

高速化データ駆動科学を用いた陽電子回折実験のデータ解析



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ポスト「京」重点課題7(次世代の産業を支える新機能デバイス・高性能材料の創成)

P1

Background: Data-driven science and material development. Includes a flowchart of the research cycle and a photo of the Oakforest-PACS supercomputer.

P2

Measurement: Total-Reflection High-Energy Positron Diffraction (TRHEPD). Includes a diagram of the TRHEPD experiment and a crystal structure diagram of rutile TiO2.

P3

Analysis method (outline): Inverse problem analysis (1/3). Includes a graph of intensity vs. scattering angle and a diagram of the scattering process.

P4

Analysis method (outline): Inverse problem analysis (2/3). Includes a graph of the residual function R and a diagram of the multi-stage search process.

P5

Analysis method (outline): Inverse problem analysis (3/3). Includes a flowchart of the program concept showing three stages of refinement.

P6

Method: Multi-stage grid calculation. Includes a diagram showing the refinement of the grid from stage 0 to stage 2.

P7

Oakforest-PACS (OFP) strong scaling test results. Includes a log-log plot of execution time vs. number of nodes and a diagram of the Si(100) surface.

P8

Test calculation: Rutile-type TiO2(110)-(1x1) surface. Includes a crystal structure diagram and a comparison of experimental and calculated intensity profiles.

P9

Prospect: Hierarchical superparallel calculation on next-generation PCs. Includes a tree diagram of the calculation hierarchy and a diagram of the scattering process.