

Preface

Only four years after the first edition was published, new developments of the augmented spherical wave (ASW) methodology made an update of this book necessary. In particular, the successful implementation and widespread application of the spherical-wave based full-potential ASW method was reflected by many requests for a comprehensive description of the new approach. This is accounted for by the present edition, which complements the variety of ASW methods dealt with in this book by a detailed outline of the spherical-wave based full-potential ASW method in Chap. 5.

It is probably not exaggerated to say that the spherical-wave based full-potential ASW method, the development and implementation of which has kept me busy over many years, marks the present highlight of the spherical wave methods. Indeed, it combines the simplicity and very high computational efficiency of Andersen's atomic sphere approximation (ASA) with the high accuracy of modern full-potential methods. This is even more remarkable, as the spherical wave methods, while being conceptionally simple and allowing for an intuitive interpretation of results in terms of atomic-like orbitals, suffered for a long time from severe approximations, which prevented highly accurate total energy calculations. So far, the latter could be achieved only by considerable loss in computational efficiency, an obstacle, which has been overcome with the present spherical-wave based full-potential ASW method.

The recent developments and the implementation of the corresponding code have been accompanied and supported by many friends and colleagues. Without being complete, I would like to thank particularly Prof. U. Eckern, Prof. R. Frésard, PD Dr. K.-H. Höck, Prof. T. Kopp, Prof. J. Mannhart, Prof. S. F. Matar, Dr. A. Mavromaras, Prof. W. Scherer, Prof. P. C. Schmidt, Dr. M. Stephan, Prof. D. Vollhardt, and Dr. E. Wimmer. Again, I want to express my gratitude to Dr. C. Caron, Mrs. G. Hakuba, and Mrs. A. Schulze-Thomin from Springer Verlag for their expertise in guiding me through the final phase of this book. Last but not least, many thanks go to all the readers of the first edition as well as the users of the ASW program package worldwide, for their interest, feedback, suggestions, and the numerous fruitful discussion on the method and its applications. I both enjoyed and

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