

Abstract Submitted
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Statistics of Data Fitting: Flaws and Fixes of Polynomial Analysis of Channeled Spectra¹ WILLIAM KARSTENS, Saint Michael's College, DAVID Y. SMITH, University of Vermont and Argonne National Laboratory — Starting from general statistical principles, we have critically examined Baumeister's procedure* for determining the refractive index of thin films from channeled spectra. Briefly, the method assumes that the index and interference fringe order may be approximated by polynomials quadratic and cubic in photon energy, respectively. The coefficients of the polynomials are related by differentiation, which is equivalent to comparing energy differences between fringes. However, we find that when the fringe order is calculated from the published IR index for silicon* and then analyzed with Baumeister's procedure, the results do not reproduce the original index. This problem has been traced to 1. Use of unphysical powers in the polynomials (e.g., time-reversal invariance requires that the index is an even function of photon energy), and 2. Use of insufficient terms of the correct parity. Exclusion of unphysical terms and addition of quartic and quintic terms to the index and order polynomials yields significantly better fits with fewer parameters. This represents a specific example of using statistics to determine if the assumed fitting model adequately captures the physics contained in experimental data. The use of analysis of variance (ANOVA) and the Durbin-Watson statistic to test criteria for the validity of least-squares fitting will be discussed. *D.F. Edwards and E. Ochoa, Appl. Opt. 19, 4130 (1980).

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