



# Contents

## Dynamical Properties of Point Defects in Metals

By P.H. Dederichs and R. Zeller. With 66 Figures

1.	Introduction and Survey .....	1
2.	Dynamical Green's Functions of Ideal and Defect Lattices .....	3
2.1	Equation of Motion and Eigenfunctions .....	3
2.2	Real and Imaginary Part of Green's Function and its Connection with Correlation Functions .....	6
2.3	The Local Frequency Spectrum .....	10
2.4	Behaviour of $G(\omega)$ for High and Low Frequencies .....	13
2.5	Asymptotic Expansion for Large Distances .....	16
2.6	Singularities at Critical Points .....	18
2.7	Analytical and Numerical Solutions for Cubic Ideal Lattices .....	22
3.	Lattice with an Isolated Point Defect .....	28
3.1	Scattering States and Localized States .....	28
3.2	The Isotopic Defect .....	33
3.3	Variational Method for Localized States .....	40
4.	Description of Resonant and Localized Defect Vibrations .....	41
4.1	Method of Krumhansl and Matthew .....	42
4.2	Resonant Modes .....	45
4.3	Effective Force Constant and Effective Mass .....	49
4.4	Damping of Resonant Modes .....	54
4.5	Localized Modes .....	57
4.6	Resonance and Localized Modes near the Band Edge $\omega_{\max}$ .....	61
5.	Dynamics of Substitutional Defects .....	65
5.1	Nearest Neighbour Model for Substitutional Defects .....	65
5.2	Mössbauer Studies of Fe, Sn and Au Impurities .....	74
5.3	Dynamical Behaviour of Vacancies .....	81
6.	Vibrational Properties of Interstitials .....	83
6.1	Vibrations of H in Metals .....	83
6.2	Qualitative Explanation of the Dynamics of Self-interstitials .....	89

6.3 Octahedral Interstitial .....	91
6.4 100-Dumbbell Interstitial .....	97
<b>7. Effects on Phonon Dispersion Curves .....</b>	<b>104</b>
7.1 The Average Green's Function .....	105
7.2 Theory of Thermal Neutron Scattering .....	112
7.3 Change of Phonon Dispersion Curves .....	116
7.4 Effects of Different Scattering Lengths and Static Displacements ..	121
7.4.1 Effects of Different Scattering Lengths .....	121
7.4.2 Incoherent Scattering .....	123
7.4.3 Effects of Static Displacements .....	125
7.5 Results of Neutron Scattering Experiments .....	128
7.5.1 Effects due to Resonance Modes .....	128
7.5.2 Observation of Localized Modes .....	134
7.5.3 Incoherent Scattering Experiments .....	136
7.6 Change of Elastic Constants .....	138
<b>8. Thermodynamic Properties .....</b>	<b>146</b>
8.1 Free Energy of Defect Crystal .....	146
8.2 Properties of the Changed Density of States $\Delta z(\omega)$ .....	149
8.3 Change of the Specific Heat .....	157
8.4 Formation Entropy of Point Defects .....	160
<b>References .....</b>	<b>165</b>

## Theory of Diffusion Controlled Reactions of Point Defects in Metals

By K. Schroeder. With 25 Figures

<b>1. Introduction .....</b>	<b>171</b>
<b>2. Diffusion in Ideal Crystals .....</b>	<b>173</b>
2.1 Lattice of Equilibrium Sites ("Diffusion Lattice") .....	176
2.2 Jump Frequency .....	179
2.3 Diffusion Equation and Green's Function .....	183
2.3.1 The Stationary Green's Function .....	186
2.3.2 Asymptotic Behaviour .....	188
2.3.3 Spectral Representation .....	188
2.3.4 Analytical Behaviour .....	189
2.3.5 Numerical Results .....	190
2.4 Experimental Methods .....	192

3.	Interaction of Defects in Metals .....	194
3.1	Static Displacements Around Defects .....	194
3.2	Point Defect Interaction .....	196
3.3	Interaction of Point Defects with Dislocations .....	199
3.4	Short-Range Interaction .....	202
4.	Diffusion in Force Fields .....	203
4.1	Derivation of Continuum Theory from Lattice Theory .....	205
4.1.1	Cubic Defects .....	205
4.1.2	Noncubic Defects .....	209
4.2	Diffusion in a Homogeneously Deformed Crystal .....	212
4.3	Discussion .....	214
5.	Phenomenological Theory for Reactions of Point Defects .....	214
5.1	Stationary Diffusion and Boundary Condition .....	215
5.2	Reaction Probability of a Single Defect with a Single Sink .....	218
5.3	Independent Sink Approximation .....	219
5.4	Reaction of Point Defects with Straight Dislocations .....	220
5.5	Finite Sink Densities .....	222
5.5.1	Spherical Cell Approximation .....	222
5.5.2	Random Distribution of Sinks .....	223
6.	Lattice Theory for the Reaction Probability .....	224
6.1	General Expression for the Reaction Probability .....	226
6.2	Asymptotic Form .....	229
6.3	Variational Principle for Calculating $R_a$ .....	229
6.4	Results .....	231
6.4.1	Exact Results for the bcc Lattice .....	231
6.4.2	Asymptotic Results .....	232
6.4.3	Other Cubic Lattices .....	233
6.4.4	Noncompact Reaction Regions .....	234
6.5	Discussion and Conclusion .....	236
7.	Influence of Long-Range Potentials on the Rate Constant .....	237
7.1	Variational Principles .....	239
7.1.1	Upper Bound for the Rate Constant .....	239
7.1.2	Lower Bound for the Rate Constant .....	241
7.1.3	Discussion .....	242
7.1.4	Variational Principle with Production .....	242
7.2	Effective Rate Constant for Spherical Sinks .....	243
7.2.1	Temperature Dependence .....	244
7.2.2	Spherically Symmetric Potentials .....	244
7.2.3	Test of Variational Principles .....	246
7.2.4	Nonspherical Potentials .....	247

7.3 Effective Rate Constant for Straight Dislocations .....	250
7.3.1 Cylindrically Symmetric Potentials .....	251
7.3.2 Edge Dislocations .....	252
7.4 Discussion and Applications .....	253
8. Summary and Outlook .....	256
References .....	258

