**Illite polytype quantification for accurate K-Ar age determination**

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**ABSTRACT**

PolyQuant, a new method to quantify illite polytypes in physical mixtures, has been coupled with Illite Age Analysis (IAA, Pevear 1992) to determine accurate K-Ar ages of the individual polytypes. K-Ar radioisotope dates from illite in shales and sandstones are typically meaningless because these rocks are mixtures of diagenetic and detrital components in unknown proportions. IAA uses linear extrapolation to unmix measured K-Ar ages and establish the end-member ages. This procedure requires samples to have a diagenetic Illite-Smectite (I-S) component mixed with a detrital discrete illite component because they are separable and quantifiable using X-ray diffraction (XRD) of oriented aggregate samples. We extend IAA for use in mixtures of diagenetic and detrital illite with no I-S component by coupling a genetic algorithm (GA) with the WILDFIRE programs (1993) of Reynolds in a new computer program, PolyQuant, which quantifies illite polytypes in a natural sample.

Based on first principles of XRD, WILDFIRE is a forward model that calculates hkl reflections by varying parameters such as rotational disorder, octahedral cation occupancy (i.e., cis- and trans-vacancies), chemical substitutions (K and Fe), orientation, and crystallite thickness. PolyQuant executes several forward models, using the GA to vary the parameters and weight percent of each polytype to automatically achieve a “best fit” with an experimental XRD pattern. Sensitivity tests reveal that changes in the weight percent of an illite polytype, disorder ($P_0$, $P_{cv}$), and the orientation function affect the pattern more than other parameters. In addition, PolyQuant successfully quantified illite components in prepared mixtures of $1M_1$ illite and $2M_1$ muscovite and $1M_1$ illite and $2M_1$ muscovite.

We show examples to validate IAA from prepared mixtures of end-members with known ages and also to obtain end-member ages of highly illitic clay fault gouge. Using K-Ar ages and PolyQuant to quantify the $1M$ and $2M_1$ components from mixtures of RM-30 ($25 \pm 1$ Ma) and a $2M_1$ muscovite from Wards ($428 \pm 9$ Ma), IAA determined end-member ages of 19.9 Ma ($0–44$ Ma) and 429 Ma ($408–459$ Ma)—in reasonable agreement with the measured results. In addition, we use clay gouge from the Canadian Rockies to date movement along thrust faults. Regional geologic data indicate movement along these faults occurred between 73 and 48 Ma. IAA determined the ages of faulting to be from 79.2 to 53.5 Ma, in good agreement with the known range of fault dates. Our results indicate that neoformation of illite in the fault zone must have modified the ages to younger dates.

**INTRODUCTION**

Illite and illite-smectite (I-S) minerals are important to sedimentary basin research for a variety of reasons: (1) reaction progress of smectite illitization can provide a geothermometer during burial subsidence; (2) they can provide an independent, radiogenic isotope date constraining basin-heating events; and (3) they may precipitate in the pores of sandstone reservoirs, decreasing permeability and fluid flow. Formation of illite fixes K during burial diagenesis and illite crystallites retain Ar, which allows this system to act as a radiometric clock. The ages derived from illite and I-S have been used to constrain the geologic timing of hydrothermal fluid migration, regional overthrusting, faulting, and oil and gas migration (Hamilton et al. 1989; Hoffman et al. 1976; Aronson and Burtner 1983; Lee et al. 1985; Hay et al. 1988; Pevear et al. 1997; Pevear 1999; van der Pluijm et al. 2001).

In sedimentary basins, the timing of hydrocarbon generation with respect to trap formation remains a primary exploration concern. The K-Ar age from illite is useful because illite forms in response to heating over the same temperature range as oil formation (Burst 1969; Perry and Hower 1972; Foscolos et al. 1976). In order for oil to have been trapped in reservoirs in an exploration area, it is critical to establish that hydrocarbon generation and migration occurred after the traps formed. If integrated geologic evaluation of outcrops or nearby wells indicate hydrocarbon generation occurred after trap formation, the risk of drilling a dry hole is reduced.

K-Ar dates from shale or sandstone are a mixture of older-than-depositional ages from detrital mica (or illite) and younger-than-depositional ages from diagenetic illite. Detrital illite is eroded from weathered slates and phyllites, whereas diagenetic