

Dispersion properties of mid-infrared optical materials

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This material is offered as a resource for calculating the dispersion of ultrafast mid-IR laser pulses through optical devices. For additional reading on this topic see:

“The role of dispersion in ultrafast optics,” Ian Walmsley, Leon Waxer, and Christophe Dorrer, *Review of Scientific Instruments* 72, 1-29 (2001).

“Dispersion compensation with optical materials for compression of intense sub-100 femtosecond mid-infrared pulses,” N. Demirdöven, M. Khalil, O. Golonzka and A. Tokmakoff, *Optics Letters*, 27, 433-435 (2002).

For refractive index data:

“Handbook of Optical Constants of Solids,” Edited by Edward D. Palik, (Academic Press, San Diego, 1998)

<http://refractiveindex.info/>

Dispersion calculations for short mid-IR pulses

The optical dispersion experienced by a short pulse propagating through an spectrometer is calculated in the frequency domain from the spectral phase $\phi(\omega)$. The field is expressed as

$$E(\omega) = \sqrt{I(\omega)} e^{i\phi(\omega)}$$

The spectral phase is related to the frequency dependent optical pathlength P as

$$\phi(\omega) = \frac{\omega}{c} P(\omega)$$

and the optical pathlength is related to the index of refraction and geometric path length ℓ as $P(\omega) = n(\omega)\ell(\omega)$. Commonly, we choose to expand ϕ about the center frequency of the pulse spectrum ω_0 :

$$\phi(\omega) = \phi_0 + \phi^{(1)}(\omega - \omega_0) + \frac{1}{2}\phi^{(2)}(\omega - \omega_0)^2 + \dots$$

$$\phi^{(1)} = \left. \frac{\partial \phi}{\partial \omega} \right|_{\omega=\omega_0} = \frac{1}{c} \left[P(\omega) + \omega \frac{\partial P}{\partial \omega} \right]_{\omega=\omega_0}$$

$$\phi^{(2)} = \left. \frac{\partial^2 \phi}{\partial \omega^2} \right|_{\omega=\omega_0} = \frac{1}{c} \left[2 \frac{\partial P}{\partial \omega} + \omega \frac{\partial^2 P}{\partial \omega^2} \right]_{\omega=\omega_0}$$

Here, the first order term $\phi^{(1)}$ is inversely proportional to the group delay for the pulse and the second order term $\phi^{(2)}$ is the group delay dispersion or group velocity dispersion (GVD). If the GVD is non-zero, the pulse is said to be “chirped.” A positive chirp means that the low frequencies within the bandwidth have a smaller group delay than the higher frequencies, i.e. that lower frequencies precede the higher frequencies.

The optical phase expressed as frequency derivatives with respect to optical path length can also be expressed in terms of wavelength derivatives

$$\omega = \frac{2\pi c}{\lambda} \quad \frac{\partial \omega}{\partial \lambda} = -\frac{2\pi c}{\lambda^2}$$

$$\begin{aligned} \frac{\partial P}{\partial \omega} &= \frac{\partial P}{\partial \lambda} \cdot \frac{\partial \lambda}{\partial \omega} \\ &= \frac{-\lambda^2}{2\pi c} \cdot \frac{\partial P}{\partial \lambda} \end{aligned}$$

$$\begin{aligned}\frac{\partial^2 P}{\partial \omega^2} &= \left(\frac{-\lambda^2}{2\pi c} \right)^2 \frac{\partial}{\partial \lambda} \left[\frac{\partial P}{\partial \lambda} \right] \\ &= \left(\frac{\lambda^2}{2\pi c} \right)^2 \left[\frac{\partial^2 P}{\partial \lambda^2} + \frac{2}{\lambda} \frac{\partial P}{\partial \lambda} \right]\end{aligned}$$

Then, the second and third order phase is given by

$$\begin{aligned}\phi^{(2)} &= \frac{\partial^2 \phi}{\partial \omega^2} \\ &= \frac{\lambda^3}{2\pi c^2} \frac{\partial^2 P}{\partial \lambda^2} \\ \phi^{(3)} &= \frac{\partial^3 \phi}{\partial \omega^3} = -\frac{\lambda^2}{2\pi c} \frac{\partial \phi^{(2)}}{\partial \lambda} \\ &= -\frac{\lambda^2}{2\pi c} \left[\frac{\lambda^3}{2\pi c^2} \frac{\partial^3 P}{\partial \lambda^3} + 3 \frac{\lambda^2}{2\pi c} \frac{\partial^2 P}{\partial \lambda^2} \right] \\ &= -\frac{\lambda^4}{4\pi^2 c^3} \left(\lambda \frac{\partial^3 P}{\partial \lambda^3} + 3 \frac{\partial^2 P}{\partial \lambda^2} \right)\end{aligned}$$

Propagating through material

To help in describing the dispersion that results from propagating through optical material characterized by a frequency dependent index of refraction $n(\omega)$, it is helpful to calculate the spectral phase in terms of the phase acquired per mm of material traversed. The expansion coefficients typically quotes in units of $(fs)^i mm^{-1}$ are

$$\gamma_i = \frac{\phi^{(i)}}{l} = \frac{1}{l} \frac{\partial^i \phi}{\partial \omega^i}$$

which can be calculated from the wavelength derivatives for the index of refraction

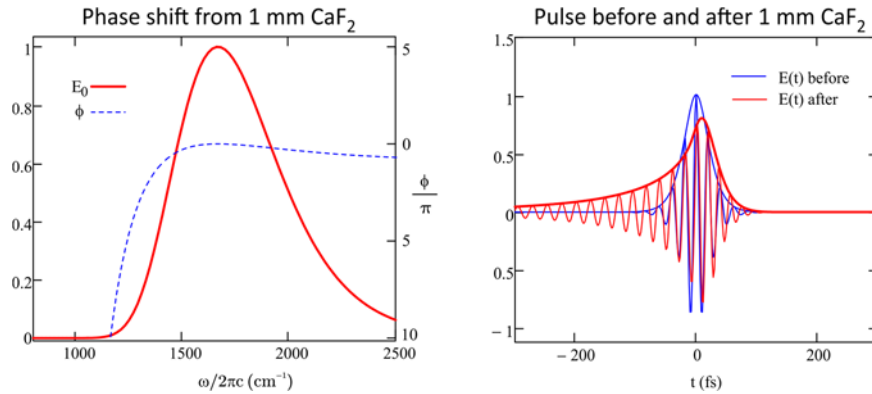
$$\beta_i = \frac{\partial^i n(\omega)}{\partial \lambda^i}$$

Following the derivation above, we see that the second and third order dispersion are

$$\begin{aligned}\gamma_2 &= \frac{\lambda^3}{2\pi c^2} \beta_2 \\ \gamma_3 &= -\frac{\lambda^4}{4\pi^2 c^3} (\lambda \beta_3 + 3\beta_2)\end{aligned}$$

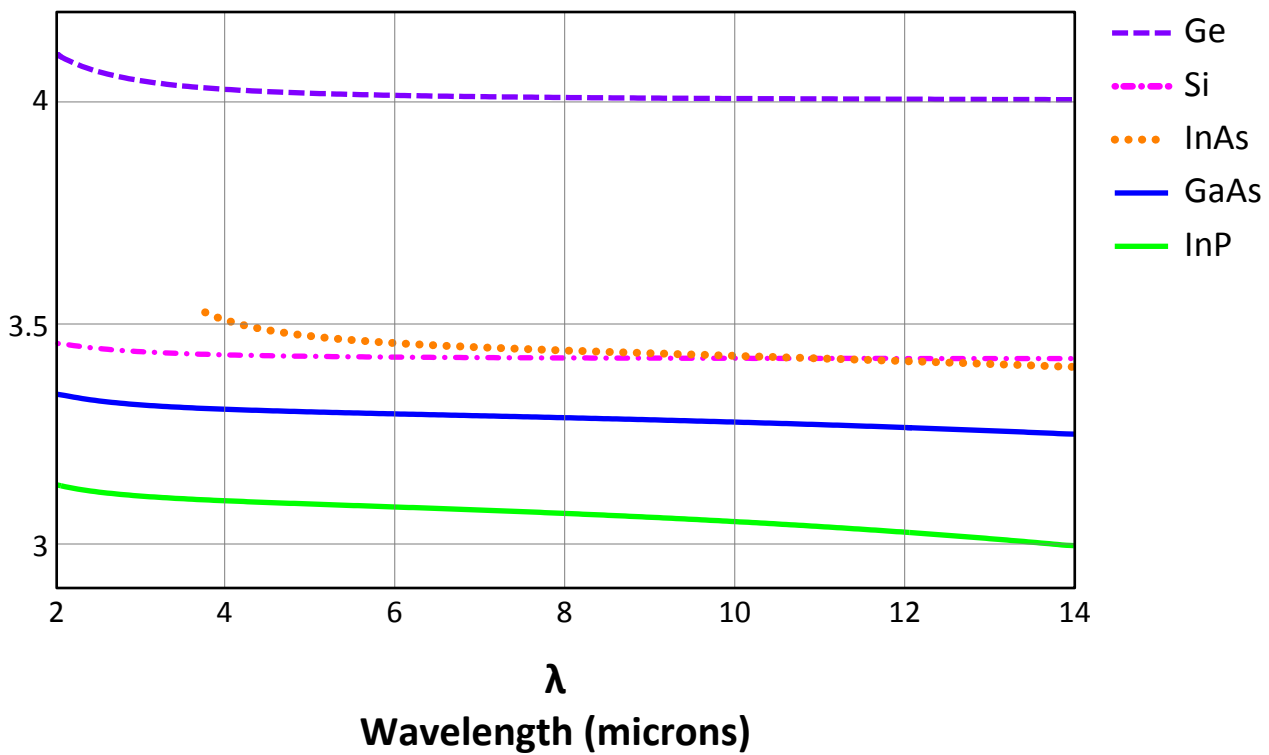
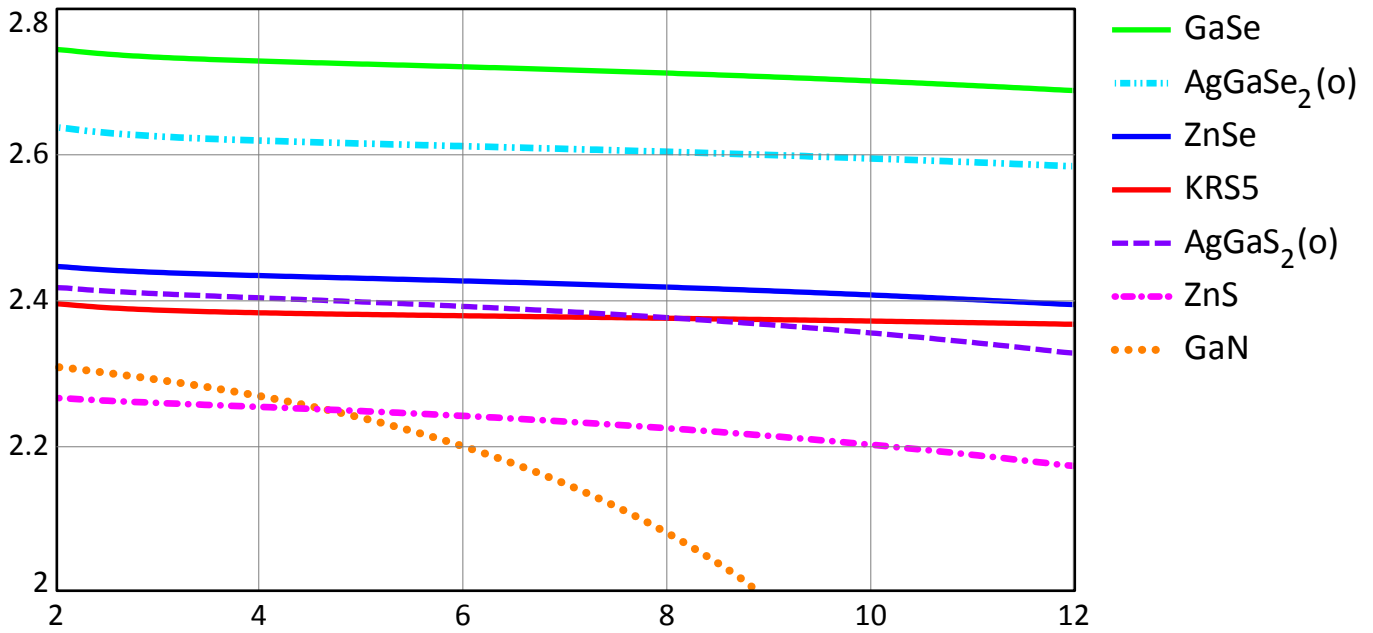
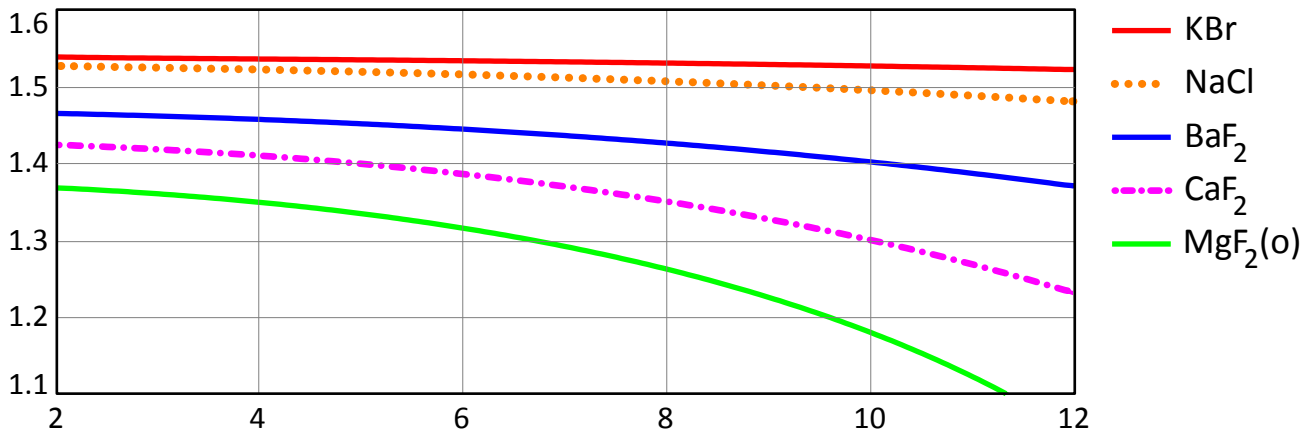
Most optical materials in the visible and near-IR spectrum have $\beta_2 > 0$, meaning that passing a transform limited pulse through this material will result in positive chirp on the pulse. The figure

below illustrates how a transform-limited pulse with a center wavelength of $\lambda_0 = 6 \mu\text{m}$ (1667 cm^{-1}) and a bandwidth of $\sigma=0.6 \mu\text{m}$ (167 cm^{-1}) is chirped after passing through 1 mm of CaF_2 . The left panel shows the spectral phase imparted by the CaF_2 . The right panel shows the pulse shape obtained by Fourier transformation before and after the material (neglecting the group delay, γ_l).

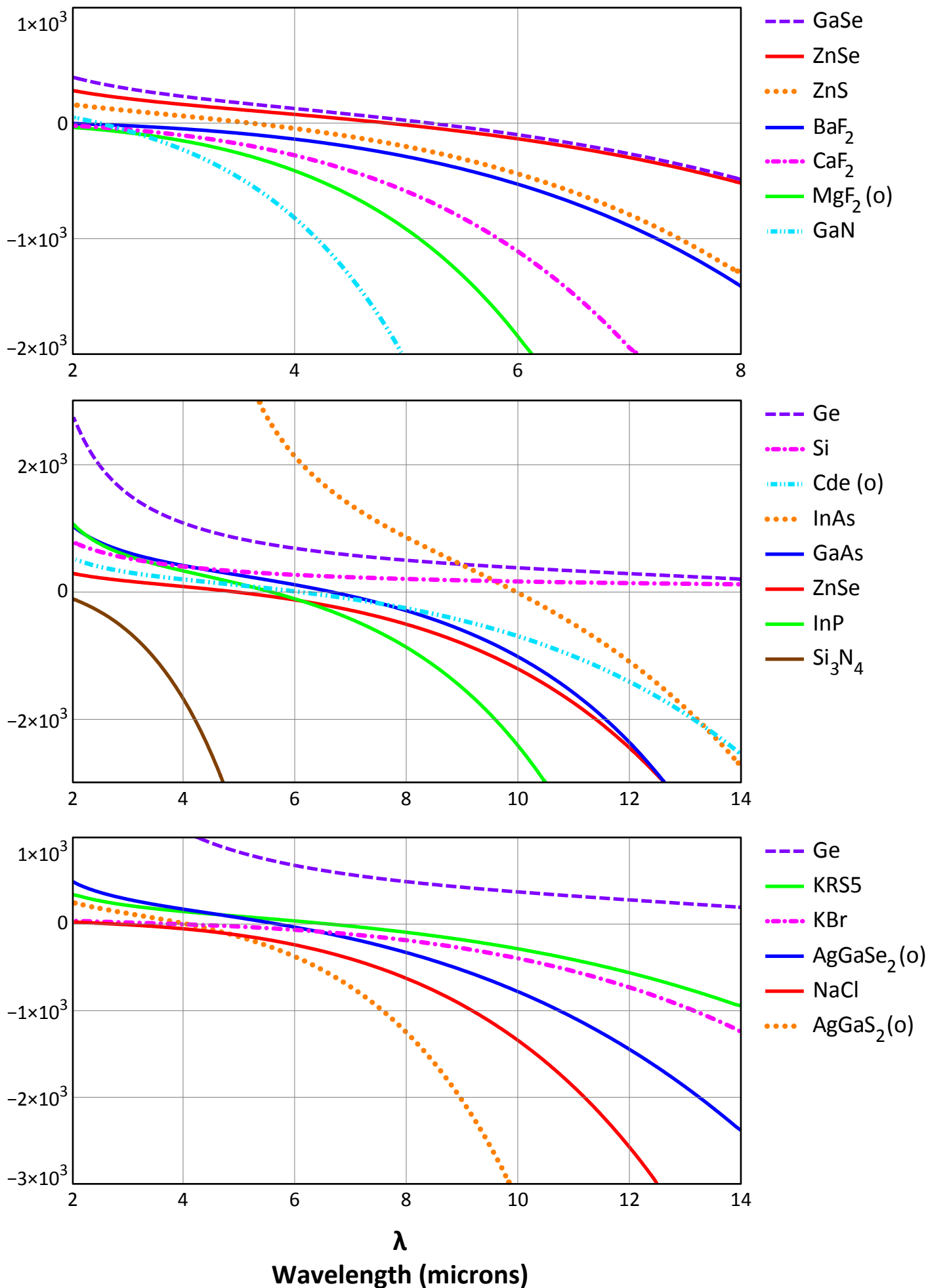


In the mid-infrared region ($\lambda=3\text{-}20 \mu\text{m}$), the sign of most transparent materials changes from positive to negative, meaning that there is a zero GVD wavelength with $\gamma_2=\beta_2=0$. Near this wavelength a pulse can propagate through material dispersion free (to second order). Also, this means that a combination of two optical materials with opposite sign for β_2 can be used to compress a pulse or zero the GVD for an optical device.

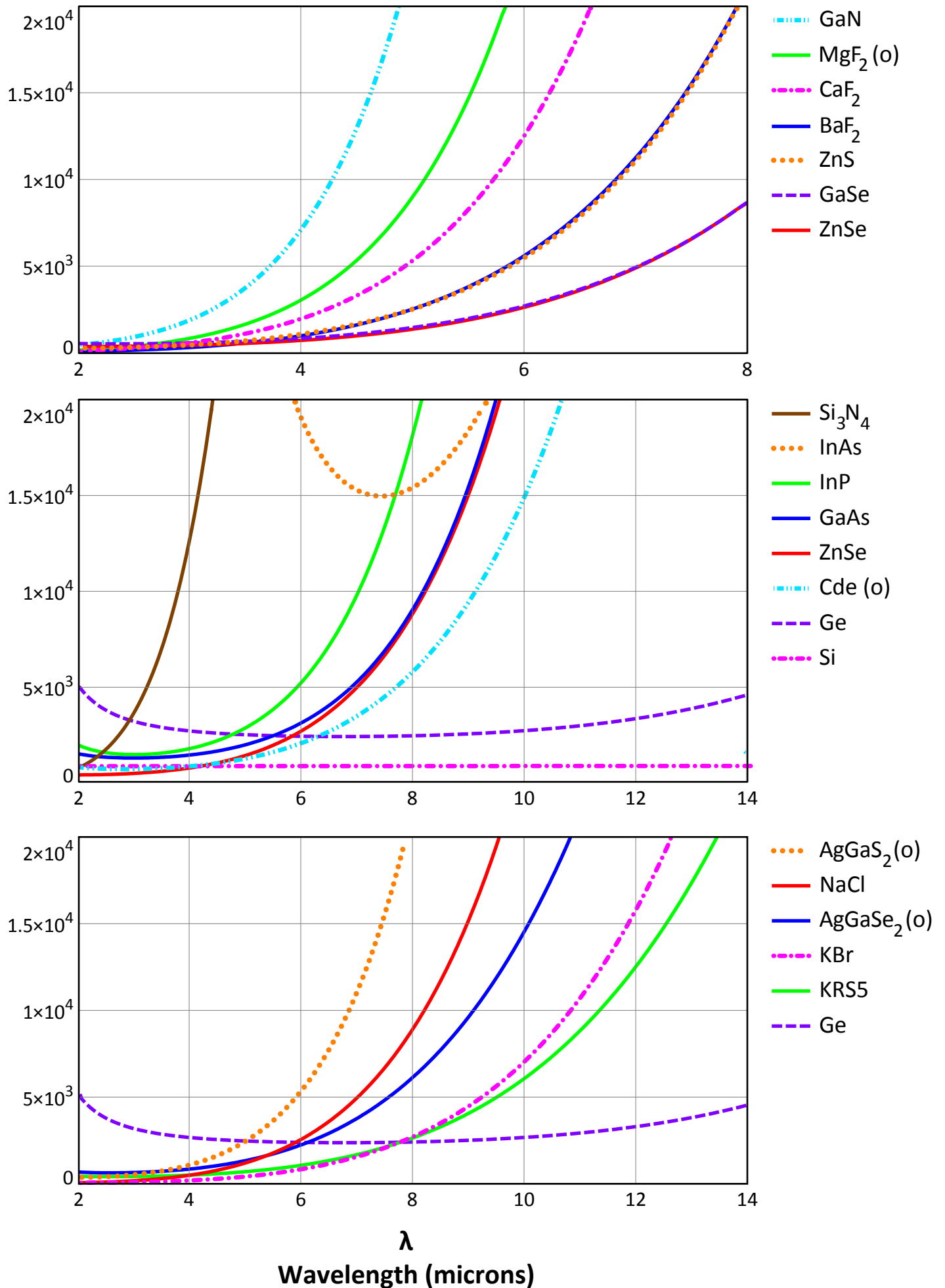
Index of Refraction for IR Materials



Second Order Dispersion for IR Materials (fs^2/mm)



Third Order Dispersion for IR Materials (fs^3/mm)



Zero Group Velocity Dispersion Wavelength

