlinger^f, Richard Cole^g, Jason Tandy^g, Chris Brockley-Blatt^g

^aEuropean Space Agency - ESTEC, Keplerlaan 1, 2200AG Noordwijk, Netherlands; ^bEADS Astrium GmbH, 81663 Munich, Germany;

^cUniversité de Lyon, Lyon, F-69003, France ; Université Lyon 1, Observatoire de Lyon, 9 avenue Charles André, Saint-Genis Laval, F-69230, France ; CNRS, UMR 5574, Centre de Recherche Astrophysique de Lyon ; Ecole Normale Supérieure de Lyon, Lyon, F-69007, France;

^dINAF - Osservatorio Astrofisico di Arcetri, Largo E. Fermi 5, 50125 Firenze, Italy;

^eCentro de Astrobiología (CSIC-INTA), Ctra de Ajalvir km 4, 28850 Madrid, Spain;

^fEuropean Space Astronomy Centre, P.O. Box 78, 28691 Villanueva de la Cañada, Madrid, Spain;

^gUniversity College London-Mullard Space Science Laboratory, Holmbury St. Mary, Dorking, Surrey RH5 6NT, United Kingdom

ABSTRACT

The Near Infrared Spectrograph (NIRSpec) is one of four science instruments aboard the James Webb Space Telescope (JWST) that is to be launched later this decade. NIRSpec is sensitive in the wavelength range from 0.6 to $5.0 \,\mu$ m and operates at temperatures $\leq 40 \,\text{K}$. It offers multi-object, fixed slit, and integral field spectroscopy with seven selectable dispersers. The on-ground spectrophotometric calibration of the instrument is performed by means of continuum and line emission lamps. NIRSpec also contains an internal calibration assembly (CAA) that will provide the wavelength and radiometric calibration in orbit. Due to thermal constraints, the CAA features low power tungsten filament lamps in combination with long-pass and Fabry-Perot-like interference filters, which need to be calibrated at instrument level. We will report on the wavelength calibration of the NIRSpec flight model and the CAA, carried out during the first cryogenic performance testing.

 ${\bf Keywords:} \ {\rm James \ Webb \ Space \ Telescope, \ JWST, \ Near \ Infrared \ Spectrograph, \ NIRSpec, \ wavelength \ calibration \ Minorphi \ Calibration \ Minorphi \ Min$

1. INTRODUCTION

The Near Infrared Spectrograph (NIRSpec) is one of the four science instruments of the James Webb Space Telescope (JWST). JWST features a deployable and passively cooled ($T \le 50 \,\mathrm{K}$) primary mirror with ~ 6.5 m diameter. A comprehensive description of the observatory and its main science goals is given by Gardner et al.¹ and at this conference.²

NIRSpec is a near-infrared multi-object spectrograph developed by the European Space Agency (ESA) with EADS Astrium Germany GmbH as the prime contractor. In March 2011, the first part of its cryogenic performance testing was completed. In this paper, we focus on the test results of this first campaign regarding the wavelength calibration of NIRSpec.

Further author information: (Send correspondence to S.M.B)

S.M.B.: e-mail: stephan.birkmann@esa.int; telephone +3171 565 8598; telefax +3171 565 4697

2. THE NIRSPEC INSTURMENT

NIRSpec features three three-mirror anastigmats (TMAs), namely the fore optics (FOR), the collimator (COL) and the camera (CAM). Furthermore, a filter and a grating wheel assembly (FWA and GWA), a refocus mechanism assembly (RMA), a calibration assembly (CAA), the microshutter assembly (MSA), and the integral field unit (IFU). Light is detected by the focal plane assembly (FPA), a mosaic of two $2k \times 2k$ HAWAII-2RG detector arrays with a ~ 5.3 μ m cut-off. Both the FPA and the MSA are provided by NASA. With the exception of the filters in the FWA and a double pass prism in the GWA, the entire optics is all-reflective and made out of Silicon Carbide, as is the optical bench.

NIRSpec offers seven dispersers. A CaF₂ prism covers the entire wavelength range (0.6 to 5μ m) in a single exposure with varying spectral resolution (30 $\leq R \leq 300$). Six gratings offer medium ($R \sim 1000$) and high ($R \sim 2700$) resolution spectroscopy in three bands covering 1 to 5μ m. A mirror is available for imaging and target acquisition.

The microshutter assembly offers an array of 730×342 individually addressable shutters over a field of view (FOV) of more than 9 arcmin², giving NIRSpec its multi-object capabilities. For isolated objects, NIRSpec features an IFU with 30 slitlets covering a 3×3 arcsec FOV. The IFU spectra fall on the same detector area as the MSA spectra, therefore the IFU aperture is blocked when doing multi-object observations, and all shutters have to be closed when using the IFU. Finally, there are five fixed slits for high contrast spectroscopy, with their spectra falling onto dedicated detector areas.

A more detailed description of NIRSpec and its optical train is given by Bagnasco et al.³ and te Plate et al.,⁴ and also in these proceedings by De Marchi et al.⁵

3. WAVELENGTH CALIBRATION STRATEGY

As mentioned above, NIRSpec will offer a number of different observing modes to the user. In terms of wavelength calibration, multi-object observations with the MSA will provide the greatest challenge. Due to the vast number of micro-shutters, a direct wavelength calibration of each of them would be very demanding, time consuming, and costly. We will therefore utilize the instrument model of the instrument performance simulator $(IPS)^6$ of NIRSpec to establish the wavelength calibration for each mode.

The IPS is a software designed to simulate NIRSpec exposures, taking into account the full optical model of the instrument. This means that for a given input (source/shutter location, spectral energy distribution), the IPS can generate data that look like as observed with the real NIRSpec, as has already been shown for the NIRSpec demonstration model.⁷ By comparing the measured positions of spectra and lines with the calculated ones, we can tweak the instrument model until we get the correct answer. In order to establish the wavelength calibration with the required accuracy – the NIRSpec science requirement is 1/8 of a resolution element – the light source has to deliver a number of preferably unresolved lines over the wavelength regime of interest, with the wavelength of these lines precisely known.

We have chosen an Argon emission line lamp as the primary source for on-ground wavelength calibration and tuning of the instrument model. The Argon spectrum has the advantage that it delivers i) a large number of unresolved lines^{*} in the wavelength range of interest for NIRSpec, and ii) that the wavelength of these lines have been very accurately determined by Kerber et al.⁸ using measurements performed at the National Institute of Standards and Technology (NIST). The Argon lamp is part of the calibration light source (CLS), which is NIRSpec's primary calibration source during the on-ground cryogenic test campaigns.

3.1 Calibration sources

The CLS consists of a 60 cm diameter, gold-coated integrating sphere and a light-box. The latter contains a Sapphire window sealed tungsten filament, and four filter and aperture wheels. These wheels hold several longand band-pass filters, as well as attenuators that are needed for the spectro-photometric calibration of NIRSpec. The Argon emission line lamp is located directly on the sphere and coupled in via a small hole. In order to avoid thermal background, the entire CLS including lamps and filters is cooled to $T < 100 \,\mathrm{K}$ by means of liquid

^{*}typical Ar linewidths $\Delta\lambda$ are such that $\lambda/\Delta\lambda > 100000$, significantly higher than the resolving power of NIRSpec

n an an ann an ann an ann an ann ann an	

Figure 1. NIRSpec count rate image of the CLS Argon lamp taken with the Band II high resolution grating and the target acquisition filter. The two dashed yellow boxes denote the position of the IFU spectra (2×15 slitlets), the solid green box the spectra of the five fixed slits. The narrow spectra in the IFU region are due to some unintentionally open shutters in the MSA. Full white corresponds to a count rate of 3 ADU s^{-1} .

Nitrogen and is attached to the NIRSpec cryo chamber. As the Argon lamp heats up during operation, we use it in conjunction with the NIRSpec target acquisition filter transmitting between 0.8 and 2.0 μ m, eliminating thermal background at long wavelengths. Therefore, the Ar lines below 2 μ m are used in higher orders to calibrate the gratings for the longer wavelength bands.

In orbit, the internal CAA will be used to verify that the instrument model is still valid. The CAA consists of a gold-coated integrating sphere with eleven telescope assemblies. Each telescope has two tungsten filament lamps for redundancy and a set of lenses and filters to provide spectral flats and wavelength references. Due to thermal reasons the CAA does not have a line emission source, but has to rely on Fabry-Perot-like interference filters for wavelength calibration and checking the dispersion solution. The main challenge with these filters is that they provide a set of rather broad and temperature-dependent lines, and thus need to be calibrated at instrument level against the Argon source (see section 4). The CAA also features an Erbium-doped filter that provides a stable wavelength reference in a narrow region around $1.5 \,\mu$ m.

Both the CLS and CAA were build by the Mullard Space Science Laboratory (MSSL), London, and the CLS was radiometrically calibrated by the National Physics Laboratory (NPL), also London.

4. DATA ANALYSIS AND RESULTS

4.1 Tweaking the instrument model

All data presented here were taken during the first part of the cryogenic on-ground calibration campaign concluded early 2011. NIRSpec was tested in the same chamber that was already used for testing the demonstration model^{9,10} at IABG, Munich. During this first campaign the MSA was not fully operational and thus we are limited to the fixed slits and the IFU.

Fig. 1 shows a NIRSpec image obtained with the fixed slits and IFU illuminated by the CLS Argon source. Using our extraction software that also uses the instrument model from the IPS,¹¹ we obtain wavelength calibrated spectra as shown in Fig. 2 for one of the fixed slits. For each of these spectra we fit the position of the Argon lines and compare the wavelengths with the ones measured by NIST. The deviations are then used to



Figure 2. Fixed slit spectrum of the Ar emission lamp, extracted from exposure shown in Fig. 1. The inlay illustrates the high dynamic range of the data, with lines well measured ranging from a few $ADUs^{-1}$ to several thousand. Argon lines seen in second and third order are dominating the spectrum.

optimize the instrument model, by minimizing the residuals for the available spectra of all dispersers together, including data obtained in imaging mode.

The achieved accuracy in wavelength calibration for the fixed slits and the IFU is meeting the requirements. This is illustrated in Fig. 3 for the Band II high resolution grating. The root mean square (RMS) residual of 0.28 Å corresponds to $\sim 1/30$ resolution element, about a factor of four better than required. The RMS residuals of other gratings and slits are similar.

Furthermore, there is still room for improvement. There are clearly some systematic deviations visible in the residual plot (like the double 'u' shape), which will be addressed with data to be taken during the second calibration campaign, then also including the MSA. This will allow us to increase the number of free parameters for the COL and CAM parts of the instrument model, including higher order distortions.

Another limiting factor for the wavelength knowledge of any observation is the limited reproducibility of the GWA, introducing slightly random tilts when changing dispersers.¹² However, this effect can be compensated using the tilt sensor of the GWA, as is demonstrated by another paper in these proceedings.⁵

4.2 Calibrating the CAA line sources

The CAA holds five spectral references: four transmission line filters for the three bands covered by the gratings and the prism, plus one Erbium doped absorption filter. All filters have in common that they produce lines that are resolved with NIRSpec and have asymmetric profiles (see Fig. 4). In order to get a usable wavelength for the lines of these filters, we compute the center of gravity (CoG) of the line. The centre of gravity calculation is based on the method described by Cameron et al.¹³ The CoG of a function $E(\lambda)$, in the region where $E(\lambda) \ge E_t$,



Figure 3. Residuals (observed minus true wavelength⁸) for Argon lines from the spectrum shown in Fig. 2 after tweaking the instrument model. The error bars denote the uncertainty due to the line fitting.

is given by:

$$\operatorname{CoG} = \frac{\int_{\lambda_j}^{\lambda_k} \lambda \left[E(\lambda) - E_f \right] d\lambda}{\int_{\lambda_j}^{\lambda_k} \left[E(\lambda) - E_f \right] d\lambda},\tag{1}$$

where E_t and E_f (the threshold and floor values respectively) are fractions f_T and f_F of the maximum value and λ_j and λ_k are the wavelengths on opposite sides of the peak maximum value at which $E(\lambda) = E_t$. If the peak is symmetric, the CoG will be the wavelength of the absorption/emission peak maximum. If the peak is asymmetric, as is the case for the CAA sources, the CoG will differ from the peak maximum by an amount dependent on the selection of f_T and f_F as well as the degree of asymmetry of the selected band. For a discrete set of spectral values E_i at wavelengths λ_i and bin widths w_i , the CoG can be calculated using

$$CoG = 0.5 \left[\frac{\sum_{i=j}^{k} \lambda_i w_i (E_i - E_k)}{\sum_{i=j}^{k} w_i (E_i - E_k)} + \frac{\sum_{i=j}^{k-1} \lambda_i w_i (E_i - E_j)}{\sum_{i=j}^{k-1} w_i (E_i - E_j)} \right],$$
(2)

where E_k is the value of $E(\lambda)$ closest to E_t , and E_j is the value closest to E_t on the other side of the peak maximum, such that $E_j \ge E_k$. The double summation is required because the separate summations are biased in opposite directions.

For the Erbium filter, we compared the line centers measured with NIRSpec to those measured by NPL at filter level. The results are summarized in Table 1 on page 7. The CoGs of the six measured lines agree to within 0.6 Å, showing that this filter can be used as reliable wavelength reference. It also has the advantage that the position of the lines is almost independent of temperature. The drawback of the Erbium filter is, however, that



Figure 4. a) Spectrum of the Erbium doped wavelength reference filter taken with the Band I high resolution grating. b) to d) Spectrum of the CAA line sources taken with the high resolution gratings in Band I to III.

Table 1. Center of gravities for six lines of the internal Erbium spectral reference source. The first three columns denoted with (a) were measured by NPL at filter level, the last two columns (b) were measured with NIRSPec.

Line	measured line CoG $[\mu m]$ at temperature					
#	$29.7\mathrm{K}^{(a)}$	$39.7\mathrm{K}^{(a)}$	$49.7 \mathrm{K}^{(a)}$	$31.2\mathrm{K}^{(b)}$	$45.1 \mathrm{K}^{(b)}$	
1	1.45795	1.45796	1.45796	1.45799	1.45801	
2	1.47881	1.47883	1.47883	1.47883	1.47884	
3	1.48657	1.48658	1.48658	1.48661	1.48662	
4	1.51094	1.51095	1.51096	1.51099	1.51100	
5	1.54085	1.54085	1.54086	1.54091	1.54091	
6	1.54556	1.54556	1.54555	1.54561	1.54561	

it only covers a narrow wavelength region and thus cannot be used to verify the dispersion solution of NIRSpec once in orbit.

This will be achieved using the Fabry-Perot-like transmission filters, which provide 5 to 10 lines across the spectral bands (see Fig. 4 b) to d)). Although the lines are heavily resolved and asymmetrical, the CoG method yields very reproducible line centers from one exposure to the other, with typical RMS values smaller than 0.1 Å (see Fig. 5 on page 9). They show, however, a non-negligible temperature dependence that has to be considered. This temperature dependence was characterized by MSSL/NPL at telescope level and found to be fairly linear in the temperature range of interest ($30 \le T \le 50$ K). During the NIRSpec calibration campaign, we also probed the extreme ranges of its operational temperature. Together, these data will allow us to derive the appropriate CoGs of the lines for the temperature finally encountered in orbit.

5. CONCLUSION

We have shown that with the available data obtained during the first cryogenic performance test of the NIRSpec flight model, we can achieve the required wavelength calibration accuracy. Furthermore, this calibration can very likely be transferred to the wavelength standards in the on-board calibration source, allowing us to verify the wavelength calibration in orbit, and also to update the instrument model if necessary.

REFERENCES

- Gardner, J. P., Mather, J. C., Clampin, M., Doyon, R., Flanagan, K. A., Franx, M., Greenhouse, M. A., Hammel, H. B., Hutchings, J. B., Jakobsen, P., Lilly, S. J., Lunine, J. I., McCaughrean, M. J., Mountain, M., Rieke, G. H., Rieke, M. J., Sonneborn, G., Stiavelli, M., Windhorst, R., and Wright, G. S., [*The James Webb Space Telescope*], 1–29 (2009).
- [2] Clampin, M. C., "JWST science and system overview," Proc. SPIE 8150-14 (2011).
- [3] Bagnasco, G., Kolm, M., Ferruit, P., Honnen, K., Koehler, J., Lemke, R., Maschmann, M., Melf, M., Noyer, G., Rumler, P., Salvignol, J., Strada, P., and Te Plate, M., "Overview of the near-infrared spectrograph (NIRSpec) instrument on-board the James Webb Space Telescope (JWST)," Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series 6692 (Oct. 2007).
- [4] te Plate, M., Holota, W., Posselt, W., Koehler, J., Melf, M., Bagnasco, G., and Marenaci, P., "Optomechanical design of the near infrared spectrograph NIRSpec," *Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series* **5904**, 185–198 (Aug. 2005).
- [5] de Marchi, G., te Plate, M. B. J., Birkmann, S. M., Böker, T., Ferruit, P., Giardino, G., Jakobsen, P., Sirianni, M., Savignol, J.-C., Gnata, X., Barho, R., Kosse, M., Mosner, P., Dorner, B., Cresci, G., Rosales-Ortega, F., Stuhlinger, M., Gross, T., and Leikert, T., "Calibrating the position of images and spectra in the NIRSpec instrument," *Proc. SPIE* 8150-12 (2011).
- [6] Piquéras, L., Legros, E., Pons, A., Legay, P.-J., Ferruit, P., Dorner, B., Pécontal, A., Gnata, X., and Mosner, P., "The JWST/NIRSpec instrument performance simulator software," in [Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series], Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series 7738 (July 2010).

- [7] Dorner, B., Ferruit, P., Gnata, X., Birkmann, S. M., Böker, T., de Marchi, G., Sirianni, M., Hupfer, W. J., Köhler, J., Kolm, M.-G., Ehrenwinkler, R., Piquéras, L., Legros, E., Legay, P.-J., Pécontal-Rousset, A., Jarno, A., and Pons, A., "Confronting the NIRSpec instrument performance simulator outputs with results of the NIRSpec demonstration model calibration campaign," in [Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series], Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series 7738 (July 2010).
- [8] Kerber, F., Nave, G., and Sansonetti, C. J., "The spectrum of Th-Ar hollow cathode lamps in the 691-5804 nm region: Establishing wavelength standards for the calibration of infrared spectrographs," *The Astrophysical Journal Supplement Series* 178(2), 374 (2008).
- [9] Birkmann, S. M., Böker, T., Jakobsen, P., de Marchi, G., Sirianni, M., Bagnasco, G., Jensen, P. L., Te Plate, M. B. J., Rumler, P., Salvignol, J.-C., Strada, P., Kolm, M., Gnata, X., Honnen, K., Köhler, J., Lemke, R., Maschmann, M., Melf, M., Pittet, J.-F., Ferruit, P., and Dorner, B., "Status of the NIRSpec instrument," in [Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series], Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series 7731 (July 2010).
- [10] Boeker, T., Birkmann, S., de Marchi, G., Jakobsen, P., Sirianni, M., Ferruit, P., Gnata, X., Mosner, P., Ehrenwinkler, R., and Beck, T., "The NIRSpec Demonstration Model Test Campaign," in [American Astronomical Society Meeting Abstracts #215], Bulletin of the American Astronomical Society 42, #439.06– + (Jan. 2010).
- [11] Dorner, B., Ferruit, P., Piquéras, L., Legros, E., Pécontal, A., Jarno, A., Pons, A., Gnata, X., and Pacifici, C., "First Simulation and Data Reduction of a JWST/NIRSpec Observation," in [Astronomical Society of the Pacific Conference Series], I. N. Evans, A. Accomazzi, D. J. Mink, & A. H. Rots, ed., Astronomical Society of the Pacific Conference Series 442, 343-+ (June 2011).
- [12] Leikert, T., "Alignment and testing of the NIRSpec filter and grating wheel assembly," Proc. SPIE 8131-25 (2011).
- [13] Cameron, D. G., Kauppinen, J. K., Moffatt, D. J., and Mantsch, H. H., "Precision in condensed phase vibrational spectroscopy," *Appl. Spectrosc.* 36, 245–250 (May 1982).



Figure 5. Scatter plot of the CoG of the five lines of the Band III CAA line filter (see Fig. 4 d)) from 20 different exposures, taken without moving the grating wheel between exposures. For each line, the mean and RMS of the CoG is denoted in the panels.