IARPA MORGOTH'S CROWN: The Kramers-Kronig Relations

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Kramers-Kronig Relations

Many surface-particle models require as inputs n and k, which are the real an imaginary parts of the index of refraction of the chemical in question, respectively. Accurately measuring n and k for solids is something for which there is an accurate, established, methodology. One common approach to estimate n and k is to use the Kramers-Kronig relations. These are bidirectional mathematical relations, connecting the real and imaginary parts of any complex function that is analytic in the upper half-plane. These relations are generally used to calculate the real part from the imaginary part (or vice versa) of response functions in physical systems, because for stable systems, causality implies the analyticity condition, and conversely, analyticity implies causality of the corresponding stable physical system. The relations are named in honor of Ralph Kronig and Hendrik Anthony Kramers. In mathematics these relations are also known under the names Sokhotski–Plemelj theorem and Hilbert transform.

The generalized form of the Kramers-Kronig relations are:

$$x1(w) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{x_2(w')}{w^1 - w} dw'$$

And

$$x2(w) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{x_1(w')}{w' - w} dw'$$

For each of the substrates and bulk chemicals, n and k estimated by Kramers-Kronig relations are provided.