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Index of refraction of germanium

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Measurements of the index of refraction of a sample of high-quality, single-crystal germanium using the minimum deviation refractometry method are presented for temperatures near 22°C and for wavelengths in the range 2 to 14 μ m. The standard uncertainty for the measurements ranges from 1.5×10^{-5} to 4.2×10^{-5} , generally increasing with wavelength. A Sellmeier formula fitting the data for this range is provided. Details of the custom system and procedures are presented, along with a detailed analysis of the uncertainty. These results are compared with previous measurements.

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1. INTRODUCTION

Since germanium (Ge) first began to be developed for transistor and infrared (IR) optics applications in the late 1940s, the material quality has continually improved to meet increasingly stringent demands. For optics applications, this has driven the need for more accurate optical properties measurements, especially the index of refraction in the high-IR transmission wavelength region ($\geq 2 \mu m$), to meet the requirements of optical system performance. Ge measurements by various methods in the 1950s reported absolute index measurement standard uncertainties ranging from a high of about 1×10^{-2} to a low of 3×10^{-4} , with results between labs differing by as much as 10^{-2} [1–4]. These materials had various doping and defect levels. The measurements by Salzberg and Villa [3,4] in 1957 and 1958 for the range 2 to 16 µm have been used extensively for IR optics design for two decades since their publication and to some extent even today.

By the mid-1970s, driven by the importance of Ge for IR applications, material quality and index measurement methods had improved to the point where reported index measurements for the range of 2 to 14 μ m generally had stated standard uncertainty estimates in the mid to low 10⁻⁴ range [5,6]. In particular, Icenogle *et al.* [5] reported measurements for the refractive indexes of Ge over the range 2.5 to 12 μ m and their variations with temperature over the ranges 95 K to 298 K, with conservative estimates of their standard uncertainties of 6×10^{-4} . These differed from previous measurements, e.g., those of Salzberg and Villa [4], by as much as 5×10^{-3} , when account is taken of the different measurement wavelengths and temperatures used. Icenogle *et al.* suggested that the difference may be due to

different sample impurities. Edwin *et al.* [6] reported measurements of a Ge sample at two laboratories over a subrange 8 to $14 \,\mu\text{m}$ by different deviation-angle methods, with a discrepancy of 3×10^{-4} between labs. These results differed from those of Icenogle *et al.* by $\leq 10 \times 10^{-4}$ over the range of wavelength overlap (with the exception of longest wavelength index). In 1980, Li [7] reviewed and tabulated all the measured index data on Ge and Si since 1949. Based on an analysis of all the data, he recommended index values for Ge for wavelength and temperature in the ranges 1.0 to 18 μ m and 100 K to 550 K, using an expression with the wavelength dispersion given by a single $1/\lambda^2$ term. The stated standard uncertainty for the index was 2×10^{-3} over the wavelength and temperature range, consistent with the uncertainties stated for the 1970s measurements discussed.

Since the late 1970s, the results of Icenogle *et al.* [5], and to some extent the previous results of Salzberg and Villa [3,4], have been widely used in IR optics design, including incorporation in commercial optics design software. These values have been recommended in well-established index data reference books, such as the *Handbook of Optical Constants of Solids* [8] and the *Handbook of Infrared Optical Materials* [9]. In 2006, Frey *et al.* [10] reported Ge index measurements over the wavelength range 1.8 to 5.5 μ m and temperature range 30 K to 295 K, with an estimated standard uncertainty of $\pm 1 \times 10^{-4}$. The difference from previous results was generally in the range $\pm 2 \times 10^{-3}$, consistent with the analysis of Li [7].

There has been a clear trend over time for reported Ge index measurements to have reduced stated uncertainties and increased consistency between measurements. However, the reports generally do not give enough information to assess how much these increased agreements are due to measurement improvements and how much is due to improvements in material quality and consistency. And it is not generally clear whether these more accurate Ge index values apply to routine commercially available material. Thus, IR optical designers have had to rely either on generic Ge index data with a standard uncertainty of at best from 1×10^{-3} to 2×10^{-3} , or make measurements on the particular material batch used, with the uncertainty improved by at most about an order of magnitude.

There have been a number of different methods used to measure the index of bulk materials, including techniques based on refraction angle, interference in slabs, surface reflection, and ellipsometry. For the transparent region of IR materials, the methods generally reporting the highest accuracy are variations of the minimum-deviation-angle refractometry method. These methods are based on measuring the angle of refraction through a prism of the material set at the angle of minimum deviation as is discussed below. The accuracy of this approach is limited by the diffraction of the beam through the prism. For a prism about 3 cm on a side, calculated diffraction-limited index uncertainty is approximately 5×10^{-7} in the ultraviolet, which has been verified [11]. This diffraction-limited uncertainty scales with wavelength approximately 2 orders of magnitude to the low-to-mid 10^{-5} range in the mid-IR. This is about an order of magnitude smaller than the uncertainties reported for Ge discussed above. Thus, with an optimized refractometer design, an order of magnitude improvement in index accuracies of Ge should be achievable. Improving the accuracy to this level would enable more precise IR optical design. In addition, this accuracy improvement would be of value to sort out index variations in samples of commercial material, feeding back to material fabricators to improve material quality.

This paper presents results of index measurements on one high-material-quality Ge sample for temperatures near 22° C and wavelengths through the range 2 to 14 μ m. The measurements were made using a custom minimum-deviation-angle refractometry system designed to achieve diffraction-limited uncertainties over this range. Attaining this performance required substantially reducing numerous sources of uncertainty compared to previous measurements, in some cases by an order of magnitude or more. This work follows up on a previous work with preliminary, less-extensive results on the index of the same Ge sample [12].

2. MEASUREMENT

A. Minimum-Deviation-Angle Refractometry

The index measurements were made using the well-established minimum-deviation-angle refractometry method, which is based on determining the angle $\delta(\lambda)$ by which a collimated beam of known wavelength λ refracts through a prism of known apex angle α [13,14]. If the prism is oriented so that the beam travels symmetrically through the prism with respect to the apex angle, then the refraction angle (deviation angle) is at a minimum and the refractive index of the prism material $n_{mat}(\lambda)$ relative to the index of the gas surrounding the prism $n_{gas}(\lambda)$ is given by [Eq. (1)]

$$n_{\rm rel}(\lambda) = n_{\rm mat}(\lambda)/n_{\rm gas}(\lambda) = \sin[(\alpha + \delta(\lambda))/2]/\sin(\alpha/2).$$
(1)

A significant benefit of measuring the deviation angle $\delta(\lambda)$ at the angle of minimum deviation is that the measurement is at an extremum condition, making it relatively insensitive to the alignment of the prism, a substantial source of uncertainty. Due to the conceptual simplicity of the index determination, not depending on any models other than Snell's law, it is relatively secure from subtle sources of systematic errors. The accuracy of the determination of $n_{mat}(\lambda)$ simply depends on the accuracy of the determination of the parameters λ , $n_{gas}(\lambda)$, α , and $\delta(\lambda)$. The uncertainties in α and $\delta(\lambda)$ depend in part on the geometric and surface properties of the prism, along with the prism index homogeneity and isotropy. Some discussion is given below on those aspects of the implementation of the minimum-deviationangle technique used in this work, relevant to the uncertainties of these various components.

One limitation of this technique is that it requires relatively large prism samples of high transmission. For finite absorption, variable transmission for different path lengths through the prism gives rise to beam apodization effects. These distort the beam profile and increase the image diffraction width at the detector, resulting in increased index uncertainty. This limits the accuracy that index measurements can be made in absorbing wavelength regions.

B. NIST Minimum-Deviation-Angle Refractometer

A custom minimum-deviation-angle refractometer system was designed with all-reflective optics to achieve diffraction-limited index measurements for wavelengths through the range 0.12 to 14 µm, near room temperature. This system can be used to measure the index of any material transmitting in this wavelength range that can be made into a prism of sufficient optical quality. A schematic diagram of the system setup for IR measurements is shown in Fig. 1. The narrowband IR radiation for the $\delta(\lambda)$ measurements was generated by filtering radiation from a broadband 1200°C blackbody source by a grating monochromator or from a 3.39 µm He-Ne laser. The grating orders were separated by the prism sample. The entire path of the radiation from the source to the detector was enclosed in custom sealed housings purged with dry N₂ gas to enable measurements in the low transmission regions of air containing natural amounts of H₂O and CO₂.

The radiation from the blackbody source (IR Systems, model IR-564/301) was chopped and imaged into a McPherson 2061 monochromator with a focal length of 1 m. A grating with 100 grooves per millimeter, blazed near 9 µm, was used. Appropriate grating orders were chosen for each wavelength desired to ensure the grating was used near the blaze angle for high efficiency. The wavelength output of the monochromator was calibrated with the 633 nm line from a He-Ne laser for the first 24 grating orders and with the 3.39 µm line from a He-Ne laser for the first 4 grating orders. The small wavelength nonlinearity of the monochromator was removed by a calibration curve. The calibrated wavelength was accurate to within ± 0.05 nm for the full 2 to 14 µm range. The monochromator slit widths were chosen for each wavelength to be as large as possible to maximize the signal-to-noise ratio, while ensuring that the bandwidth contributed less than 20% of the overall uncertainty budget for the index. The entrance- and exit-slit heights were 4 mm.



Fig. 1. Schematic diagram of the top view of the NIST minimum-deviation-angle refractometer system with all reflective optics. Mirror M1 collects radiation from the blackbody source and images it, via M2, into a monochromator. The output of the monochromator is imaged into the higher refractometer entrance slit via a pair of parabolic mirrors M3 and M4. The radiation through the entrance slit is turned and angled down by plane mirror M5 and collimated by spherical mirror M6. The collimated beam is refracted by the prism and imaged to the exit slit by spherical mirror M7 and plane mirror M8. This radiation is re-imaged into the HgCdTe detector by a pair of parabolic mirrors M9 and M10.

The narrowband radiation from the monochromator was collected and focused into the entrance slit of the refractometer by a pair of parabolic mirrors (effective focal lengths: 203.2 mm). The optics of the refractometer had a focal length of 0.5 m and an f-number of 10. The entrance and exit slit widths of the refractometer were chosen as above to maximize signal-to-noise ratio without degrading the index uncertainty above the diffraction limit. A folding mirror and a spherical mirror (focal length: 508 mm, diameter: 50.8 mm) collimated the radiation to the prism, and the refracted radiation was focused onto the exit slit by a spherical mirror and a folding mirror. A ray trace analysis of the system (using Zemax OpticStudio Professional) showed that aberrations, from using spherical mirrors for the slit heights of 4 mm, were less than the diffraction spread.

The prism sample holder was mounted on a pair of stacked computer-controlled goniometers. The bottom goniometer (Huber, model 430), which holds the detector arm, incorporated an angle encoder (Heidenhain, model RON 905) with absolute accuracy of ± 0.2 arcseconds. The top goniometer (Huber, model 420) was controlled by the drive program to ensure that after initial minimum deviation alignment, the minimum deviation condition of the prism was maintained. It incorporated an angle encoder (Heidenhain, model ROD 880) with absolute accuracy of ± 1.0 arcseconds. The prism tilts were aligned by an autocollimator, and the minimum deviation alignment was determined by multiple scans at various prism angles at the wavelength of 3.39 µm.

The radiation exiting the refractometer was imaged by a pair of parabolic mirrors (effective focal lengths: 101.6 mm and 50.8 mm) onto a liquid-nitrogen-cooled HgCdTe detector (InfraRed Associates, model MCT-13-2.00). The parabolic mirrors were intentionally misaligned so that the resulting aberrations distorted the image of the narrow-width, 4 mm height slit to approximately the size of the 2 mm square detector. Lock-in detection was used. The deviation angle for each wavelength $\delta(\lambda)$ was determined by introducing each wavelength in turn into the entrance slit of the refractometer and scanning the detector arm. The prism angle was scanned at half the angular rate to ensure that the minimum-deviation condition was maintained. For each wavelength, the encoder-determined angle of the center of the peak (obtained by fitting) was compared to that of the undeviated beam to obtain the deviation angle $\delta(\lambda)$. Measurements were made on both sides of the prism repeatedly to cancel the effects of absolute angle drifts. The uncertainty of the center of each peak was estimated to be less than 10% of the FWHM (full width at half-peak-maximum). This uncertainty was a dominant contribution to the total estimated uncertainty for all wavelengths. The peak widths broadened as the wavelength increased as expected from diffraction. Thus, the total uncertainty increased as the wavelength increased as discussed in Section 3.A.

Due to the very high temperature dependence of the index of Ge of about 4×10^{-4} /°C [5], special care was taken to control the temperature throughout the prism to near the target temperature of 22.000°C. The concern was both to minimize the impact of temperature gradients in the prism on the index measurements and to minimize the uncertainties of the index at the reported temperature due to absolute temperature errors. This goal of ensuring absolute temperature control of the Ge prism within the range $(22.000 \pm 0.005)^{\circ}$ C was accomplished by the use of a feedback control loop in the following fashion. The prism was mounted between two hollow copper plates with good thermal contact to the top and bottom triangular surfaces of the prism. Two water baths had separate temperatures maintained at approximately 1°C above and 1°C below the set point temperature of 22.000°C. Water from the two baths was mixed and sent through the two hollow copper plates. The mixing of the two fluids was accomplished by a valve, which set the mixing ratio by the error in the sample temperature from the set point in a proportional-integral-derivative (PID) feedback control loop. The sample temperature was determined by two platinum resistance thermometers mounted on the top copper plate and two mounted on the bottom plate. These were calibrated by a standards-grade platinum resistance thermometer (Minco, model S1059) calibrated against the triple point of water and the melting point of gallium, according to the ITS-90 international temperature standards protocol [15]. The standard uncertainty of the calibration of each of the mounted thermometers used was 0.002°C.

During temperature control operation, all four thermometers were monitored. One of the thermometers was used to determine the feedback error signal for the temperature control loop. The control loop kept the readings of all four thermometers within a range of $\pm 0.004^{\circ}$ C centered at 22.000°C, ensuring an absolute temperature throughout the prism within the range $(22.000 \pm 0.005)^{\circ}$ C for the duration of the multi-day measurements. This symmetric temperature control of the top and bottom of the prism limited possible temperature gradients across the prism. The temperature gradient contribution to the index uncertainty is subsumed in the prism temperature contribution in Table 2. The temperature of the nitrogen gas was controlled by a second, similar PID control loop. The gas temperature within the sample housing was monitored by two calibrated platinum resistance thermometers and was controlled to maintain the absolute temperature within the range $(22.000 \pm 0.020)^{\circ}$ C.

C. Ge Sample

The single-crystal Ge material measured was made into a prism with sides 39 mm long and 29 mm high and an apex angle of nominally 15°. Both prism transmitting surfaces had figure errors less than 5 nm root mean squared (RMS, $\lambda/120$ RMS at 633 nm) over the 90% clear aperture as measured by an interferometer (Zygo, model VeriFire). The apex angle was determined by use of two stacked indexing tables and an autocollimator, making angle difference measurements between both sides of the prism with all combinations of indexing table angles separated by 15° intervals. The standard deviation of all the measurements from the various indexing table angle combinations was 0.12 arcseconds. Including other sources of error, such as the surface figure errors, gave a standard uncertainty of the apex angle of 0.15 arcseconds.

The sample resistivity, determined by a four-probe measurement, was 17 $\Omega \cdot cm$, within the range of about 10 to 40 $\Omega \cdot cm$, generally targeted for optimal Ge transmission properties [16]. The index homogeneity was measured on a 10 mm thick, 27 mm diameter Ge disk, taken from a location in the Ge ingot close to where the prism material was taken. The measurements were made at 3.39 µm, using a M3 Measurements Solutions MWAVE 339 IR phase-shifting interferometer with a calibrated accuracy of 0.002λ RMS wavefront error at 3.39 μ m [17]. Due to the very high temperature dependence of the index of about 4×10^{-4} /°C [5], there was concern that temperature gradients in the sample would give rise to substantial index inhomogeneities during the characterization. To minimize this, the sample was mounted between two large apertured copper blocks thermally connected with copper side plates. The homogeneity measurement result was 9.1×10^{-6} RMS, 72.8×10^{-6} peak to valley (PV). Due to possible residual temperature gradient effects, this represents an upper bound for the grown-in inhomogeneity.

The transmittance of the sample was measured through the center of the face of the prism with a 6 mm diameter aperture, using a Fourier-transform spectrometer and an integrating sphere to collect the transmitted light [18]. It was found that there was no change in transmittance structure using smaller apertures. The results are shown in Fig. 2. The spectrum shows



Fig. 2. Transmittance versus wavelength of the Ge prism measured using a Fourier-transform spectrometer and an integrating sphere. The illumination was apertured to 6 mm diameter at the center of the prism, with the first face at 23° to the illumination and the back face 8° to the illumination.

a transmittance of about 44% through the range just below 2 through 11 µm. A calculation using our measured index values predicts a value of within 2% of this; the specific value depends on assumptions about what happens to the multiple reflections in this highly refracting prism window. This spectrum is similar qualitatively and quantitatively to transmittance spectra of high-quality Ge in the literature [9]. The absorption structure at 12 µm and longer wavelengths is due to phonon absorption. The sharp drop in transmittance to zero near 2 μ m is due to the onset of electronic transitions at the semiconductor conduction band edge [8]. This is the approximate lower limit wavelength for use of Ge as thick transmitting windows and optics. For 1.875 µm, the data from Fig. 2 gives an absorption coefficient of about 2.2 cm⁻¹, causing beam apodization effects, discussed in Section 2.A. These result in a substantial increase in index uncertainty due to diffraction broadening and systematic errors, which are difficult to assess quantitatively. For this reason, 2.0 µm was used as the lower limit for the measurements.

D. Measurement Procedures

Deviation angle measurements were made at minimum deviation with transmission through the prism in each direction in separate measurements by rotating the prism around and measuring the deviations on each side of the undeviated beam. This required establishing minimum deviation settings on each side by multiple index scans as a function of prism position. On each side, deviation angle measurements were made at 21 wavelengths, as shown in Table 1, within the range 2.0 to 14.0 μ m. The deviation angle at each wavelength was determined by the average of the deviation angles from both sides. This was repeated 4 times. During the measurements, the temperature of the prism and the N₂ gas in the sample chamber were continuously monitored, but because they were controlled to 22.000°C, no temperature corrections were necessary. The pressure of the

Table 1. Vacuum and Air Wavelengths, Absolute and Relative Indices, and Combined Standard Uncertainties for Measurements of Ge at 22.000°C

λ ^{vac} (μm)	λ^{air} (μm)	Index ^{vac}	Index ^{air}	$u_c(n) (10^{-5})$
2.00000	1.99947	4.109725	4.108630	1.6
2.12500	2.12443	4.095492	4.094401	1.5
2.25000	2.24940	4.084070	4.082982	1.5
2.37500	2.37437	4.074715	4.073629	1.5
2.50000	2.49933	4.066925	4.065842	1.5
2.75000	2.74927	4.054785	4.053705	1.5
3.00000	2.99920	4.045796	4.044719	1.6
3.39224	3.39133	4.035736	4.034661	1.6
4.00000	3.99894	4.025816	4.024744	1.7
4.50000	4.49880	4.020584	4.019514	1.8
5.00000	4.99867	4.016867	4.015798	1.9
5.50000	5.49854	4.014131	4.013062	2.0
6.00000	5.99840	4.012071	4.011003	2.2
7.00000	6.99814	4.009192	4.008126	2.4
8.00000	7.99787	4.007321	4.006255	2.6
9.00000	8.99761	4.006019	4.004953	2.9
10.00000	9.99734	4.005079	4.004013	3.1
11.00000	10.99707	4.004360	4.003294	3.4
12.00000	11.99681	4.003824	4.002758	3.7
13.00000	12.99654	4.003358	4.002293	4.0
14.00000	13.99627	4.002979	4.001914	4.2

 N_2 gas in the chamber was monitored throughout the measurements by an internal precision pressure sensor and was nearly the ambient pressure. It was not controlled, and it drifted with the ambient pressure during measurements. The varying pressure was corrected for in the data analysis.

The calibrated wavelengths from the monochromator were the wavelengths in N₂ gas. The wavelengths shown in the first column of Table 1 are wavelengths corrected to vacuum wavelengths. The wavelengths in the second column of Table 1 are wavelengths corrected to dry-air wavelengths at 22.000°C and a pressure of 101.325 kPa (1 standard atmosphere). To make the conversions, the well-established indices of air and N₂ gas as functions of temperature and pressure were used [19,20]. For air with 50% relative humidity, the air wavelengths and relative indices are both changed by a relative fraction of approximately 5×10^{-7} . This difference is negligible compared to the index uncertainties discussed in Section 3.A.

3. RESULTS

A. Index of Refraction

The indices of refraction determined by the procedures discussed above are presented in Table 1. The indices are presented as absolute (vacuum) indices (column 3) and relative indices in air (column 4). The last column gives, for each wavelength, our estimate of the combined standard uncertainty of the index $u_c(n)$. This was determined from summing in quadrature our estimates of the standard uncertainties of the various uncertainty components $u_x(n)$ listed in Table 2. The combined standard uncertainties range from near 1.5×10^{-5} near the shortest wavelengths, increasing to 4.2×10^{-5} at 14μ m. The magnitudes of these uncertainties are approximately what we

Table 2.	Sources of	Uncertainty	and T	heir	Impacts	on
the Index	Uncertainty					

Sources x	Magnitude of Uncertainty <i>u</i> (<i>x</i>)	Index Uncertainty $u_x(n) (10^{-5})$
Peak position	(0.7 to 5) arcseconds	0.6–4
	(1/10th of diffracted	
	peak width FWHM)	
Prism apex angle	0.15 arcseconds	0.9
	[including $\lambda/120$ (at	
	633 nm) RMS surface	
	flatness error]	
Index inhomogeneity	0.91×10^{-5} RMS for	0.91
	10 mm thickness at	
	$\lambda = 3.39 \ \mu m$	
Encoder angle	0.15 arcseconds	0.17
Prism temperature	0.005°C	0.26-0.20
Wavelength calibration	0.05 nm	0.6-0.002
Alignment	0.05 arcseconds	0.08
N ₂ gas and air	2×10^{-7}	0.08
dispersion formulas		
N ₂ gas temperature	0.02°C	0.01
N ₂ gas pressure	0.02 kPa	0.02

would have expected on the basis of diffraction-dominated measurements as discussed in the Introduction.

The measurements reported in this work were made on the same sample for which preliminary results were previously reported in conference proceedings [12]. For these new measurements, the entire refractometer system and prism sample were completely realigned. In addition, the temperature sensors and the monochromator output wavelengths were recalibrated. The measurement wavelengths used were the same as those used in the preliminary work, except for some additional wavelengths at the short-wavelength end. Improvements to the system and procedures resulted in more accurate measurements with reduced uncertainties. The index results presented here are consistent within the standard uncertainties of the results of the preliminary work.

Table 2 gives our assessment of the principal sources of uncertainty in the index results in Table 1. Column 2 gives the magnitudes of the sources, and column 3 gives the resulting contribution to the index uncertainties. When the uncertainties vary with wavelength, the uncertainties are shown as a range corresponding to wavelengths from the shortest to the longest. The largest contributions to the total uncertainty come from the uncertainties due to the determination of the peak positions and the prism apex angle, the uncertainty due to the sample index inhomogeneity, and the wavelength uncertainty. The radiation wavelength uncertainty of 0.05 nm is independent of wavelength, but its contribution increases rapidly as the wavelength gets shorter. The peak position uncertainty increases with wavelength as the peak widths increase due to diffraction, and it dominates the uncertainty for wavelengths longer than about 3 µm. The measurements are nearly diffraction limited for wavelengths longer than about 3 µm. Though Ge has a very large thermo-optic coefficient, the uncertainty due to this is held to a minor contribution by the tight control of the prism temperature to $22.000 \pm 0.005^{\circ}$ C.

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Table 3.	Sellmeier	Constants	of	ΓEα.	(2)] ^a

Sellmeier Constants			
K1	0.362471		
K ₂	14.640402		
K ₃	0.008175		
L	1.243341 μm		
L ₂	0.4120985 μm		
L ₃	26.5311 μm		

"Range of validity: $2 \,\mu m < \lambda < 14 \,\mu m$.

B. Sellmeier Fit and Residuals

The air index values at the air wavelengths listed in Table 1 were fit by standard least-squares nonlinear curve fitting procedures to several types of dispersion formulas. It was found that a good fit resulted from a standard three-term, six-parameter Sellmeier formula shown in [Eq. (2)], valid for the range $2 \ \mu m \le \lambda \le 14 \ \mu m$. Adding more terms or more adjustable parameters does not significantly improve the fit:

$$n^{2} - 1 = \frac{K_{1}\lambda^{2}}{\lambda^{2} - L_{1}^{2}} + \frac{K_{2}\lambda^{2}}{\lambda^{2} - L_{2}^{2}} + \frac{K_{3}\lambda^{2}}{\lambda^{2} - L_{3}^{2}}.$$
 (2)

The Sellmeier parameters are listed in Table 3. The best fit places two divergent terms (poles) below the transmission region, in the electronic absorption band wavelengths, as expected. One pole at 1.24 μ m is close to the band edge, and the other at 0.41 μ m is rather lower. The pole at a wavelength longer than the measured wavelengths is at 26.5 μ m, in the phonon absorption band region, is also as expected. For the six Sellmeier parameters in Table 3, the decimal places from the best fit were truncated without introducing errors above one part in 10⁻⁷.

The residuals of the fit (the difference between the measured values and formula values) are shown in Fig. 3. The residuals are less than or equal to 1×10^{-5} for all wavelengths, except at 11 µm, where the residual is -1.1×10^{-5} . This is consistent with the lowest estimated uncertainty, $u_c(n) = 1.5 \times 10^{-5}$, listed in Table 1. That the residuals are below all the estimated uncertainties by at least a factor of 1.5 indicates that the random



Fig. 3. Plot of residuals of the fit to the data of the Sellmeier formula [Eq. (2)], using the parameters in Table 3.

errors are reasonably assessed, though this does not rule out the possibility of unaccounted for systematic errors. Systematic errors were guarded against by careful consideration of the uncertainty components listed in Table 2.

4. COMPARISON WITH PREVIOUS MEASUREMENTS

Comparison of the Sellmeier equation values of this work with the extensively used data of Salzberg *et al.* [3,4] and of Icenogle *et al.* [5] is given in Fig. 4. Temperature corrections were made to the values of this work to compare the values at the temperatures of previous work, using the thermo-optic coefficient from Icenogle *et al.* The plot gives the difference between the previous data and the Sellmeier formula values at each of the previous authors' measured wavelengths. The error bars correspond to the reported standard uncertainties for each of the measurements. The error bars $[u_c(n)]$ for the results of Salzberg *et al.* are all below those of this work by $(13 \text{ to } 38) \times 10^{-4}$, well outside their estimated standard uncertainty of 2×10^{-4} . The Ge material they measured may well have had a substantial difference in quality, and this could account for the difference.

The newer data of Icenogle *et al.* are generally closer to the values of this work, with a trend of relatively lower values at the shortest wavelengths to relatively higher values at longer wavelengths crossing at about 2.5 μ m. Their error bars include, or nearly include, the Sellmeier values for all wavelengths except for the value at 12.36 μ m.

Figure 5 gives similar comparisons of the more limited range of measurements of Edwin *et al.* [6] (8 to 14 μ m) and of Frey *et al.* [10] (1.8 to 5.5 μ m) to the results of this work. In all cases, the error bars of these authors include the values of this work. The Edwin *et al.* values are all slightly outside the error bars of this work, which are 7 to 11 times smaller. The Frey *et al.* values range from above to slightly below the values of this work, with uncertainties larger by a factor of about 5 to 6.6.



Fig. 4. Plot of differences between the measurements of Salzberg *et al.* [3,4] and the values of this work and differences between the measurements of Icenogle *et al.* [5] and the values of this work, using the fitted Sellmeier formula. The error bars represent standard uncertainties.



Fig. 5. Plot of differences between the measurements of Edwin *et al.* [6] and the values of this work and the differences between the measurements of Frey *et al.* [10] and the values of this work, using the fitted Sellmeier formula. The error bars represent standard uncertainties. The heavier-set error bars correspond to the results of this work.

5. CONCLUSIONS

The IR optics community has generally relied on index data for Ge measured 40 or more years ago for optical design with Ge. It seems that these values should be revisited, especially because improvements in material fabrication may have produced higher-quality materials with potentially different index properties. We have demonstrated that we have developed a refractometry facility and procedures that are at least at the state of the art for index measurements in the near- to mid-IR. We have used this facility to measure the index of recently produced high-quality Ge. Our measurements cover the wavelength range 2 to 14 μ m at 22.000°C. We provide a Sellmeier formula for the relative index for this range, with a standard uncertainty ranging from 1.5 × 10⁻⁵ near the short-wavelength end to 4.2 × 10⁻⁵ at the long-wavelength end.

Our measured Ge index values are substantially outside the measurement uncertainties of values reported in commonly used index databases. They are within the measurement uncertainties of the most recent published measurements. Our analysis of measurement uncertainties gives values smaller than those of all previous reported measurements of Ge by at least a factor of 5, and our uncertainties are essentially diffraction limited for the sample sizes used for wavelengths longer than 3 μ m.

Comparing our new Ge index data to the widely used data starting from the late 1950s, there seems to be convergence of the data over time and more consistency of the uncertainties with the differences. The remaining differences may be genuine, resulting from actual material differences, such as doping and impurity levels. A verified improvement in accuracy should be of value to assess the material differences for the new generation of Ge and other materials. We suspect that the short-wavelength band edges would be particularly sensitive to defect and impurity differences, and that this would be reflected in the index behavior in this region. For future exploration of this, we made measurements with relatively smaller wavelength increments at the short-wavelength end. We intend to exploit our improved index accuracy capability to measure Ge samples from diverse sources to explore correlations of index with properties such as absorption edge transmission and impurity content and to assess the range of sample variations of index of commercial Ge material.

Acknowledgment. Commercial equipment, instruments, materials, or software are identified to specify adequately the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology nor does it imply that the items identified are necessarily the best available for the purpose.

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