LETTER

Identification of randomly interstratified illite/smectite with basal peak widths

IL MO KANG,1,* MYUNG HUN KIM,2 YUNGOO SONG,3 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

This study formulates the following relationship for identifying randomly interstratified illite/smectite using the integrated peak widths (β) for the first-order reflections after ethylene-glycolation (EG) and thermal dehydration (TD) treatments:

\[ \beta_I = \frac{\beta_{EG} - 0.589\beta_{TD}}{1.324\beta_{TD} - 3.911} \]

where \( \beta_I \) is the proportion of interstratified illite layers. The relationship minimizes the effect of crystallite thickness on the evaluation of \( \beta_I \), which has been a critical source of error in the previous methods using peak position and intensity.

Keywords: Illite/smectite, interstratifications, peak width, crystallite thickness

INTRODUCTION

Smectite progressively transforms into randomly interstratified illite/smectite (random I/S) as burial depth increases (Hower et al. 1976; Altaner and Ylagan 1997). Because this transformation is irreversible in the circumstance of progressive diagenesis, random I/S identified from X-ray diffraction has been used for gathering information on thermal maturation of sedimentary basins with hydrocarbon potential (Pollastro 1993).

Theoretically, the distinctive basal reflections of random I/S result from the Fourier series of the product between the scattering factor from a unit layer and the Laue interference function when the Lorentz-polarization factor is normalized (Reynolds 1980). The Fourier series demonstrates how the layer-by-layer interference of a given coherent scattering crystallite domain (CSCD) affects the basal peak position, intensity, and width of random I/S. Among these parameters, the basal peak position has been routinely applied for identifying random I/S because it systematically shifts with the proportion of interstratified illite layers (Šrodoň 1980; Tomita et al. 1988; Moore and Reynolds 1997). However, most of the peak position methods proposed previously are not sufficiently accurate. The reason is that the extent of peak shift is influenced by not only interstratifications but also by the thickness (Reynolds 1980) and the fluctuation of smectite basal spacing (Šrodoň 1980). The effect of CSCD thickness is especially critical for ultra-fine clay minerals such as random I/S, which generate broad reflections shifted from the original Bragg angles in the direction of which the layer scattering amplitude increases (Kang et al. 2006). Inoue et al. (1989) proposed an alternative method using the peak intensity of random I/S instead of the peak position (so-called, saddle/peak method). However, the method also requires detailed information on the CSCD thickness since the maximum peak intensity is proportional to the number of silicate layers composing the CSCD as is described by the interference function (Reynolds 1980). The effect of CSCD thickness should therefore be considered for the accurate measurement of \( \beta_I \). Kang et al. (2005) have previously demonstrated that the peak widths of random I/S measured after ethylene-glycolation (EG) and thermal dehydration (TD) treatments are useful for minimizing the effects of crystallite thickness for the \( \beta_I \) measurement. The goal of this paper is to formulate an equation for quantifying \( \beta_I \) using basal peak widths of EG and TD treated samples.

COMPUTATIONAL METHOD

Basal peak parameters of random I/S were calculated using Reynolds’ NEWMOD program (Reynolds 1985). The basal reflections of random I/S were simulated in the range of 0 ≤ \( \beta_I \) ≤ 0.4, assuming the chemical compositions are respectively Na0.35(Al1.8Fe0.05Mg0.15)Si2O10(OH)2 for the smectite layer and K0.9(Al1.8Fe0.05Mg0.1)Si2Al0.2O10(OH)2 for the illite layer (Šrodoň et al. 1992). The reason for restricting the \( \beta_I \) range is that the basal reflection of EG sample is extremely broad at \( \beta_I = 0.5 \) and its peak width is difficult to measure. The dimica (\( d_{001} = 0.998 \) nm) and dismectite-2gly (\( d_{001} = 1.69 \) nm) layers were randomly interstratified (Reichweite = 0) (Moore and Reynolds 1997). On the other hand, the basal reflections of TD samples were obtained by using dimica layers and 0.35 potassium atoms per SiO4(OH)2 instead of the dismectite-2gly layers. The calculation matched the structure of thermally dehydrated smectite after K-saturations.

To determine the influence of CSCD thickness on the peak parameters, eight crystallite thickness distribution models were considered for the accurate measurement of \( \beta_I \). Kang et al. (2005) have previously demonstrated that the peak widths of random I/S measured after ethylene-glycolation (EG) and thermal dehydration (TD) treatments are useful for minimizing the effects of crystallite thickness for the \( \beta_I \) measurement. The goal of this paper is to formulate an equation for quantifying \( \beta_I \) using basal peak widths of EG and TD treated samples.

\[ f(n) = \frac{1}{\sqrt{2\pi} \beta_I} \exp \left\{ -\frac{[\ln(n) - \alpha]^2}{2\beta_I^2} \right\} \]

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