Critical performance differences of monocrystalline versus polycrystalline germanium for optical applications

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Introduction

Germanium (Ge) is a useful optical material over the mid-wave and long-wave infrared wavelength region. It can be used as a window, dome or lens substrate, and it can be coated with thin film layers to enhance its optical performance and durability.

It can be obtained in the form of a single crystal or as polycrystalline material.

In general, polycrystalline germanium is less expensive and is available in larger sizes than monocrystalline material.

In a number of cases, it is worthwhile for an optical designer/fabricator to consider which material class is the better choice for a particular application. Generally, material suppliers can readily quantify one set of trade-offs associated with material cost and availability. However, EEO has found that the corresponding trade-offs related to technical performance differences are not well defined, at present.

To address this apparent deficiency, EEO has investigated the reported differences in optical, mechanical and thermal properties between the two classes of germanium. It was determined that, with respect to optical applications, there are two fundamental performance differences: (a) the level of refractive index homogeneity in a given component; and (b) the degree of optical absorption. Each can have measureable implications on the operational performance of a given germanium component depending on the specific application.

This paper describes the pertinent material characteristics investigated by the EEO team and its findings; provides a semi-quantitative evaluation of the practical effect of the differences in index homogeneity and absorption based on optical modeling and measurements of specimens; and makes a set of recommendations for specifying germanium material for generalized applications.

Potential differences in performance characteristics (based on a literature review)

There are a number of material properties that are important to the performance of germanium in typical optical applications. As a first step, a review of the published literature was completed to determine which, if any, of these properties were likely to exhibit differences in performance for monocrystalline versus polycrystalline material. The overall list of properties was divided into three categories: mechanical, thermal and optical. Information collected for each category and property of interest is detailed below.

- Mechanical properties

  The following set of mechanical properties was identified as particularly pertinent to the use of germanium in typical opto-mechanical applications. It is recognized that other properties may also be considered critical for specific applications but this a good general list. As detailed below, based on a review of the published literature, it was found that no practical performance differences in terms of mechanical characteristics should be expected between monocrystalline and polycrystalline germanium for typical optical applications.

- Density
  - The contribution of the density difference of the grain boundaries in polycrystalline material is trivial. No measureable difference between the two material classes is expected to be observed.
- Young's Modulus (Elastic Modulus)
  - No explicit comparisons of elastic modulus values could be found in the open literature for monocrystalline versus polycrystalline germanium. In general, in the single crystal form, it is known that the elastic modulus varies in cubic crystals according to the crystalline orientation. The highest atomic density yields the highest modulus value.[1] Germanium exhibits a cubic lattice structure. In a polycrystalline material, the grains have a randomized crystalline orientation so the modulus is isotropic.
- Hardness
  - No explicit comparisons of hardness values could be found in the open literature for monocrystalline versus polycrystalline germanium. Similar to the note above regarding elastic modulus, it is known that the hardness varies in cubic crystals according to the orientation.[1] In a polycrystalline material, the grains have a randomized orientation so the hardness is isotropic. No discussion of a practical effect of any crystal orientation induced difference was reported, for example, with respect to polishability. In other words, there were no reported observations of issues with respect to material removal rate, surface roughness or final surface quality directly associated with grain-to-grain variation in material hardness.
- Strength (Rupture Modulus)
  - Adams reported that data collected for over one hundred polished germanium specimens indicated no difference in modulus of rupture between monocrystalline and polycrystalline samples.[2] As such, no practical difference in mechanical strength is expected in parts intended for optical applications.

- Thermal properties

  The following set of thermal properties was identified as pertinent to the use of germanium in typical opto-mechanical applications. It is recognized that other properties may also be considered critical for specific applications but that this list is a general one. As detailed below, it was found that, based on a review of the published literature, no practical performance differences in terms of thermal characteristics would be expected between monocrystalline and polycrystalline germanium.

  - CTE
    - For typical grain sizes, over the temperature range of interest, grain size/boundary effects are expected to be minimal and no observable difference between the materials is expected.
    - Also, due to its cubic diamond structure, no crystal orientation effects are expected in single crystal germanium.

- Thermal conductivity
  - For typical grain sizes, over the temperature range of interest, grain size/boundary effects are expected to be minimal and no observable difference between the materials is expected.
  - Also, due to its cubic diamond structure, no crystal orientation effects are expected in single crystal germanium.

- Optical properties

  The following set of optical properties was identified as pertinent to the use of germanium in typical opto-mechanical applications. It is recognized that other properties may also be considered critical for specific applications, but that this list is a general one. As detailed below, it was found that, based on a review of the published literature, two specific performance differences between monocrystalline and polycrystalline germanium could be a concern: index homogeneity and absorption.

  - Index
    - No measureable differences in refractive index at a given wavelength and temperature between monocrystalline and polycrystalline germanium have been reported. This is expected due to the cubic crystal form of germanium. Likewise, no difference in the change in index with temperature (dn/dT) has been identified. Standard textbook values, such as those defined by Umicore, have been successfully employed by optical designers. [3]
  - Index homogeneity
    - Due to the presence of the grain boundaries, polycrystalline germanium generally exhibits a higher level of inhomogeneity of refractive index compared to single crystal germanium. Umicore quantifies the typical range of refractive index variation within a given part as 10-100 ppm for monocrystalline germanium and 50-200 ppm for a polycrystalline germanium.[3] Van Goethem reported comparable data, indicating around 20 ppm of inhomogeneity for monocrystaline germanium and around 60 ppm for polycrystalline material.[4]
    - In the subsequent section of this paper, the team will employ optical modeling to illustrate the practical effect of index homogeneity differences associated with monocrystalline versus polycrystalline germanium.
  - Absorption coefficient
    - Again, due to the presence of the grain boundaries, polycrystalline material typically absorbs/scatters more light and, therefore, transmits less. Van Goethem reported data for absorption coefficients on polished germanium samples measured via laser calorimetry.[4] The paper reported a typical absorption coefficient of </= 0.020 cm-1 for monocrystalline germanium and 0.035 cm-1 for polycrystalline. Umicore reports the same limiting value for monocrystalline germanium and a range of 0.020 – 0.035 cm-1 for polycrystalline material.[3]
    - It is important to note that the absorption coefficient of germanium in either form is strongly influenced by the conduction type and electrical resistivity of

the material. Most optical grade germanium is specified to be n-type material with a resistivity within the range of 5 – 40 ohm-cm at room temperature for optimum optical transmission.

- In the subsequent section of this paper, the team will employ classical textbook calculations to illustrate the practical effect of the optical absorption differences associated with monocrystalline versus polycrystalline germanium.

- Birefringence
  - No measureable difference in stress-induced birefringence between monocrystalline and polycrystalline germanium have been reported. This is expected due to the cubic crystal form of germanium. [5]

Comparisons performed by EEO

Optical absorption

To address the practical implications of the reported absorption differences between monocrystalline and polycrystalline material, the team calculated the effect of absorption on a prototypical germanium window assuming the upper limits for absorption coefficients for each material class and using standard optics textbook equations for absorption and transmission. [5,6]

- EXP(-abs coeff*thickness) : internal transmission per Beer's law
- T=(1-R)*(1-R)exp(-a*t)/(1-R*R*exp(-2a*t)) : bare germanium slab transmission
- Toa=(T1T2T3)/(1-R1'R2T32) : AR-coated germanium slab transmission

For a 1 cm thick window coated with a typical anti-reflection coating on each surface at 10.6 um, an absorption coefficient of 0.020 cm-1 gives a transmission of 97.8%. For a coated window of identical thickness at the same wavelength but with an absorption coefficient of 0.035 cm-1, the calculated transmission is 96.4%. This example utilizes an almost perfect anti-reflective coating (R </= 0.1%) on each surface, so the absolute transmission values will be different for coatings exhibiting less than perfect performance. However, the absolute difference between the two forms of germanium would remain consistent at approximately 1.4%.

These results are summarized in the table below.

		Monocrystalline		**Polycrystalline**	
Description	**symbol**	**values**	**percent**	**values**	**percent**
Reflectance	R	0.360	36.00%	0.360	36.00%
Abs Coeff (/cm-1)	a	0.020		0.035	
Thickness cm	t	1.000		1.000	
uncoated Transmittance	T	0.4586	45.86%	0.4499	44.99%
internal transmittance	T3	0.9802	98.02%	0.9656	96.56%
AR (non abs) reflectance	R1'&R2	0.001	0.10%	0.001	0.10%
Overall Transmittance coated	Toa	0.9782	97.82%	0.9637	96.37%

Table 1: Absorption characteristics of germanium. Values in shaded boxes are entered constants.

Index homogeneity

To address the practical implications of the reported index homogeneity differences between monocrystalline and polycrystalline material, the team took an optical modeling approach.

Determining whether one requires monocrystalline germanium or polycrystalline material depends on the system requirements and component wavefront specifications. It is generally safer to specify monocrystalline material but this comes at a higher cost. We have attempted to bound the maximum and typical wavefront error to expect from index inhomogeneity. Then we can determine if polycrystalline germanium is obviously suitable, needs analysis, or is not suitable for a given application. We can also characterize the type of aberration one can expect for a given aperture size.

We present a simple analysis to help the user decide "mono or poly?"   Technical purists should object to this analysis, but it will provide quick guidelines for engineers and program managers who want to know if they can reduce materials budgets and still hope to meet spec. A more rigorous development of the homogeneity analysis is can be found in Rogers.[7,8] As noted previously, the principle differences between polycrystalline and monocrystalline germanium materials are cost and index of refraction homogeneity. Homogeneity affects wavefront distortion. We will attempt to provide general guidelines to help the user in the material selection decision. We must first establish the requirements for homogeneity.

Since this analysis is intended to support a general discussion, we will outline basic rules-of-thumb estimates for tolerances that can be applied across a broad spectrum of optical systems. We will assume commercial, precision and research grade optical systems with 0.05, 0.25 and 1.0 wave Optical Path Difference (OPD wavefront distortion), respectively, as tabulated below. "Typical" optical systems consist of 1-10 optical elements. For each element in the system, wavefront error may be allocated between power, irregularity, wedge, homogeneity and "residual" aberrations. Systems with more elements, shorter wavelength and higher resolution will have tighter homogeneity tolerances as shown in the tables below. The magnitude of the allowed distortion can be compared to estimated OPD for various sizes of optics.

Tolerances for a Commercial Grade Optical System

# elements	System RSS WF	Allocation/ Element, RMS	OPD Allocation Homogeneity
1	1.0	1.000	0.350
2	1.0	0.707	0.247
3	1.0	0.577	0.202
4	1.0	0.500	0.175
5	1.0	0.447	0.157
6	1.0	0.408	0.143
7	1.0	0.378	0.132
8	1.0	0.354	0.124
9	1.0	0.333	0.117
10	1.0	0.316	0.111

Figure 2: Tolerances for commercial grade optical system. OPD from inhomogeneity allowed for commercial grade optics is 0.11 to 0.35 waves.

Tolerances for a Precision Grade Optical System

# elements	System RSS WF	Allocation/ Element, RMS	OPD Allocation Homogeneity
1	0.25	0.250	0.088
2	0.25	0.177	0.062
3	0.25	0.144	0.051
4	0.25	0.125	0.044
5	0.25	0.112	0.039
6	0.25	0.102	0.036
7	0.25	0.094	0.033
8	0.25	0.088	0.031
9	0.25	0.083	0.029
10	0.25	0.079	0.028

Figure 3: Tolerances for a precision grade optical system. OPD from inhomogeneity allowed for precision grade optics is 0.03 to 0.09 waves.

Tolerances for a Research Grade Optical System

# elements	System RSS WF	Allocation/ Element, RMS	OPD Allocation Homogeneity
1	0.05	0.050	0.018
2	0.05	0.035	0.012
3	0.05	0.029	0.010
4	0.05	0.025	0.009
5	0.05	0.022	0.008
6	0.05	0.020	0.007
7	0.05	0.019	0.007
8	0.05	0.018	0.006
9	0.05	0.017	0.006
10	0.05	0.016	0.006

Figure 4: Tolerances for a research grade optical system. OPD from inhomogeneity allowed for research grade optics is 0.018 to 0.006 waves.

Now that we have estimated the wavefront quality required for germanium components, we can assess whether polycrystalline germanium can meet these requirements. EEO's experience producing thousands of high quality optics from both monocrystalline and polycrystalline Ge provide us with an extensive database to correlate material homogeneity and transmitted wavefront error (TWE). EEO evaluated some samples of polycrystalline and monocrystalline germanium to characterize the index of refraction homogeneity in a typical germanium boule from poly and monocrystalline material. Boules can vary in diameter and length; the ends of the boule are usually sliced off and recycled. The remaining cylinder has a characteristic radial gradient index profile but is fairly homogenous over the length. The monocrystalline boules have a similar characteristic index profile, but are 5-10x smaller in magnitude. We measured maximum inhomogeneity and "typical" inhomogeneity across the diameter in order to characterize a nominal "worst case" and a conservative "best case" estimate of material behavior if one was reasonably careful about how they create lens blanks from raw boules of material. An effective means to control wavefront distortion from material inhomogeneity is to select the maximum diameter and radial location in the boule from where optics blanks can be cut. The central 60% of a boule has significantly lower homogeneity and it tends to be dominated by power with very low tilt and astigmatism. We have estimated the amount of index variation across the diameter of the optic and related that to a transmitted wavefront error on windows or distortion in lenses. We also estimated the contribution to wavefront error from tilt, power, astigmatism and other aberrations so the designer can predict whether the residual inhomogeneity distortion adversely affects their system performance.

Optical window and lens blanks tend to be thin disk-shaped objects that are sliced out of the boule across the diameter to take advantage of the invariant longitudinal index. Larger diameter optics tend to be thicker. The characteristic shape and magnitude of the index profile in an optic blank will depend on where in the boule it came from. A slice across the center of the boule will have a radial gradient index that results in mostly power. If that slice is cut into smaller disks, then there will be a strongly asymmetric gradient that is mostly wedge, some astigmatism and other aberrations. We can estimate how much tilt, power, astigmatism and residual aberration to expect by extending the glass homogeneity analysis by Rogers to polycrystalline Ge. EEO intends to collect more homogeneity data on our material to refine estimates of wavefront distortion in the future.

Estimated MWIR OPD Due to Inhomogeneity of Germanium

Lens Dia	10	25	50	75	100	125	150	200	mm
Lens Thickness	3.5	4.25	5.5	6.75	8	9.25	10.5	13	mm
OPD Max Factor Poly	0.002	0.007	0.018	0.034	0.053	0.077	0.104	0.172	Waves MWIR
OPD Typical Factor Poly	0.001	0.002	0.005	0.008	0.013	0.019	0.026	0.043	Waves MWIR
OPD Max Factor Mono	0.000	0.001	0.002	0.004	0.007	0.010	0.013	0.022	Waves MWIR
OPD Typical Factor Mono	0.000	0.000	0.000	0.001	0.001	0.002	0.003	0.004	Waves MWIR

Table 5: MWIR Wavefront vs. Germanium Substrate Blank Dimensions.

Table 5 indicates that the expected OPD contribution from germanium inhomogeneity is insignificant for many blank sizes in the MWIR waveband.

Estimated LWIR OPD Due to Inhomogeneity of Germanium

Lens Dia	10	25	50	75	100	125	150	200	mm
Lens Thickness	3.4	4	5	6	7	8	9	11	mm
OPD Max Factor Poly	0.001	0.002	0.006	0.011	0.017	0.025	0.034	0.055	Waves LWIR
OPD Typical Factor Poly	0.000	0.001	0.002	0.003	0.004	0.006	0.008	0.014	Waves LWIR
OPD Max Factor Mono	0.000	0.000	0.001	0.001	0.002	0.003	0.004	0.007	Waves LWIR
OPD Typical Factor Mono	0.000	0.000	0.000	0.000	0.000	0.001	0.001	0.001	Waves LWIR

Table 6: LWIR Wavefront vs. Germanium Substrate Blank Dimensions.

Table 6 indicates that the expected OPD contribution from polycrystalline germanium inhomogeneity is insignificant for most blank sizes in the LWIR waveband. If tilt and power can be compensated (via fabrication or alignment) or neglected, the OPD will be about 2x lower.

Estimated Relative Tilt, Power and Other OPD Contributions Due to Inhomogeneity of Germanium

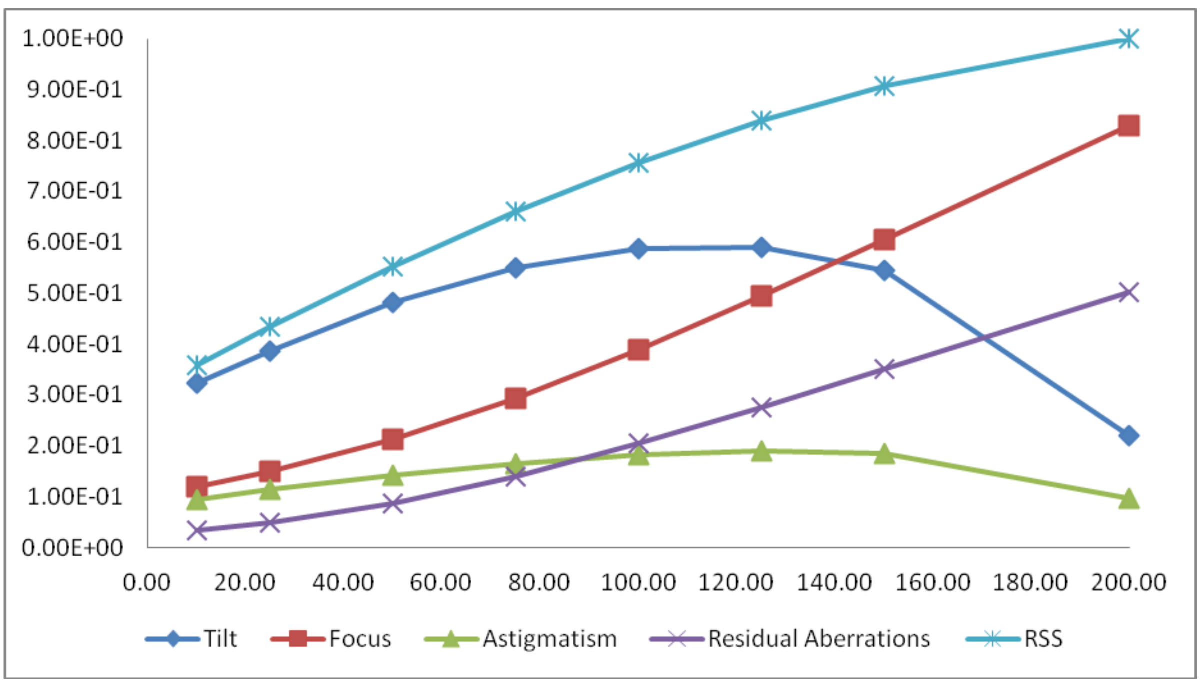

Chart 1. Normalized contribution to wavefront error vs. optic diameter from an 8" dia. Ge boule.

Chart 1 indicates the changing character of the distortion as the optic diameter increases. At smaller diameters, the OPD is dominated by tilt. As the diameter of the element increases to the maximum boule diameter, the OPD is dominated by power. Power and tilt may be allowed or compensated/corrected in component fabrication and during the assembly and alignment of the optical system. One can also reduce astigmatism by clocking individual optics in an assembly to balance figure irregularity and astigmatic inhomogeneity. Interferometry can be used measure radial gradients to tune optical figure, validate TWE on finished optics for critical applications.

Aberrations for polycrystalline germanium wavefront tilt tends to be 0.2-1.0 arc-second for 10-200mm diameter optics. This can be compensated by fabricating a wedge of appropriate magnitude and orientation into the substrate or adjusting boresight through the optical system by decentering. Power varies inversely with the F/number of the optic. Power is 0.5 waves peak-to-valley (p-v) at 3.39 microns and 0.16 waves at 10.6 microns for 8" diameter F/1 lens. Power is 0.12 waves at 3.39 microns and 0.04 at 10.6 microns for 8" diameter F/4 optics. This defocus can be corrected by changing the radius of curvature of the optic if the index profile is known or refocusing the optic. Inhomogeneity tends to have little impact on chromatic aberration since germanium has very low dispersion. The astigmatism due to inhomogeneity behaves like surface irregularity on the optic and is smaller in magnitude than power. Astigmatism may be effectively corrected by properly clocking astigmatic components in a multi-element system. The remaining irregularities (spherical and other residuals) will contribute to mid spatial frequency aberrations and degrade resolution but this is bounded by the max OPD calculated for the various optics. The residuals are more problematic to reduce with fabrication or alignment techniques so it is reasonable to assume this will limit the system performance.

Recommendations for specifying germanium material

Taking the two performance differences into consideration, absorption and index homogeneity, the following basic rules of thumb can be employed.

- In the case of a component for which a 1% improvement in optical transmittance is a critical performance criterion, the use of single crystal germanium is suggested. This is not typically an issue for single pane germanium windows but would be a more significant consideration for systems containing multiple germanium lenses in series.
- As described above, aperture diameter is a principal governing factor for deciding whether monocrystalline germanium is required to minimize the effects of index homogeneity. For relatively small apertures, as demonstrated above, use of polycrystalline material does not significantly degrade system optical performance. This determination is best made via optical modeling of the opto-mechanical system in question.
- As noted in passing above, two other pertinent requirements typically defined for optical grade germanium include uncompensated, n-type material with a bulk resistivity of 5 – 40 ohm-cm. Imposition of these specifications will ensure optimal levels of optical transparency.
- Polycrystalline germanium is potentially suitable for most small to medium diameter optics, even for research grade optical systems.

EEO has complete control over boule production and the cutting process to produce germanium blanks. EEO routinely produces 8" polycrystalline windows with diffraction-limited transmitted wavefront error (TWE) for LWIR and MWIR systems. These results are not intended to substitute for serious analysis of all requirements and specifications evaluating tolerances for selecting germanium material. However, it does offer practical, helpful insight into whether one can even consider polycrystalline germanium for precision optical applications.

References

1. B. P. O'Connor, E. R. Marsh, J. A. Couey, "On the effect of crystallographic orientation on ductile removal in silicon," Precision Engineering, vol. 29, (2005), p. 124.

2. J. H. Adams, "Specifications for optical grade germanium and silicon blanks," SPIE vol. 406, (1983), p. 51.

3. "Umicore Germanium Optics," accessed at http://eom.umicore.com/en/materials/library/brochuresAndMarketingMaterial/show_GermaniumOpticsBrochure.pdf on 10/08/12.

4. L. Van Goethem, L. Ph. Van Maele, M. Van Sande, "Trade-offs using poly versus monocrystalline germanium for infrared optics," SPIE Vol 683, (1986), p. 160.

5. D. C. Harris, Materials for Infrared Windows and Domes: Properties and Performance, SPIE Press, (1999).

6. P. W. Baumeister, Optical Coating Technology, SPIE Press, (2004).

7. J. R. Rogers, "Homogeneity tolerances for optical elements", SPIE Optifab, TD-0736, (2011).

8. J. R. Rogers, "Modeling homogeneity for elements made of block glass", accessed at http://www.cybernet.co.jp/codev/example/developer/2012_Rogers_ModellingHomogeneity.pdf, (2012).