# Fundamentals of Dispersive Optical Spectroscopy Systems

# Fundamentals of Dispersive Optical Spectroscopy Systems

Wilfried Neumann

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## **Table of Contents**

Pr Gl	eface ossary	of Symbols and Notation	xiii xv
1	Introduction, Terminology, and Scales		
	1.1	General Introduction	1
	1.2	Photon Energies	2
	1.3	Photon-Energy Conversion Equations	3
	1.4	Naming Convention	4
	1.5	The Spectral Line	5
	1.6	General Rule of Optical Transfer	5
	1.7	Definitions	6
		1.7.1 Exponential functions and signal damping (attenuation)	6
		1.7.2 Low-pass filter functions	8
		1.7.2.1 A note on the dB interpretation	9
		1.7.3 Definition of bandwidth in electric versus optical	
		spectroscopy systems	10
	1.8	Spectral Distribution of Thermal Radiation by Planck's Law	10
	1.9	Keeping Optics Clean	11
	Refe	rences	11
2	Spect	rometer Concepts	13
	2.1	Basic Principle of an Optical Spectrometer	13
		2.1.1 Attributes of modular spectrometers	14
	2.2	Basic Grating Parameters and Functions	15
		2.2.1 The free spectral range	16
		2.2.2 Dispersion of gratings and prisms	16
	2.3	Existing Basic-Spectrometer Concepts	17
		2.3.1 The Littrow configuration	17
		2.3.2 Ebert–Fastie configuration	20
		2.3.2.1 Origin of astigmatism	23
		2.3.3 Czerny–Turner configuration	23
	2.4	Impacts and Distortions to Spectrometers	24
		2.4.1 The influence of the internal angles on the wavelength	25
	2.5	Other Spectrometers, Including Those for the Vacuum Range	25

	2.5.1	Curved-	grating spectrometer: Wadsworth setup	27
	2.5.2	Normal	incidence	27
	2.5.3	Seya–N	amioka	27
	2.5.4	Grazing	incidence	27
	2.5.5	Rowland	circle spectrometer and Paschen-Runge mount	28
2.6	Other	Paramete	rs and Design Features	28
	2.6.1	Straight	slits versus curved slits	28
	2.6.2	Aperture	e and light flux (luminosity)	29
		2.6.2.1	Real aperture or f-number?	29
		2.6.2.2	Examples of the influence of the internal angles	
			on the light flux	30
		2.6.2.3	Calculating the <i>f</i> -number versus $\Omega$ for light	
			flux/luminosity	31
	2.6.3	Dispersi	on of spectrometers	36
	2.6.4	Intensity	distribution in the exit	37
	2.6.5	Spectral	resolution	39
		2.6.5.1	Does one measure the resolution of the	
			spectrometer or that of the experiment?	42
		2.6.5.2	When is a spectral curve completely reproduced?	43
		2.6.5.3	Rayleigh diffraction limit	44
		2.6.5.4	Resolution of a monochromator compared to	
			that of a spectrograph	45
		2.6.5.5	Numerical resolution $R_{\rho}$ and $R_{r}$ , and their	
			wavelength dependence	48
	2.6.6	Image c	uality: Q-factor or fidelity	51
		2.6.6.1	Calculating aberrations	51
		2.6.6.2	A reflecting spectrometer has two	
			or even three axes	52
		2.6.6.3	The slit height also influences the total	
			aberrations	52
		2.6.6.4	The quality factor	53
		2.6.6.5	Image-transfer issues	53
		2.6.6.6	Spectrometers with internal image correction	56
		2.6.6.7	General aberrations and coma	57
	2.6.7	False a	nd stray light, and contrast	58
	0.0.0	2.6.7.1	Reducing stray light	59
07	2.6.8	Contras		60
2.7	Mecha	inical Stat	bility and inermal influence	60
	2.7.1	Defecute	ing inermal variations	01
	2.1.2	Delocus	thermel constants	61
	2.1.3	i ypical	na anvironmental influence	01
20	2.1.4 Doduo	ivin III IIIZI	ny environmental innuence	60
2.0			es filtore	62
	2.0.1	Long-pa	33 III(CI 3	03

		2.8.2	Band-pass filters and prism	64
		2.8.3	Short-pass filters	65
		2.8.4	General filtering techniques	66
		2.8.5	Notch filters	66
	2.9	Genera	al Collection of Performance Parameters of Spectrometers	66
	Refe	rence		67
3	The D	ispersio	on Elements: Diffraction Grating and Refraction Prism	69
	3.1	Introdu	ction	69
	3.2	Diffract	ion Efficiencies and Polarization of Standard Gratings	69
	3.3	Types	of Dispersers	71
		3.3.1	Holographic gratings	71
		3.3.2	Echelle gratings	72
		3.3.3	Concave and other curved gratings	73
		3.3.4	Transmission gratings	73
	3.4	The Pr	ism	73
	3.5	The Gr	rism	75
	3.6	Other I	Features of Diffraction Gratings	77
		3.6.1	Polarization anomaly	77
		3.6.2	Polarization of Echelle gratings	78
		3.6.3	Scattering effects	79
		3.6.4	Grating ghosts	79
		3.6.5	Shadowing and diffusion	80
		3.6.6	Surface coating	80
	Refe	rences		81
4	Desig	n Consi	derations of Monochromator and Spectrograph Systems	83
	4.1	Beam	Travel inside a Spectrometer	83
		4.1.1	Beam travel in a symmetric spectrometer	85
		4.1.2	Variations of the basic Ebert–Fastie and	
			Czerny–Turner concepts	87
		4.1.3	Output wavelength as a function of the source position	88
		4.1.4	Local output dispersion as a function of the lateral	
			position in the field output	89
		4.1.5	Output dispersion and fidelity as a function of the	
			tilt angle of the field output	90
		4.1.6	Correction methods for spectral imaging	92
			4.1.6.1 External imaging correction	92
			4.1.6.2 Internal imaging correction by toroidal mirrors	93
			4.1.6.3 Internal imaging correction by a curved grating	94
		4 4 <del>-</del>	4.1.6.4 Internal imaging correction by a Schmidt corrector	94
		4.1.7	Prism spectrometer	95
		4.1.8	Dispersion of a prism spectrometer	96
		4.1.9	Ecnelle grating spectrometers	99
		4.1.10	I ransmission spectrometers	99

4.2	Grating	g Rotation and Actuation	100
	4.2.1	Classical driving system	101
	4.2.2	Grating actuation by a rotating system	102
4.3	Multipl	e-Stage Spectrometers	105
	4.3.1	Double-pass spectrometers	106
	4.3.2	Double spectrometers	107
		4.3.2.1 Subtractive spectrometers	108
		4.3.2.2 Efficiency behavior and analysis	110
		4.3.2.3 Energy transmission and bandwidth of single-,	
		double-, and triple-stage spectrometers	110
		4.3.2.4 Effects of photon traveling time (time of flight)	111
	4.3.3	Construction considerations for double spectrometers	112
		4.3.3.1 Additive setup	112
		4.3.3.2 Subtractive setup	113
		4.3.3.3 Modern off-axis double spectrometers	114
		4.3.3.4 Mechanical filtering in double spectrometers	118
	4.3.4	Various configurations of flexible double spectrometers	118
	4.3.5	General performance data of double spectrometers	
		versus similar single-stage systems	119
	4.3.6	Triple-stage spectrometers	120
4.4	Echell	e Spectrometers	122
	4.4.1	Echelle monochromators and 1D spectrographs	123
	4.4.2	High-resolution Echelle spectrometer designed as	
		a monochromator and 1D spectrograph	124
		4.4.2.1 Echelle aberrations	127
		4.4.2.2 Thermal drift assuming an aluminum chassis	127
	4.4.3	Two-dimensional Echelle spectrometer for the parallel	
		recovery of wide wavelength ranges at high resolution	128
		4.4.3.1 Concept of a compact 2D Echelle	131
		4.4.3.2 Comparison of an Ebert–Fastie and a folded	
		Czerny–Turner	133
		4.4.3.3 Constructive precautions	136
4.5	Hypers	spectral Imaging	137
	4.5.1	Internal references	137
	4.5.2	Example of hyperspectral imaging	137
		4.5.2.1 Image reproduction and spectral recovery	139
		4.5.2.2 Overlaid hyperspectral image recovery	139
		4.5.2.3 Separated hyperspectral image recording	140
		4.5.2.4 Hyperspectral imaging supported by filters	140
	4.5.3	General design for hyperspectral imaging	141
		4.5.3.1 Design considerations	141
Refe	rences		142

5	Detec	tors for	Optical Spectroscopy	143
	5.1	Introdu	uction	143
		5.1.1	Work and power of light signals	143
		5.1.2	Basic parameters of detectors	143
			5.1.2.1 Pre-amplifier considerations and wiring	144
			5.1.2.2 General signals and sources of noise in optical	
			detector systems	145
		5.1.3	Detection limit, noise, and SNR	146
		5.1.4	Detection limit, noise, and SNR in absolute measurements	146
		5.1.5	Detection limit, noise, and SNR in relative measurements	147
	5.2	Single-	-Point Detectors	147
		5.2.1	Phototubes	147
		5.2.2	Comments on the interpretation of PMT data sheets	150
		5.2.3	A sample calculation for PMTs, valid for an integration	
			time of 1 s	150
		5.2.4	Photon counter	150
		5.2.5	UV PMTs and scintillators	151
	5.3	Illumin	ation of Detectors, Combined with Image Conversion	152
	5.4	Chann	eltron <sup>®</sup> and Microchannel Plate	153
	5.5	Intensi	fied PMT and Single-Photon Counting	157
	5.6	Solid S	State Detectors	157
		5.6.1	General effect of cooling	159
		5.6.2	Planck's radiation equals blackbody radiation	159
		5.6.3	Detectors and the ambient temperature	160
			5.6.3.1 Signal modulation and synchronized detection	162
			5.6.3.2 Estimation of the modulated measurement	168
		5.6.4	Tandem detectors	169
		5.6.5	Typical parameters of solid state detectors,	
			and their interpretation	170
	5.7	Design	n Considerations of Solid State Detectors	171
		5.7.1	Illumination of small detector elements	171
		5.7.2	Charge storage in semiconductor elements, thermal	
			recombination, and holding time	171
		5.7.3	PIN and avalanche diodes	172
		5.7.4	Detector coupling by fiber optics	172
	5.8	Area D	Detectors: CCDs and Arrays	173
		5.8.1	Mounting of area detectors, the resulting disturbance,	
			and the distribution of wavelengths	173
			5.8.1.1 Popular versions of area detectors	174
		5.8.2	Basic parameters of arrays and CCDs with	
			and without cooling	175
			5.8.2.1 Pixel size, capacity, sources of noise, dynamic	
			range, shift times, read-out time, and ADC	
			conversion time	176
			5.8.2.2 Applicability of CCDs for spectroscopy, image	
			processing, and photography	178

	5.8.3	Signal tr	ansfer and read-out	178
		5.8.3.1	Combining the read-out in imaging mode and the	
			display in spectroscopy mode	181
	5.8.4	CCD arc	hitectures	181
	5.8.5	CCD and	d array efficiency	183
		5.8.5.1	Front-illuminated CCDs	183
		5.8.5.2	Rear-side-illuminated CCDs	183
		5.8.5.3	Interference of rear-side-illuminated CCDs:	
			Etaloning	186
	5.8.6	Time co	ntrol: synchronization, shutter, and gating	187
		5.8.6.1	Shutter control	187
		5.8.6.2	Microchannel-plate image intensifiers	188
	5.8.7	Current	formats of area detectors	188
	5.8.8	Read-ou	t techniques: Multi-spectra spectroscopy,	
		binning,	and virtual CCD partition	189
		5.8.8.1	Virtual CCD programming	192
	5.8.9	CCDs ar	nd array systems with image intensification	193
		5.8.9.1	CCDs with on-chip multiplication or electron	
			multiplication (EMCCD)	193
		5.8.9.2	CCDs with an additional microchannel-plate	
			image intensifier (MCP-CCD)	194
	5.8.10	Data acc	quisition in the ms–µs time frame	195
		5.8.10.1	Kinetic measurements	195
		5.8.10.2	Double-pulse measurements	197
	5.8.11	Extendin	g the spectral efficiency into the deep UV	198
	5.8.12	NIR and	IR area detectors	198
5.9	Other A	Area Dete	ctors	200
	5.9.1	CID and	CMOS arrays	200
		5.9.1.1	Typical CMOS parameters, and comparison	
			to CCDs	200
	5.9.2	Position-	sensitive detector plate	203
	5.9.3	Streak a	nd framing camera	203
Refe	rences			205
Illumir	nation o	f Snectro	meters and Samples: Light Sources	
Transf	fer Svst	ems and	Fiber Ontics	207
6 1	Introdu	otion and	Paprocentation of Symbols	207
6.0	Dedier	cuon anu		207
0.Z	Advont		sing $\Omega$ and ar	200
0.3 6.4	Difforor	aye or os	of Padiation and Their Collection	210
0.4			diation	210
	0.4.1		anad radiation	210
	0.4.Z	Doll char	aped radiation from point acurace. Lampa	213
	0.4.3	Dall-Shap	Thermal filement lemna	210
		0.4.3.1	Are discharge lamps	210
		0.4.J.Z	ALC UISCHALGE IAMPS	∠10

6

			6.4.3.3 Spectra of the various lamp types	217
			6.4.3.4 Light collection and transfer into a spectrometer	218
		6.4.4	Diffuse radiation collected by integrating spheres	219
			6.4.4.1 Collecting lamp radiation	222
			6.4.4.2 Approaching the parameters of a sphere	222
		6.4.5	NIR radiation	224
		6.4.6	IR radiators	225
	6.5	Examp	les of Optimizing Spectrometer Systems	227
		6.5.1	Optimization of gratings	227
		6.5.2	Change-over wavelengths of lamps, gratings, and detectors	228
	6.6	End Re	esult of an Illumination Monochromator System	230
	6.7	Light T	ransfer and Coupling by Fiber Optics	231
		6.7.1	Fiber guides, light-wave guides, and fiber optics	231
		6.7.2	Fiber optics for the UV–Vis–NIR range	232
		6.7.3	Fiber optic parameters and effects	233
		6.7.4	"Flexible optical bench," and a precaution about its handling	236
		6.7.5	Typical kinds and variations of single fibers and fiber cables	236
			6.7.5.1 Basic versions	236
	6.8	Transfe	er Systems	239
		6.8.1	Coupling by bare optical fibers	239
		6.8.2	Coupling by lens systems	240
		6.8.3	Coupling by mirror systems	242
	Refer	rences		243
7	Calibra	ation of	Spectrometers	245
	7.1	Calibra	tion of the Axis of Dispersion, Wavelength,	
		and Ph	noton Energy	245
		7.1.1	Parameters that define the angular position of a dispersion	
			element	245
		7.1.2	Driving a grating or prism spectrometer	245
			7.1.2.1 Grating spectrometers with a sine-functional drive	246
			7.1.2.2 Calibrating a scanning system with a sine drive	247
			7.1.2.3 First calibration of a sine-driven system	247
			7.1.2.4 Parameters that can degrade the linearity	248
			7.1.2.5 Timing calibration checks and recalibration	248
			7.1.2.6 Recalibration requirements	249
		7.1.3	Grating spectrometers with a rotary drive	249
		7.1.4	Calibration of the field output	251
			7.1.4.1 Output dispersion as a function of the lateral	
			position in the field output	252
	7.2	Calibra	ting the Axis of Intensity, Signal, and Illumination	253
		7.2.1	Requirements for a useful calibration and portability	
			of data	253
		7.2.2	Light sources for radiometric calibration	253
		7 7 2	Procedures to produce reliable calibrated data	254
		1.2.5	Trocedures to produce reliable calibrated data	204

277

	7.3	Transfer Efficiency of Spectrometers	256
		7.3.1 General behavior	256
		7.3.2 Measurement of transfer efficiency	256
	Refe	rences	258
8	Stray	and False Light: Origin, Impact, and Analysis	259
	8.1	Origin of Stray Light	259
	8.2	Impact of Stray Light	261
		8.2.1 Disturbance in the application of discrete spectral signals	261
		8.2.2 Disturbance in the application of broadband spectral	
		signals	263
	8.3	Analysis and Quantization of Stray Light in Spectrometers	
		and Spectrophotometers	264
	8.4	Minimizing the Impact of Disturbance through Optimization	266
	8.5	Reducing Stray Light	267
	Refe	rences	268
9	Relate	ed Techniques	269
	9.1	Compact, Fiber-Optic-Coupled Spectrographs	269
	9.2	Programmable Gratings	272
	9.3	Bragg Gratings and Filters	272
	9.4	Hadamard Spectrometer	273
		9.4.1 Principle of Hadamard measurements	274
		9.4.2 Hadamard setups	274
	Refe	rences	275

### Preface

My search for universal and comprehensive literature on dispersive optical spectroscopy revealed many gaps. The books on very basic information are rather theoretical and dig deep into arithmetic derivations to calculate spectrometers, illumination, and detection. The books on the different applications of optical spectroscopy are mainly "cookbooks" and do not explain why something should be done in a certain way. Books with comprehensive content are available from the vendors of dispersers, spectrometers, detectors, and systems—they naturally feature the advantages of the supported products but offer no overall view.

For more than twenty years, I have calculated and delivered special dispersive spectroscopy systems for different applications. In the time between inquiry and decision, the customers wanted to justify my presentation and compare it. A common problem was finding useful references that could be used to verify my calculations and predictions. So, again and again, I wrote long letters combining the different parameters of the project presented. Several of my customers-industrial project managers as well as researchersnot only acknowledged the proposals but also often used the papers to check the instrumental performance at delivery. Because the proposals fit the requirements and the predictions were at least reached, their confidence was earned. Customers used my papers for internal documentation and teaching. Several asked me to provide the know-how in a general, written database in order to close the gap between theory, practice, and applications. After my retirement from regular work, I did just that, and published my writing on my homepage (www.spectra-magic.de). Now, the content has been improved and extended into a pair of printed books, the first of which you are reading now.

The aim of this book is to supply students, scientists, and technicians entering the field of optical spectroscopy with a complete and comprehensive tutorial; to offer background knowledge, overview, and calculation details to system designers for reference purpose; and to provide an easy-to-read compendium for specialists familiar with the details of optical spectroscopy.

#### Acknowledgments

My thanks are first addressed to my wife, Heidi, for her patience during the months spent investigating, reviewing, and writing. I also thank those who urged me to start writing in the first place and who collected data and calculations. The trigger to turn the homepage into written books came from Dr. Karl-Friedrich Klein, who kept me going and contacted SPIE. The section on fiber optics was supported by Joachim Mannhardt, who provided specifics and added features and ideas. After the manuscript was given to SPIE, external reviewers spent much effort on the content, providing corrections and suggestions for improvement; that valuable support came from Mr. Robert Jarratt and Dr. Alexander Sheeline. Last but not least, I'd like to thank Tim Lamkins, Scott McNeill, and Kerry McManus Eastwood at SPIE for the work they invested into the project.

I hope that readers will find useful details that further their interest or work.

Wilfried Neumann May 2014

# **Glossary of Symbols** and Notation

A	Absorbance (extinction) in photometric absorption
	measurements
A	Geometric area
A	Light angle inside a prism
ADC (A/D-C)	Analog-to-digital converter
$A_{iG}$	Effective disperser area at a given disperser angle
$A_{iM}$	Illuminated area of the focusing mirror
В	Bandwidth
С	Capacity
С	Contrast; ratio of useful signal/disturbance
$c_0$	Speed of light
CCD	Charge-coupled device
d	Deflection angle at the prism
d	Dispersed beam after a grating
$D^*$	Numeric capability of an IR detector for the recovery of
	low signals
dB	Decibel
$d_x$	Focus displacement after thermal change
$d_y$	Focus increase after thermal change
e	Base of the natural logarithm
E	Deformation factor at the exit of a spectrometer
e <sup>-</sup>	Electron
$E_{(\lambda)}$	Irradiance of a light beam on a normalized surface
el	Elbow angle
eV	Electron volt
f	Focal length
f	Frequency
$f_c$	Angular frequency
FSR	Free spectral range
FWHM	Full width at half maximum
h	Planck's constant ( $6.626 \times 10^{-34}$ Js)

h	Slit height
Н	Total aberration
hb	Number of pixels binned together
I	Parallel incident beam to grating or prism
<i>i</i> <sub>1</sub>	Angle of the prism's incident light related to N
J	Joule
k	Absorption coefficient of a material
k	Boltzmann's constant $(1.381 \times 10^{-23} \text{ JK}^{-1})$
k	Grating constant for the distance of the grating lines
K	Kelvin
Κ	Thermal dilatation coefficient
L	Inductivity
L	Luminosity, light flux in spectrometers
$L_{(\lambda)}$	Radiance
LN	Liquid nitrogen
т	Modulation factor in lifetime measurements
	by phase/modulation
т	Spectral order number
M	Magnification factor
M	Radiant emittance/exitance
MCP	Microchannel plate; also, microchannel-plate
	image-intensifier system
$m_s$	Minimum slit width
n	<i>f</i> -number
п	Refractive index
п	Total number of lines in a grating
Ν	The normal of a grating or prism
0	Aberration
$O_1$	Basic aberration
$O_{ss}$	Additive aberration
P	Power
PMT	Photomultiplier tube
PPS	Pulses per second; also, events per second
PSD	Phase-sensitive detector (in the lock-in); also, position-
	sensitive (counting) detector
Q	Energy of radiation R; also, the numerical resolution
$\tilde{Q}$	Ratio of the numerical resolution $R_r/R_p$
$\tilde{\varrho}$	Quality factor
ÕΕ	Quantum efficiency
r	Radius of curved slits; also, the distance of the slit to the
	instrument's center
R	Normalized reflectance of a sample
R	Numeric resolution
R	Resistance

RD	Reciprocal dispersion
ROI	Region of interest
$R_{p}$	Theoretical resolution of a dispersing element
$r_p$	Absolute value of parallel polarization
r <sub>s</sub>	Absolute values of perpendicular polarization
$R_r$	Real experimental resolution
S	Constant of thermal diffusion
SL	Number of vertical lines of a CCD
SNR (S/N-R)	Signal-to-noise ratio
sr	Steradian
SR	Number of horizontal register pixels of a CCD
STD	Standard deviation
Т	Temperature; also, thermal change
Т	Normalized transmission in photometric applications
W	Median distance of a mirror to the center line or grating
	center axis
W	Active grating or mirror width
W	Electrical or optical work
X	Geometric dilation as a function of thermal change
X	Half the inclusion angle at the grating
У	Geometric increase of the focal spot as a function of
	thermal change and dilatation
α	Angle of the light illuminating the grating or prism with
	respect to N
β	Angle of the diffracted or refracted light leaving the
	disperser with respect to N
δ	Inclusion angle of the light at the disperser originating from
	the lateral distance and width of the mirrors
δ	Phase angle or phase shift ellipsometry (SE)
$\Delta$	Imaginary part of ellipsometric data
$\epsilon_1$	Angle of the grating-impinging beam
ε <sub>2</sub>	Angle of the beam leaving the grating
L	Internal off-axis angle
ι <sub>h</sub>	Horizontal off-axis angle in a spectrometer
L <sub>V</sub>	Vertical off-axis angle in a spectrometer
λ	Wavelength
ν ~	Oscillation frequency of a light wave
ν	Frequency of a light wave presented as a wavenumber
ρ	Complex result of ellipsometric data
σ	Statistical parameter often used for deviations
τ	Time constant
Φ	Angle of sample illumination in ellipsometry
Φ	Median grating angle

$\Phi$	Phase angle/phase shift in phase/modulation lifetime measurements
Φ	Radiant power/flux
$\Psi$	Real part of ellisometric data
ω	Angular frequency
ω	Normalized cone angle of illumination
Ω	Acceptance angle
Ω	Real and normalized aperture of a spectrometer; also,
	light-guiding factor