

Finding the layer scattering origin of rectorite for basal peak calculations

IL MO KANG,^{1,*} MYUNG HUN KIM,² AND HI-SOO MOON³

¹Korea National Oil Corporation, 1588-14, Gwanyang-dong, Dongan-gu, Anyang, Gyeonggi-do, 431-711, Korea

²Department of Chemistry, Yonsei University, 134, Shinchon-dong, Seodaemun-ku, Seoul, 120-749, Korea

³Department of Earth System Sciences, Yonsei University, 134, Shinchon-dong, Seodaemun-ku, Seoul, 120-749, Korea

ABSTRACT

We calculate here the basal peak profiles of Na-rectorite (regularly interstratified Na-illite-smectite) with two different scattering origin choices, one based on the octahedral cationic plane and the other on the basal oxygen plane of the tetrahedral sheet. Our calculation shows that the scattering origin of the octahedral cationic plane, which has been often used in previous diffraction models, is ineffective for profiling the measured peak skewness and irrationality. Alternatively, the calculation using the scattering origin of the basal oxygen plane better mimics the measured peak profiles and provides more reliable crystallite thickness distributions for Bertaut-Warren-Averbach analyses. This origin is also useful for demonstrating the scattering sequence, the layer chemistry heterogeneity, and the effect of the crystallite margin on rectorite scattering.

Keywords: Rectorite, X-ray diffraction, scattering origin, basal reflections, layer boundary