Textbook of First-Principles Plane-Wave Methods: Purpose, Contents, Important Points and New Ideas in My Recent Publication

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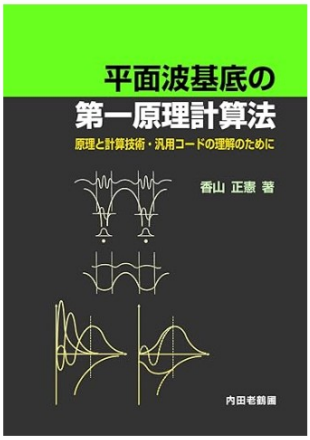
Nowadays, a lot of researchers use package software of the first-principles plane-wave methods such as VASP, CASTEP, ABINIT and so on, which significantly contributes to recent high research activities of computational materials science and engineering. However, not all the users fully understand the basic theory, practical plane-wave methods or efficient techniques for large-scale calculations. One can obtain basic information through web sites or original papers, although it is not so easy for researchers in the field of materials science and engineering to fully understand the above issues. Thus, I have published a textbook on the first-principles plane-wave methods in Japanese [1], which explains the theory, methods and techniques commonly used in such plane-wave codes within a proper size (226 pages), based on my notes for AIST original code, QMAS [2]. This book is aimed at intervening between introductory ones and high-level theoretical ones, and including both theory and techniques in codes. Such a book is demanded, while rare. The first part deals with the density-functional theory (DFT) and the band theory concerning Bloch's theorem and Brillouin-zone integration. The second part deals with the norm-conserving pseudopotential (NCPP), ultrasoft pseudopotential (USPP), and projector augmented wave (PAW) methods to describe valence electrons' behavior by plane waves. The third part deals with the efficient techniques to solve huge-size eigen-value problems, including fast Fourier transformation (FFT). Careful, self-contained and *understandable* explanations are provided with selected equations. The derivation and meaning of each equation are clearly explained. As novel features of my book, first, the meaning of the Monkhorst-Pach k-point sampling (which is often misunderstood) is clarified from both views of special points and discrete Fourier transformation. Second, the evolution of the plane-wave method from NCPP to PAW via USPP is clearly described from unified perspective, which enables us to understand how the PAW method can describe *all-electron behavior* of valence electrons without increasing computational efforts. Third, various computational techniques to attain rapid convergence to the ground state of a large system are explained with our own experiences in the code development [3].



[1] Masanori Kohyama: "First-Principles Plane-Wave Method (Japanese)" (Uchida Rokakuho, 2024, ISBN: 978-4753655601)
[2] https://qmas.jp; S. Ishibashi *et al.*: Phys. Rev. B **76**, 153310 (2007)
[3] M. Kohyama: Modell. Simul. Mater. Sci. Eng. **4**, 397 (1996); T. Tamura *et al.*: *ibid.* **12**, 945 (2004)