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Stacking structure in disordered talc: Interpretation of its X-ray diffraction pattern by using pattern simulation and high-resolution transmission electron microscopy

TOSHIHIRO KOGURE,[1,*] JUN KAMEDA,[1] TOMOYUKI MATSUI,[1] AND RITSURO MIYAWAKI[2]

[1]Department of Earth and Planetary Science, Graduate School of Science, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo, 113-0033, Japan
[2]Department of Geology, The National Science Museum, 3-23-1 Hyakunin-cho, Shinjuku-ku, Tokyo 169-0073, Japan

ABSTRACT

Stacking structure in disordered talc, $Mg_3Si_4O_{10}(OH)_2$, has been investigated by using high-resolution transmission electron microscopy (HRTEM) and by comparison between experimental and simulated powder X-ray diffraction (XRD) patterns. The talc specimen investigated was massive aggregates of fine platy crystals from the Shirakashi mine, Nagasaki-Prefecture, Japan, formed from regional metamorphism. HRTEM observations revealed that the orientation of the 2:1 layer, which is described by the direction of the lateral shift of $a/3$ from the lower tetrahedral sheet to the upper tetrahedral sheet within the 2:1 layer (intralayer shift), is almost completely disordered. In contrast, lateral displacement between the adjacent tetrahedral sheets across the interlayer region (interlayer displacement) is relatively ordered. The interlayer displacement parallel to the intralayer shift in lower or upper 2:1 layers tends to be avoided.

A Gandolfi camera was used to record XRD patterns from a small fragment of the aggregates, to avoid preferred orientation and artifacts in stacking sequence by grinding. XRD patterns were simulated using the DIFFaX program and compared with experimental patterns. The experimental pattern from $hk = 02$, 11, and $1\bar{1}$ reciprocal lattice rows is explained by a mixture of the stacking sequence with almost random directions of intralayer shift and a small amount of 1*A* dominant stacking sequence. The peak profiles for the reflections indexed with 20*l*, 13*l*, or $1\bar{3}l$ are reproduced by considering their variance, and a slightly different interlayer displacement from that reported in talc-1*A*.

Keywords: Crystal structure, talc, electron microscopy, order-disorder, polytypism, XRD data