## **Contents**

1.	Distribution of the Scattering Intensity.				
	Gen	eral Asp	pects		
	1.1	Diffrac	ction Techniques		
			alyzing Imperfections in Crystals		
	1.2	Kinem	natical Theory of Scattering		
		1.2.1	Dynamical and Kinematical Theories		
		1.2.2	X-Ray Scattering Intensity		
		1.2.3	· · · · · · · · · · · · · · · · · · ·		
		1.2.4	Applicability Range for the Kinematic Theory 19		
	1.3	Scatter	ring by Perfect Crystals of Finite Size		
		1.3.1	Intensity Distribution in Reciprocal Lattice Space:		
			Form Function		
		1.3.2	Intensity Distribution in the		
			Debye Diffraction Pattern		
	1.4	Scatter	ring in Undistorted Crystals Containing		
		Micros	scopic Cavities or Inclusions		
	1.5	Scatter	ring by Crystals Containing Defects		
		of Arb	pitrary Type. Classification of Defects		
		1.5.1	Analysis of Scattering by Imperfect Crystals 3		
		1.5.2	Scattering by Crystals		
			with Randomly Distributed Defects		
		1.5.3	Classification of Defects		
		1.5.4	Diffuse Scattering by Crystals Containing		
			First-Class Defects Under Weak Overlap		
			of the Displacement Fields of Individual Defects 4		
		1.5.5	Approximation of Smoothly Varying Distortions 4		
		1.5.6	Scattering Intensity with		
			Correlated Arrangement of Defects		
	1.6	Harmo	onic Analysis of the X-Ray Line Shapes 5		
		1.6.1	Fourier Coefficients for the Intensity Distributions		
			of X-Ray Lines		
		1.6.2	Limiting Cases of Nondistorted		
			and Large-Size Crystallites 6		
		1.6.3	Analysis of Crystallite Size and Distortions 6		



2.	Stati	ic Displa	cements in Crystals with Bounded Defects	75		
	2.1	Fluctuation Waves of Defects Concentration				
		and Sta	itic Displacements	75		
		2.1.1	Symmetry of Defects	77		
		2.1.2	The Defect Distribution in Terms of Static			
			Concentration Waves	80		
		2.1.3	Static Displacement Waves	83		
	2.2	Macros	copic Theory for the Static Displacement Waves	85		
		2.2.1	Long-Wavelength Fluctuation Waves			
			and the Free Energy of the Anisotropic			
			Elastic Continuum	85		
		2.2.2	Amplitudes of the Fluctuation Waves			
			of Static Displacements	87		
		2.2.3	Fourier Components of the Static Displacements			
			in the Continuum Description	92		
		2.2.4	Simplifications Introduced by Symmetry	95		
		2.2.5	Fluctuation Waves in Thin Films	99		
	2.3	Micros	copic Theory for the Static Displacement Waves	103		
		2.3.1	Free Energy of Distorted Crystal			
			with Bravais Lattice	103		
		2.3.2	Transition to the Long-Wave Approximation			
			and the Related Force Constants	106		
		2.3.3	Crystals of Arbitrary Structure	111		
	2.4	Static I	Displacement Fields Around Bounded Defects	112		
		2.4.1	Atom Displacements Far from Defects	112		
		2.4.2	Atomic Displacements Near Defects, Green Functions			
			and Mean Squares of Static Displacements	124		
	2.5 Static Distortions in Quasi-One-Dimensional					
			asi-Two-Dimensional Crystals	130		
		2.5.1	Discreteness of the Lattice and Spatial Dispersion	130		
		2.5.2	Static Distortion Fields of Defects			
			in Strongly-Anisotropic Crystals	136		
3.	Posit	ions and	Intensities of Regular Reflection Peaks	147		
	3.1	Shift of X-Ray Lines in Imperfect Crystals				
			Determination of Defect Concentrations	147		
		3.1.1	Influence of Defects on X-Ray Line Positions			
			and Estimated Crystal Sizes	147		
		3.1.2	Studies of Vacancies in Crystals	152		
		3.1.3	Complexes in Solid Solutions and Their Effect			
			on the Lattice Parameters	155		
		3.1.4	Dilation Effects Caused by Dislocation Loops			
	3.2	Regular	Reflection Intensities in Perfect Crystals			
			Intensity Attenuation Factors	166		

			Contents	XVII
		3.2.2	Debye-Waller Factor in Perfect Harmonic Crystals .	. 168
		3.2.3	Chain-Like and Layered Crystals	
		3.2.4	Effect of Anharmonicity on the Debye-Waller Factor	
	3.3		of Static Displacements on Intensities	
		of Regi	ular Reflections	. 194
		3.3.1	Debye-Waller Factor Due to Static Displacements .	
		3.3.2	Effects in Crystals Containing Particles	
			of a New Phase or Dislocation Loops	. 201
		3.3.3	Layered and Chain-Like Crystals	. 206
		3.3.4	Concentrated Solutions	. 211
		3.3.5	Experimental Results on Regular Reflection	
			Intensities in Imperfect Crystals	. 218
	3.4	Effect of	of Thermal Vibrations in Imperfect Crystals	. 223
		3.4.1	Crystals with Low Defect Concentrations	
		3.4.2	Concentrated Solutions	
	3.5	Debve-	Waller Factors in Dynamical Diffraction Effects	
		3.5.1	Anomalous Transmission	
		3.5.2	X-Ray Fluorescence	
		3.5.3	Spatial Intensity Oscillations	
		3.5.4	Critical Potentials	
		0.0		
4.	Diffu	ıse Scatt	ering of X-Rays and Neutrons	
	by C	rystal D	efects	. 241
	4.1	Weakly	Distorted Crystals	. 241
		4.1.1	Scattering by Single Defects	. 241
		4.1.2	Scattering Intensity Near Reciprocal Lattice Points:	
			Symmetry of Defects and Force Dipole Tensors	. 244
		4.1.3	Scattering Intensity Distribution at Large Distances	
			from Reciprocal Lattice Points and Determination	
			of the Defect Configuration and the Force Field	. 251
		4.1.4	Diffuse Scattering and the Correlation	
			in Defect Positions	. 254
		4.1.5	Experiments on Scattering by Point Defects	
			in Irradiated Crystals and Dilute Solutions	. 257
		4.1.6	Scattering by Self-localized Electrons	. 268
		4.1.7	Diffuse Scattering Representation in Various	
			Experimental Techniques	. 271
	4.2	Effects	of Groups of Point Defects, New-Phase Particles,	
			ll-Radius Dislocation Loops	. 275
		4.2.1	Scattering by Large Bounded Defects	
			in Weakly Distorted Crystals	. 275
		4.2.2	Diffuse Scattering by Weakly Distorted Crystals	
			with Particles of a Second Phase	
			and Ageing of Solutions	. 283

XVIII	Contents

		4.2.3	<u> </u>		
			in Strained and Irradiated Materials	294	
	4.3	Intensi	ity Distribution for Scattering by Strongly		
		Distor	ted Crystals with Finite Defects	303	
		4.3.1	Change in Scattering Intensity Distribution		
			with Increasing Defect Strength	303	
		4.3.2	Integrated Intensity from Strongly		
			Distorted Crystals	305	
		4.3.3	Intensity Distribution in the Reciprocal Space		
		4.3.4	The Debye Diffraction Pattern		
		4.3.5	Experiments on Strongly Distorted Ageing Alloys		
		****	and Irradiated Materials	323	
		4.3.6	Nonrandom Arrangement of Finite Defects		
	4.4		ly Anisotropic Crystals		
		4.4.1	Quasi-Two-Dimensional Crystals		
		4.4.2	Quasi-One-Dimensional Crystals		
	4.5		of Finite Defects in Thin Films		
			urface Layers on X-Ray Scattering	349	
		4.5.1	Scattering Intensity for Imperfect Finite Crystals		
		4.5.2	Diffuse Scattering by Defects in Thin Films		
		4.5.3	Broadening of Regular Reflection Peaks		
			in Free Films with a Large Surface Area	354	
		4.5.4	Diffuse Scattering by Defects		
			in a Thin Surface Layer	355	
5.	Scatt	tering o	f X-Ray and Neutrons in Crystals		
	with	Disloca	ntions	357	
	5.1	Broadening of Peaks by Randomly Distributed Defects			
			Second Class	358	
		5.1.1			
		5.1.2			
			Dislocation Dipoles		
		5.1.4	Stacking Faults and Split Dislocations		
	5.2	Effect	of Nonrandom Dislocation Arrangement		
			attering Intensity Distribution	381	
		5.2.1	Scattering by Crystals with Dislocation Walls		
			and a Dislocation Description for the Effects		
			Caused by Blocks and Cells	381	
		5.2.2	Correlation in the Uniform Dislocation		
			Ensemble and in Crystals with Nonuniform		
			Dislocation Arrangement	392	
	5.3	Diffrac	ction Methods of Investigation		
			location Ensembles	406	
		5.3.1	Determination of Dislocation Density		

	5.3.2 Correlation and Inhomogeneity			
	in Dislocation Arrangement 41	1		
	5.3.3 Dislocations in Narrow Small-Angle Walls (Boundaries)			
	and Excess Dislocations of a Given Sign 41	14		
	5.3.4 Diffraction Techniques for Analyzing			
	the Grain Boundaries 41	18		
Append	ices	21		
Α.	Cumulant Expansion	21		
В.	Equations for Amplitudes of Static Displacement Waves			
	for Various Crystal and Defect Symmetries 42	28		
C.	Microscopic Theory of $A_k$ in Cubic Crystals			
D.	Mean Squares of Static Displacements in fcc Crystals 43			
E.	Calculation of the Function $T''(\rho)$			
	and the First Moment of the Intensity Distribution			
	for Strongly Deformed Crystals Containing			
	Limited-Size Defects	38		
F.	Calculation of $T(\rho)$ for Homogeneous			
	Dislocation Ensemble	10		
Referen	ces	<b>‡</b> 7		

Contents

XIX