

# Contents

|          |  |           |
|----------|--|-----------|
| <b>1</b> | <b>Balancing Detail and Completeness in Collisional-Radiative Models</b> | <b>1</b>  |
|          | Stephanie B. Hansen  |           |
| 1.1      | Introduction   | 1         |
| 1.2      | State-Space Completeness   | 2         |
| 1.3      | Degree of State Detail   | 6         |
| 1.4      | Application-Driven Approaches to Balancing Detail and Completeness       | 9         |
| 1.4.1    | Coronal Fine-Structure Models  | 10        |
| 1.4.2    | General Models for Moderate-Density Plasmas                              | 10        |
| 1.4.3    | Self-consistent Field Models for Dense Plasma                            | 13        |
| 1.5      | Conclusions  | 14        |
|          | References   | 15        |
| <b>2</b> | <b>Self-consistent Large-Scale Collisional-Radiative Modeling</b>        | <b>17</b> |
|          | Christopher J. Fontes, James Colgan and Joseph Abdallah Jr               |           |
| 2.1      | Introduction   | 18        |
| 2.2      | Large-Scale Collisional-Radiative Modeling                               | 20        |
| 2.2.1    | The Los Alamos Suite of Atomic Physics Codes                             | 20        |
| 2.2.2    | Selecting a List of Configurations                                       | 22        |
| 2.2.3    | Selecting the Level of Refinement  | 26        |
| 2.2.4    | Constructing the Rate Matrix   | 28        |
| 2.2.5    | Steady-State Solutions Versus Time-Dependent Solutions                   | 29        |
| 2.2.6    | Boundary Conditions for the Steady-State CR Equations                    | 29        |
| 2.2.7    | Different Methods of Solving the Steady-State CR Equations               | 31        |
| 2.3      | An Illustrative Example  | 33        |
| 2.4      | Summary and Outlook  | 40        |
|          | References   | 42        |

|   |     |
|---|-----|
| <b>3 Generalized Collisional Radiative Model Using Screened Hydrogenic Levels . . . . .</b> | 51  |
| H.-K. Chung, S.B. Hansen and H.A. Scott   |     |
| 3.1 Introduction . . . . .  | 52  |
| 3.2 Formalism . . . . .   | 53  |
| 3.2.1 Generalized Collisional-Radiative Atomic Levels. . . . .                              | 53  |
| 3.2.2 Atomic Transition Rates. . . . .  | 58  |
| 3.2.3 Plasma Effects. . . . .   | 64  |
| 3.2.4 Spectroscopic Emissivity and Opacity . . . . .  | 66  |
| 3.3 Applications . . . . .  | 68  |
| 3.3.1 Steady-State Plasmas Generated by Long-Pulse Lasers . . . . .                         | 68  |
| 3.3.2 Two-Temperature Plasmas Generated by Short-Pulse Lasers . . . . .                     | 69  |
| 3.3.3 Photoionization Equilibrium Plasmas . . . . .   | 70  |
| 3.3.4 Photo-Ionized Plasmas Generated by X-Ray Free Electron Lasers . . . . .               | 71  |
| 3.3.5 Radiative Loss Rates of Heavy Elements . . . . .                                      | 73  |
| 3.4 Validities and Limitations . . . . .  | 73  |
| 3.4.1 Completeness . . . . .  | 74  |
| 3.4.2 Improvement on SH Model Spectra . . . . .   | 75  |
| 3.4.3 Dielectronic Recombination . . . . .  | 76  |
| 3.4.4 Radiative Power Losses . . . . .  | 76  |
| 3.4.5 Continuum Lowering . . . . .  | 77  |
| 3.4.6 CR Models in High-Energy-Density Radiation-Hydrodynamic Simulations . . . . .         | 78  |
| 3.5 Summary . . . . .   | 78  |
| References . . . . .  | 78  |
| <b>4 Collisional-Radiative Modeling for Radiation Hydrodynamics Codes . . . . .</b>         | 81  |
| Howard A. Scott   |     |
| 4.1 Introduction . . . . .  | 81  |
| 4.2 Governing Equations . . . . .   | 83  |
| 4.3 Non-LTE Material Response . . . . .   | 87  |
| 4.4 High Density Effects . . . . .  | 91  |
| 4.5 Detailed Balance, Energy Conservation and Discretization . . . . .                      | 98  |
| 4.6 Conservation and Consistency in Non-LTE Thermal Radiation Transport . . . . .           | 101 |
| 4.7 Summary . . . . .   | 104 |
| References . . . . .  | 104 |
| <b>5 Average Atom Approximation in Non-LTE Level Kinetics . . . . .</b>                     | 105 |
| Vladimir G. Novikov   |     |
| 5.1 Introduction . . . . .  | 105 |
| 5.2 Level Kinetics Equations . . . . .  | 106 |

|   |     |
|---|-----|
| 5.3 The Rates of Collisional and Radiative Processes. . . . .   | 108 |
| 5.3.1 Excitation by Electron Impact. . . . .  | 108 |
| 5.3.2 Electron-Impact Ionization and Three-Body Recombination . . . . .                               | 111 |
| 5.3.3 Autoionization and Dielectronic Capture. . . . .  | 113 |
| 5.3.4 Rates of Radiative Processes. . . . .   | 114 |
| 5.4 Configuration Accounting in the Extended CR-AA Model . . . . .                                    | 116 |
| 5.5 Reducing Detailed Level Kinetics to Extended CR-AA Model . . . . .                                | 117 |
| 5.6 The Calculation Algorithm . . . . .   | 120 |
| 5.7 Results of Calculation for Tin Plasma . . . . .   | 121 |
| References . . . . .  | 125 |
| <b>6 Collisional-Radiative Modeling and Interaction of Monochromatic X-Rays with Matter . . . . .</b> | 127 |
| O. Peyerusse  |     |
| 6.1 Introduction . . . . .  | 127 |
| 6.2 Atomic Model Construction for the Modeling of X-Ray Interaction with Matter . . . . .             | 128 |
| 6.3 Interaction with Gas. . . . .   | 130 |
| 6.4 Interaction with Small Objects. . . . .   | 135 |
| 6.5 Interaction with Solids . . . . .   | 136 |
| 6.5.1 Population Kinetics and Atomic Structure at Solid Density . . . . .                             | 137 |
| 6.5.2 Temperature and Population Evolution . . . . .  | 139 |
| 6.5.3 Energy Deposition . . . . .   | 144 |
| 6.5.4 Modeling of Al, V and Ag Samples Irradiated in the X-UV or X-Ray Range . . . . .                | 146 |
| 6.6 Conclusion . . . . .  | 150 |
| References . . . . .  | 150 |
| <b>7 Spectral Modeling in Astrophysics—The Physics of Non-equilibrium Clouds . . . . .</b>            | 153 |
| G.J. Ferland and R.J.R. Williams  |     |
| 7.1 Introduction . . . . .  | 154 |
| 7.2 Working with Real Nebulae: The Observational Questions We Are Trying to Answer . . . . .          | 155 |
| 7.3 Approaches to Astronomical Spectral Modelling . . . . .   | 162 |
| 7.4 Spectral Calculations . . . . .   | 166 |
| 7.4.1 The Ionization Balance in the ISM Limit . . . . .   | 166 |
| 7.5 The Physics of the Astronomical Problem. . . . .  | 173 |
| 7.6 Future Opportunities and Challenges . . . . .   | 174 |
| 7.6.1 New Spectroscopic Opportunities . . . . .   | 174 |
| 7.6.2 And the Grand Challenges to Exploiting Them . . . . .   | 177 |
| References . . . . .  | 178 |

|  |     |
|--|-----|
| <b>8 Validation and Verification of Collisional-Radiative Models . . . . .</b> | 181 |
| Yu. Ralchenko  |     |
| 8.1 Introduction . . . . .   | 181 |
| 8.2 Tests and Uncertainty Analysis of CR Models. . . . .                       | 182 |
| 8.3 Overview of NLTE Code Comparison Workshops . . . . .                       | 186 |
| 8.4 Code Comparison Parameters . . . . .                                       | 188 |
| 8.4.1 List of Parameters for Steady-State Cases . . . . .                      | 188 |
| 8.4.2 Global Parameters . . . . .  | 190 |
| 8.4.3 Ion Parameters . . . . .   | 192 |
| 8.4.4 Data for Atomic States. . . . .  | 197 |
| 8.5 Concluding Remarks . . . . .   | 205 |
| References . . . . .   | 207 |
| <b>Index . . . . .</b>   | 209 |