Impact of Depositional and Diagenetic Heterogeneity on Multiscale Mechanical Behavior of Mancos Shale, New Mexico and Utah, USA

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Abstract

Shales are enigmatic rock types with compositional and textural heterogeneity across a range of scales. This work addresses pore- to core-scale mechanical heterogeneity of Cretaceous Mancos Shale, a thick mudstone with widespread occurrence across the western interior of the USA. Examination of a ~100m core from the eastern San Juan Basin, New Mexico, suggests division into seven lithofacies, encompassing mudstones, sandy mudstones and muddy sandstones, displaying different degrees of bioturbation. Ultrasonic velocity measurements show small measurable differences between the lithofacies types, and these are explained in terms of differences in allogenic (clay and sand) and authigenic (carbonate cement) mineralogy. Variations in ultrasonic velocities can be related to well log velocity profiles, which allows correlation across much of the eastern San Juan Basin. A quarry block of Mancos Shale from eastern Utah, USA, a common target for unconventional exploration and ultrasonically, compositionally, and texturally similar to the laminated muddy sandstone (LMS) lithofacies of the San Juan core, is examined to sub-laminae or micro-lithofacies scales using optical petrographic and electron microscopy. This is mapped to results from axisymmetric compression and indirect tensile strength testing of this

facies at the core-plug scale, and nanoindentation measurements at the micron scale. As anticipated, there is a marked difference in elastic and failure response in axisymmetric and cylinder splitting tests relating to loading orientation with respect to bedding or lamination. Shear bands and Mode-I fractures display contrasting fabric when produced at low or high angles with respect to lamination. Nanoindentation, mineralogy distribution based on MAPS^{TM} (Modular Automated Processing System) technique, and high resolution backscattered electron images show the effect of composition, texture phases, and interfaces of phases on mechanical properties. A range of Young's moduli from nanoindentation is generally larger by a factor of 1 to 4 compared to axisymmetric compression results, showing the important effect of pores, microcracks, and bedding boundaries on bulk elastic response. Together these data sets show the influence of cement distribution on mechanical response. Variations in micro-lithofacies are first-order factors in determining the mechanical response of this important Mancos constituent, and are likely responsible for its success in hydrofracture-based recovery operations as compared to other Mancos lithofacies types.

Introduction

Shale mechanical properties under *in situ* loading determine geometry and extent of fracture networks produced during unconventional reservoir stimulation. Given that identifying "sweet spots" for horizontal drilling and well completion in such reservoirs remains a major challenge (e.g., Rickman et al., 2008), an ability to predict mechanical behavior in the subsurface can significantly improve cost effective oil and gas recovery. In addition, shale mechanical attributes determine the likelihood that a shale caprock will fracture, and thus be compromised, due to elevated pore fluid pressures caused by waste disposal or carbon storage in the underlying reservoir sandstone (Rutqvist and Tsang, 2002; Chiaramonte et al., 2008; Pasala et al., 2013; Bourg, 2015). Nonetheless, predicting the mechanical behavior of shales remains difficult, in large part due to their heterogeneity and anisotropic nature (Slatt and Abouslemain, 2011; Hart et al., 2013). Mudstone mechanical properties are controlled by a variety of geologic variables, including mineralogy, grain size, grain contacts, organic content, cementation, and the spatial distribution of these characteristics (i.e., heterogeneity). Lithology (e.g. mineralogy, grain size, grain contact, organic content, and cementation) has a major impact on mudstone mechanical properties at the macroscopic (cm) and microscopic (<mm) scales (Dewhurst and Siggins, 2006; Harris et al., 2011; Hart et al., 2013).

Previous studies have identified common shale lithofacies visible in core and outcrop, and their microscopic characteristics (Macquaker and Gawthorpe, 1993; Schieber, 1989; Macquaker and Adams, 2003; Hickey and Henk, 2007; Loucks and Ruppel, 2007; Slatt et al., 2009; Macquaker et al., 2014; Bruner et al., 2015; Lazar et al., 2015a; b; Li and Schieber, 2018). The mineralogical characteristics of such facies have been linked to mechanical properties, with the proportions of quartz, carbonate, and clay commonly cited as controlling elastic moduli which has been correlated to "brittleness" or "frackability" (Jarvie et al., 2012; Rickman et al., 2008; Wang and Carr, 2012). To our knowledge, however, few studies have mapped lithofacies at the millimeter scale, nor attempted to directly relate millimeter scale attributes to shale mechanical properties (see, e.g., Slatt et al., 2012). Such data are necessary to place small-scale mechanical measurements in a broader context and to allow the accurate determination of key multiscale constitutive properties. Additionally, the processes of fracture vary with stress state, anisotropy and microstructure of the rock. Generally, opening-mode and mixed-mode fractures have a process zone of millimeters to centimeters, and include a tensile stress state. Most proxy measurements of elastic properties and strength focus on average properties of centimeters to tens of centimeters, and are then scaled up to seismic length scales. However, a question remains as to what is the heterogeneity of shale at process zone length scales, and how does this influence fracture propagation.

Most studies of shale mechanics examine the influence of bedding or lamination direction with respect to maximum principal effective stress, but not in the context of depositional lithofacies or diagenetic effects. Fjaer and Nes (2013) study unconfined compressive strength (UCS) of Mancos Shale, noting a "plane of weakness" model adequately predicts failure and Young's moduli variation as a function of orientation. Orientation effects on elastic and inelastic behavior of shales are also examined by Gao et al. (2015), Holt et al. (2011), Ajalloeian and Lashkaripour (2000), Ibanez and Kronenberg (1993) and many others. Sone and Zoback (2013) examine various shales by linking bulk composition to static and dynamic mechanical anisotropy. In addition, nanoindentation test has been used to evaluate the impact of elemental composition and mixture phases on mechanical properties at the mineralogical scale (Ulm and Abousleiman, 2006; Deirieh et al., 2012; Abedi et al. 2016).

In this study we address the influence of scale and heterogeneity of a common shale type by describing textural and mineralogical heterogeneity of a core of Mancos Shale (Landis and Dane, 1967; Leckie et al., 1997; Ridgley, 2000; Broadhead, 2013) from the eastern San Juan Basin, New Mexico, USA, and a quarry block of Mancos Shale from eastern Utah, USA. We differentiate between bulk lithofacies at the core scale, and macro- and micro-lithofacies at the bedding and lamination and sub-lamination scale respectively. We use a variety of methods to determine geologic and mechanical attributes of the mudstone at these length scales, including ultrasonic (1 MHz) velocity measurements, optical and electron microscope petrography, and mechanical measurement with interrogation volumes ranging from 10s of centimeters to microns. Together this data set shows the importance of primary depositional, and secondary diagenetic heterogeneity (e.g., carbonate cement, clay, and porosity distributions) as first-order factors in the multiscale mechanical response of the Mancos Shale.

Geologic Background

The Mancos Shale is a dark grey to black calcareous mudstone with interbedded sandstone, reaching a maximum thickness of over 2,000 feet in the San Juan Basin (Landis and Dane, 1967; Leckie et al., 1997; and Ridgley, 2000) to over 5,000 feet in the Uinta and Piceance Basins (Hettinger and Kirschbaum, 2003). Much literature considers Mancos Shale deposition in the Late Cretaceous Interior Seaway primarily in offshore and open-shallow marine environments (Hazenbush, 1973; Fassett, 1974; Hettinger and Kirschbaum, 2003; Li and Schieber, 2018) with sediments sourced from the Sevier Orogeny to the west (Hettinger and Kirschbaum, 2003; Edwards et al., 2005). Recent work considers that much of the laminated lithofacies within the Mancos to representative of prodeltaic hyperpycnal or turbiditic deposition along mud-dominated coastlines (Bhattacharya and MacEachern, 2009). The Mancos Shale has moderate to low TOC (total organic carbon; less than 2% in shelf marine systems tract and 2-5% in transgressive systems tracts) and is commonly thought to be a source rock within Cretaceous Interior Seaway basins (Pasley et al., 1991; Ridgely, 2000). It intertongues with several groups or members of limestone, marine and coastal sandstones, as well as non-marine fluvial deposits (Landis and Dane, 1967; Hazenbush, 1973; and Hettinger and Kirschbaum, 2003).

Samples of the Mancos Shale described in this study include a cored interval from the Davis-Federal 3 No. 15 well, located in the eastern San Juan Basin, Rio Arriba County, New Mexico (Figure 1) and detailed in Weatherford (2010) and Rosandick (2014). Cored portions described herein include the lower part of the Upper Mancos Shale and the upper portions of the Lower Mancos Shale, as described by Ridgely (2000) after Molenaar (1974) and Pentilla (1964). While we have used the stratigraphy of Ridgely (2000), the stratigraphic correlation of the Tocito-El Vado-Gallup Sandstones is plagued by large, relatively unexplained erosional gaps in the geologic record and a lack of tightly constrained biostratigraphy (Nummedal and Molenaar, 1994; Cheney et al., 2016). In stratigraphic order from oldest to youngest, units/members of the cored interval are: the Middle Shale Unit, the Cooper Arroyo Sandstone Member (equivalent to the Tocito Sandstone Member of Ridgely, 2000, and the Smoky Hill Member in the Mancos Shale reference section of Leckie et al., 1997), and the El Vado Sandstone Member (Figure 1; Emmendorfer, 1992). The base of the Cooper Arroyo Sandstone Member is hypothesized to correspond to the Carlile-Niobrara Unconformity (Dane, 1960; Lamb, 1968) which represents a low stand between the R5 regression and T6 transgression of Kauffman (1977), or, equivalently, the boundary between Turonian and Coniacian stages (Leckie et al., 1997; Nummedal and Molenaar, 1994). The Cooper Arroyo represents deposition in an offshore bar environment (Molenaar, 1977). Several offshore bar muddy sandstones have been referred to as transgressive Gallup, Tocito, or basal Niobrara sandstones (Molenaar, 1974; 1977). The Cooper Arroyo Sandstone Member is also described as being a transgressive lens of basal Niobrara sandstone (Molenaar, 1977).

In addition to the Davis Federal 3 No. 15 core, we examine a block of Mancos Shale quarried near East Carbon, Utah, USA, from a silty/sandy interval in the Ferron Tongue in the upper Mancos Shale (Peter Nielsen, Utah Geological Survey, Personal Communication, 2018). The Ferron Tongue more proximal to the paleo-coast corresponds primarily to a prograding delta-mouth bar depositional environment, or a series of clinoformal, interbedded sandstone-mudstone beds dipping into the seaway (Enge et al., 2010). The quarry block appears to be distal offshore hyperpycnal/turbiditic deposits, similar to the LMS facies of the Davis Federal 3 No. 15 core. The Ferron Tongue is Turonian in age, and has an erosional contact at its top, which is the unconformity between Turonian and Coniacian stages (i.e., the Carlile-Niobrara Unconformity of above; Leckie et al., 1997; Nummedal and Molenaar, 1994). The quarry block of the Ferron Tongue permitted us to obtain many samples for mechanical testing from a lithofacies commonly used as a unconventional reservoir in the Mancos Shale and its equivalents through much of the Cretaceous North American Inner Seaway.

Methods

Core Description and Logging

An exceptionally intact shale core taken from the Davis Federal 3 No.15 well in Rio Arriba, New Mexico (Figure 1) was obtained from the New Mexico Bureau of Geology and Mineral Resources Core Library. The core spans an interval of 341.70 feet (7076.50 ft to 7418.20 ft below ground surface; 104.2 m) with very few missing sections. Facies were assigned based on visual description within the core library. Sections of core containing natural fractures were also described and sampled for analysis. Electric logs taken from the Davis Federal 3 No.15 well (and other wells of interest) were examined and assessed for quality control. Well logs (in the form of scanned paper images) were accessed and digitized from online files on the Oil Conservation Division of the New Mexico Energy, Minerals and Natural Resources Department. For this study we focus on gamma ray, caliper, and sonic logs. Details on core descriptions and well log analysis can be found in Rosandick (2014).

Quarry Block Handling

Mancos Shale samples for characterization and mechanical testing were taken from a cylindrical quarry block provided by Schlumberger/TerraTek, measuring 30 cm in height by 40 cm in diameter and encased in wax. Prior to description of the rock, the block was cut into several blocks using a quarry diamond wire saw with mineral oil lubricant. After cutting, cut faces were immediately dried and cleaned with isopropanyl to limit wetting by oil. Details of the block sectioning and analysis can be found in Grigg (2016).

Ultrasonic Measurements

Compressional (P-wave) and shear (S-wave) wave velocities were measured using an Olympus® HV Pulser/Receiver set to a 20 Hz pulse repetition rate and 1 MHz resonant-frequency transducers. The transducers and samples were coupled with pistons pressurized to 40 psi with compressed air, and by applying corn syrup to transducers before measurement. The distance between transducers were measured using a Fowler & NSK® Max-Cal 0.001inch-resolution electronic digital caliper. Details on the ultrasonic measurements can be found in Rosandick (2014).

Macroscopic Characterization

Macroscopic characterization on the block samples was performed following the workflow of Lazar et al. (2015b). The relative amount of clay and silt within the fine-grained intervals was determined using a "scratch test" by scratching the clean surface with a steel knife and then observing the scratch luster and the powder color as described by Lazar et al. (2015a). After observation of grain size, beds were classified according to a textural classification scheme of Lazar et al. (2015a) by Grigg (2016). Additional features noted include degree of bioturbation, skeletal grains, organic content, sedimentary structure, fractures, and estimations of proportions of clay, carbonate and quartz. For macroscopic classification all sides of the quarry block sections were scanned with a flatbed scanner at 600 dpi resolution. Classification maps were produced by highlighting macroscopic lithofacies by color; detailed descriptions are found in Grigg (2016).

Microscopic Characterization

Oriented thin sections were prepared by Wagner Petrographic™ from slices of the core block mapped to locations, with one set perpendicular to the other. Each thin section was paired with a facing "billet" or small parallel piped of the sample. All thin sections and facing billets were polished and impregnated with epoxy dyed with rhodamine fluorochrome. One thin section was selected for a detailed textural and compositional study, and divided into preliminary lithofacies boundaries by observations of texture changes within lamina based on optical analysis. Observations of texture (including mean grain size, degree of bioturbation, fossil identification, organic content, sedimentary structure and fractures) and composition were performed. Each preliminary micro-lithofacies were then analyzed following a procedure detailed in Grigg (2016).

Polished, carbon coated thin sections were analyzed using a CAMECA® SX-100 electron microprobe equipped with back-scattered and secondary electron detectors. Three WDS spectrometers were used for quantitative chemical analysis using a 15-kV beam. For micron-scale characterization, 2-3 mm thick samples were prepared from billet samples. Each sample was polished by argon ion milling (Fischione 1060 SEM Mill) and then analyzed with backscattered electron scanning (BSE) and energy dispersive spectroscopy (EDS). The MAPS (Modular

Automated Processing System) platform (ThermoFisher Scientific^{TM}) was used for SEM-based automated mineralogical measurement, analysis, and data integration. With spectral matching of EDS data each pixel was identified as single or multiple minerals. In this work we employed BSE and EDS analysis at 0.2 or 2 μm and 2 or 20 μm resolution, respectively.

Axisymmetric Compression Tests

A series of axisymmetric compression testing determine mechanical properties of 2.54 cm (1 inch) diameter and 5.48 cm (2 inch) length core plugs sampled at mapped locations within the quarry block. Testing was performed to characterize the mechanical anisotropy of Mancos Shale samples in two primary directions, parallel and perpendicular to bedding/lamina, and to examine differences in fracture behavior associated with loading in these two directions. The test matrix consisted of five experiments each in parallel and perpendicular directions to lamination orientation, including one unconfined, three confined, and one hydrostatic conditions. All axisymmetric compression tests with confinement were performed under constant mean stress conditions from 45 MPa to 200 MPa to allow tracking of shear moduli during deformation.

For all testing, core plug samples were stored immediately after coring in a chamber held at a constant humidity of 70% (non-condensing) for at least two weeks. This ensured that moisture content was consistent between samples. During testing, humidity was maintained by placing a salt solution (~5 molal calcium nitrate) at the bottom of a desiccator column (with the desiccant removed) so that flow into or out of the sample passed through the 70% relative humidity environment. During testing samples were vented to atmospheric pressure with vent line held at 70% relative humidity to ensure that samples did not dry out during testing.

Samples were instrumented with four LVDTs prior to testing. Two axial gages mounted on halos were attached to the top and bottom endcaps affixed to the sample. Two LVDTs were spring-mounted on rings placed around the center of the sample to measure changes in diameter. When samples were cored parallel to bedding one of these sensors was placed parallel to bedding, and one placed perpendicular to the bedding plane. This assembly was placed inside a pressure vessel and installed within a load frame. Pressure inside the vessel was raised at a rate of 0.2 MPa/s to a pre-determined mean stress. During hydrostatic pressure increase, unload-reload loops were performed to determine changes in bulk modulus of samples at different mean stresses and strain conditions, and to ensure consistency between samples. After the desired mean stress was achieved, loading was switched to axial displacement control with a piston advancement rate of 10^{-5} in/sec while confining pressure lowered to maintain a constant mean stress. Changes in shear moduli were enabled from unload-reload loops along the constant mean stress path. This procedure continued (again with unload-reload loops) until peak stress was achieved followed by stress drop. This occurred in all cases except the hydrostatic. Tests were typically allowed to run slightly longer after failure to ensure that a failure feature or shear band was visible and there was not secondary failure after the primary stress drop.

Two samples were examined to characterize post-failure features using a North Star Imaging X50 micro-computed tomography (μCT) scanner with a Varian Medical Systems PaxScan 2520DX detector, using a 220KV-vortex scan and 30 μm voxel size. Following scanning, the samples were unjacketed and one of the facing shear band facets was scanned using a Nanovea ST400 White Light Profilometer with 5 μm resolution.

Indirect Tension (Brazilian) Tests

Four disks of Mancos Shale, measuring 2.54 cm in diameter and 1.27 cm thick, were prepared and tested for indirect tensile strength. As in the axisymmetric testing, samples were cored parallel and perpendicular to the bedding direction. To evaluate the impact of anisotropy, two samples cored parallel to the bedding were loaded at 45° and 90° with respect to the bedding direction, while two samples cored perpendicular to the bedding were loaded parallel to the lamination direction. Displacements were measured with a platen-mounted extensometer. Samples were cushioned between the edge of the sample and the platen interface with a single thickness of masking tape (to reduce stress concentration at the loading point and to contain the sample after failure). Tests were performed at a rate of 2×10^{-6} mm/sec, with failure occurring approximately 2.5 minutes after contact, just within the rate limits of ASTM D3967-8 (2008). After testing, post-analysis consisted of thin-section analysis of crack features and detailed analysis of BSE and MAPS for one sample loaded at 45° with respect to the bedding direction.

Nanoindentation

Nanoindentation of ion-milling polished Mancos Shale was conducted on a Hysitron TriboIndenter 900 using a Berkovich geometry diamond tip. Indentation was performed at multiple locations within the clay-rich areas based on the BSE and MAPS analysis in a 5 × 5 grid array of indents spaced 20 μm apart with an indentation strain rate of 0.1 (Lucas, 1997) to a maximum load of 10 mN. Individual hardness and modulus measurements were computed using the standard Oliver-Pharr method (Oliver, 2004) where hardness, *H*, can be found from

$$H = \frac{P_{max}}{A} \qquad (1)$$

where P_{max} is the maximum load for the indentation cycle and A is the contact area. The reduced indentation modulus, E_r is

$$S = \beta \frac{2}{\sqrt{\pi}} E_r \sqrt{A} \qquad (2)$$

where S is the stiffness, and β is a geometrical constant that is equal to 1.14 for a Berkovich tip. The stiffness was calculated as the slope of initial unloading stage where it is assumed that the initial unloading is purely elastic (Doerner and Nix, 1988; Oliver and Pharr, 1992).

The plastic zone size underneath a Berkovich indent was estimated following (Chen and Bull, 2006) where

$$\frac{R_p}{\delta_m} = -12.907\frac{H}{E_r} + 4.5451 \qquad \frac{H}{E_r} < 0.35 \qquad (3)$$

R_p is the plastic zone radius and δ_m is the maximum displacement. This equation is valid for H/E_r ratios less than 0.35. Plastic zone volume is estimated by assuming a hemispherical region, $V = (4/3)\pi R_p^3$. After testing, each indentation was imaged using a FEI Helios Nanolab G3 CX DualBeam FIB/SEM at 6.7 nm resolution.

Results

Lithofacies Description and Sonic and Ultrasonic Properties of the Davis Federal 3 No. 15.

Nomenclature

The nested scales of bedding structures of shales challenge current sedimentary nomenclature. In our study, we focus on lithofacies that range in scale from the 10s or 100s of microns to the meter scale. Traditionally, lithofacies are described in terms of beds (> 2 cm thick) and lamina (< 2 cm thick). However, the sedimentary structures of the quarry block display complicated lateral relationships between grain-size, degree of lamination, cross-bedding, and overprinting of bioturbation and soft sediment deformation. As cm-scale sedimentary structures are constructed from smaller, sub-mm-scale sedimentary structures, lithologic variations within a bed and even within a lamina can be simplified into hierarchically scaled sets of lithofacies. For the purposes of this work, we define three scales of lithofacies: a *bulk lithofacies*, which we use to break out variations in core behavior, and will use to describe the entire quarry block; *macro-lithofacies*, which occur in mm- to cm-scale sedimentary structures; and *micro-lithofacies* found in sub-mm-scale sedimentary structures. Each higher level is made up of the next levels down. This classification allows us to discuss the architecture and scaling of mechanical variations systematically, without blurring between sedimentary structural scales.

Core Lithofacies Identification

Detailed observation of composition, grain size, sedimentological features, and degree of observable bioturbation yields seven identifiable lithofacies in the Davis Federal 3 No.15 core, and, arranged in order of decreasing sand content, these are (Rosandick, 2014): (1) laminated, muddy sandstone (LMS); (2) highly bioturbated, muddy sandstone (HBMS); (3) bioturbated, sandy mudstone (BSM); (4) moderately bioturbated mudstone (MBM); (5) fossiliferous, laminated mudstone (FLM); (6) bioturbated, fossiliferous mudstone (BFM); and (7) nonfossiliferous, strongly bioturbated mudstone (NSBM); (Figure 2). In general, the sandier LMS and HBMS facies can be recognized based on the negative gamma ray kick and the largest values of slowness (ΔT) amongst the lithofacies, and are more abundant above the Carlile-Niobrara unconformity. For the sonic and ultrasonic measurements to follow, it suffices to group these lithofacies into muddy sandstone (LMS and HBMS), sandy mudstone (BSM), and mudstone (FLM, BFM, and NSBM) categories.

Overall, the lithofacies within the Davis Federal 3 No.15 core appear to fall into the FAS-1 succession of Bohacs et al. (2014). This is storm-wave dominated based on the abundance of sedimentary structures that typify FAS-1. However, the core is dominated by the medial to distal facies and does not display an entire succession from proximal to distal. Some sections of the core display subtle, gradational changes between lithofacies that makes it difficult to define precise boundaries. Nonetheless, these lithofacies can be correlated across the eastern portion of the San Juan Basin (Rosandick, 2014). Having identified lithofacies variation in the core, we investigate the role of depositional differences in controlling velocity variations, as suggested by the range in slowness observed in the sonic log.

Ultrasonic Velocities of Lithofacies and Comparison to Well Log Sonic Velocities

A total of 189 core samples were analyzed for P- and S- wave velocities, and are plotted alongside sonic and gamma ray logs in Figure 3 in terms of slowness, the inverse of velocity. These measurements were taken at intervals of about five feet along the entire core and about six inches along two 30- ft intervals of the core (labeled “a” in Figure 3; see Appendix A in Rosandick, 2014). These two 30-ft intervals helped determine whether the five-ft sample spacing would be adequate for comparison to electric logs. The detailed sections of core were also sampled using a narrower sample size (between 0.5 and 2.0 inches in vertical height) for consistency purposes.

All compressional (orange dots) and shear (green dots) slowness measurements taken along the five-ft spacing of core samples both perpendicular and parallel to bedding are displayed in Figure 3. Sonic slowness from well logging is plotted by the red line. The entire core interval shows large fluctuations in both compressional and shear slowness perpendicular to, and less variation parallel to, the lamination direction. The sonic log changes a maximum of ~25 μs/ft across the same interval of core and shows much less variation in comparison to the “perpendicular” core velocity measurements, but a similar variation compared to the “parallel” measurements. However, the sonic log appears to generally align with perpendicular measurements that had fast travel times (further to the left on the sonic log), despite the differences in frequencies of the two methods. In general, the “parallel” measurements show a consistently lower slowness compared to the sonic log. The agreement between sonic log response and velocity measurements is surprising given the different frequencies of the laboratory transducers and sonic logging tool, the damage associated with coring and storage of the core, and uncertainties inherent in determining travel times in small samples.

To the left of the log profiles, we plot lithofacies in terms of the three major types, and suggested “mechanical facies” on the basis of velocity response and amount of sand. Historical production in the San Juan Basin to date would suggest that the sandier portions of the Mancos Shale are targeted more frequently for unconventional exploration (Ridgley, 2000). As shown by Rosandick (2014), these mechanical facies can be traced regionally in the eastern San Juan Basin. Also in

Figure 3, we show interpretations of transgressive (arrows advancing to the right and up) and regressive (arrows advancing to the left and up) sequences, which could aid in placing the Davis Federal 3 No. 15 lithofacies distributions across a broader regional framework in the San Juan Basin, but this is beyond the scope of our study.

In Figure 4, we plot P- and S-wave velocities as a function of lithofacies type, measured perpendicular and parallel to primary lamination direction. P-waves are the upper values, and S-waves the lower values per lithofacies. The box and whisker plot brackets show the upper and lower range in observed velocities. The median value in velocity from the measurements is represented by the line between the colored boxes, with the grey box displaying the upper quartile and the orange box showing the lower quartile. In general, there is much less variability in the "parallel" velocity measurements, which, as shown in Figure 3, are higher (or lower in slowness) than the "perpendicular" measurements. While there is not a major difference in median values across the lithofacies types, the sandier LMS and HBMS lithofacies have slightly lower compressional velocity magnitudes compared to the MBM, NSBM, BFM and FLM mudstone lithofacies.

Ultrasonic measurements were made on a few Davis Federal 3 No.15 samples by Weatherford (2010) during axisymmetric compression (ASC) testing at 21 MPa confining pressure, and are compared to our measurements and those calculated from the sonic well logs in Table 1. The results from ASC testing are about 400 m/s higher than sonic log values, and over 1000 m/s higher than bench top measurements. The depths of sonic measurements yield an estimate of in situ effective confining pressure (i.e., confining pressure minus pore pressure) of roughly 25 MPa (using gradients of pore pressure of 0.010 MPa/m and confining pressure of .022 MPa/m), so these results are roughly comparable. The bench top measurements were performed under unconfined conditions, and so would be expected to have lower velocity magnitudes associated with open microcracks and slit-like pores that would close under confining pressure. It is possible that the values from Weatherford (2010) reflect a sampling bias, in that measurements were restricted to portions of the core that could withstand drilling plugs (and commensurate higher velocity magnitudes), which is notoriously difficult for even the most lithified shale.

Mechanical Behavior of the LMS Lithofacies in the Quarry Block

Ultrasonic Behavior of Quarry Block Samples

Using the same techniques as for the Mancos Shale Davis Federal 3 No.15 core, we measured P- and S-wave velocities on a representative one-inch diameter and two-inch length core plug of the quarry block as a function of angle from main lamination direction (for the "parallel to lamination" case), and from an arbitrary chosen plane in the "perpendicular" to bedding case (Figure 4C). There is not large dependence on angle observed in the data. In general, values of velocities of the LMS lithofacies in the quarry block fall into lower portions of the range measured for the LMS lithofacies of the Davis Federal 3 No. 15 core. Despite the geographic separation of these two Mancos Shale samples, these results may suggest that we can gain understanding of the static geomechanical properties of this important Mancos lithofacies applicable to a wide region in the intermontane western U.S. by examining in detail the behavior of the quarry block.

Macro- and Micro-Lithofacies Interpretations

Because the LMS lithofacies is an important constituent of the Mancos Shale Davis Federal 3 No. 15 core as shown above, and important as well for oil and gas exploration and production in the San Juan Basin (Ridgley, 2000), we examine static and dynamic geomechanical properties of this lithofacies in detail in the following section. The quarry block, shown in Figure 5A, was cut into sections to examine lateral continuity and extent of heterogeneity. The so-called "large block" in Figure 5A (Grigg, 2016) was used to obtain small core plugs for geomechanical testing; the locations of all plugs are mapped in Grigg (2016, Figure 30) and shown approximately in Figure 5A and E.

The Mancos Shale quarry block (Figure 5A), overall consistent with the LMS lithofacies designation in the Davis Federal 3 No.15 core described in previous sections, consists of interlaminated fine mud, medium/coarse mud, and very fine sand and silt (Grigg, 2016). These constituents form thin 1-3 mm medium/coarse mud and very fine sand parallel lamina, wavy-lenticular lamina, and ripple forms with fine mud lamina. To distinguish the block descriptions from the larger scale lithofacies designations used in the core in previous sections, we delineate macro-lithofacies at the mm- to cm-scale, definable by visual inspection, and micro-lithofacies at the sub-mm scale, discernable by investigation with optical microscopy and applicable to scales associated with individual laminae. Macro-lithofacies include medium Mudstone (mM), sandy medium Mudstone (smM), sandy coarse Mudstone scM, and muddy Sand (mS), Fig. 5B, after Grigg, 2016). Sand grains within samples fall within the very fine range (62.5-125 µm). The mM lithofacies is often associated with lenticular mS. Sandy medium mudstone (smM, dark green in Figure 5B), sandy coarse mudstone (scM; light green in Figure 5B) and medium mudstone (mM, light blue in Figure 5B), are visible in a plane-light photograph in Figure 5C and laterally continuous through the entire core sample. Figure 5B depicts sedimentological and bioturbation features observable in the macro-lithofacies types. The mixed mS and scM macro-lithofacies contain common ripple forms and planar laminae, whereas the mM lithofacies is dominated by planar laminae. Bioturbation features interpreted by Grigg (2016) are common in the smM and mM mudstone lithofacies.

Thinner layers of mixed muddy sandstone and sandy coarse mudstone are laterally discontinuous (yellow patterns in Figure 5B). A larger view of the so-called "core-block" portion of the quarry block shows that these macro-lithofacies descriptions are continuous throughout the quarry block (Figure 8 in Grigg, 2016). Also, continuous throughout the quarry block are two large lamina-parallel extension fractures approximately one-thirds and two-thirds vertically through the quarry block, with smaller fractures extending off and interacting with these main fractures (Figure 5D). All fractures contain carbonate and/or trace sulfate cement (calcite, dolomite, gypsum and barite are observable as fracture-fills, Grigg, 2016), suggesting that these are natural fractures produced either at depth or associated with weathering processes in the near-surface, and not associated with the quarry block drilling.

Locations for sub-sampling for X-ray diffraction (XRD) analysis are shown in Figure 5B. Methods for XRD analysis are discussed by Grigg (2016). The bulk mineralogical results of the phases found within each macro-lithofacies (Table 2) do not vary widely, as seen in the quartz, carbonate, and clay (QCC) ternary diagram (Figure 6A). This is also illustrated by the limited range of phase values between samples. The apparent lack of mineralogical diversity in samples 1-9 (Figure 5B) may be due to the inability to separate samples directly on macro-lithofacies boundaries (sample contamination), or more likely because macro-lithofacies are made of the same micro-lithofacies in different proportions. The fracture fill sample (10) does contain sample from the surrounding lithofacies so it does not give a good estimate of the fracture fill composition (Grigg, 2016). Based on XRD results, the macro-lithofacies in the quarry block would be categorized as siliceous mudstone based on the scheme of Ulmer-Scholle et al. (2014) as shown in Figure 6A.

Micro-lithofacies were identified based on point count analysis of several thin sections; these definitions are important for the mechanical testing results to follow. For the purposes of our study, we show results of the thin section "A5" of Grigg (2016), presented in Table 3 and plotted in the ternary diagram (after Lazar, 2015a) in Figure 6B to define the micro-lithofacies designations. The identified microfacies include fine mud (fM), medium mud (mM), sandy medium mud (smM), sandy coarse mud (scM), and muddy sand (mS). Each of these micro-lithofacies are illustrated in thin section A5 in Figure 7A and in photomicrograph in Figure 7B. For example, the fM micro-lithofacies is found in intervals 2, 5, 7, 9, 11, 13, 15, and 18 of Figure 7A and is matrix-supported with mixed clay content. Intervals 5, 7, 9 and 13 contain planar laminated fM. Intervals 15 and 18 show bioturbation features and interval 11 shows possible ripple forms and bioturbation. This lithofacies consists of 7 to 14% identifiable quartz, about 1 to 8% carbonate, and 71 to 80% clay (non-normalized data). The fM micro-lithofacies has organic matter ranging from about 2 to 4.5% and appearing as thin elongate features that run up to 1mm along bedding planes (Figure 7B). Normalized amounts of carbonate, clay, and quartz of micro-lithofacies determined from MAPS^{TM} data of quartz+feldspar+pyrite (QFP), clays, and carbonates are plotted in Figure 6C. These all plot in the "siliceous mudstone" field of Ulmer-Scholle et al. (2014), and display a similar range in composition to the macro-lithofacies. Both macro- and micro-lithofacies plot in the "brittle" field delineated by the blue lines as described by Ulmer-Scholle et al. (2014). We explore the influence of lithofacies type on mechanical response in the next sections.

<u>Axisymmetric Compression Testing of LMS Lithofacies</u>

One-inch (2.54 cm) diameter and two-inch (5.08 cm) length core plugs from the quarry block were sampled from portions of the quarry block sufficiently far from the through-going fractures (Figure 30 in Grigg, 2016). Visual inspection suggests that samples of this size, while extremely heterogeneous, contain similar proportions of the macro- and micro-lithofacies. These core plugs were subjected to differing stress paths in ASC testing configuration, listed in Table 4, with results summarized in Figures 8-10. Overall, all the samples tested, up to 200 MPa mean stress (except those loaded hydrostatically), demonstrate dilatant behavior prior to failure (note the "turn-around" between compaction and dilation in volume strain by the green curves in Figure 8A-D), and in none of the sample testing did we observe any indication of pore-collapse. The small lines extending beneath the main stress-strain curves are unload-reload loops performed to monitor the evolution of elastic parameters up to and just preceding, sample failure. The change in these parameters with stress is discussed below; there is some evidence of modulus degradation due to post-yield plastic strain (Dewers et al., 2017).

Overall, stress-strain results in Figure 8 show that samples loaded parallel to bedding ($S_{l\parallel}$) have lower axial strain, but higher volumetric strain, compared to those loaded perpendicular to bedding ($S_{l\perp}$) except under the hydrostatic condition. Experimental results also show that $S_{l\perp}$ have more lateral expansion at failure, while $S_{l\parallel}$ have more lateral compression under confined conditions until stress exceeds apparent yield points. All the samples tested (except those loaded hydrostatically) demonstrated dilatant behavior prior to failure. In addition, $S_{l\parallel}$ under confined conditions have higher failure strength than $S_{l\perp}$, and vice versa under unconfined condition. These anisotropic behaviors clearly demonstrate that deformation and strength are closely related to the loading orientation with respect to the bedding direction and confining pressure.

Visual measurements of the primary fracture after failure (Table 4) reveal that the fracture angle with respect to the axial loading direction increased with increasing confining pressure for both $S_{l\parallel}$ and $S_{l\perp}$. Fracture planes were steeply inclined with respect to the axial direction of the sample regardless of the bedding orientation and $S_{l\parallel}$ tend to have steeper fracture angles than $S_{l\perp}$. For $S_{l\parallel}$ unconfined sample (16B), the fracture angle of 4° with respect to the vertical loading direction was apparently aligned with the lamination direction, indicating the major failure mechanism would be due to the extension of the lamination plane. This can be seen in Figure 8A where lateral strain 2 for sample 16B was measured perpendicular to bedding. Interestingly, unconfined sample 32A ($S_{l\perp}$) also has a high fracture angle (6°) and strong dilation behavior on the volumetric strain curve in Figure 8A suggests fracturing through the bedding layers.

Change of fracture angle under confined conditions can be also correlated to stress-strain behaviors (Figure 8B-D). With a constant mean stress of 45 MPa (Figure 8B), $S_{l\parallel}$ (15B) shows significantly less strain in the individual directions, but more volumetric strain than $S_{l\perp}$ (28A) due to the disproportion of the strains in the axial and lateral directions. Both samples experienced brittle failure, with relatively steep fracture angles. With a constant mean stress of 100 MPa (Figure 8C),

$S_{l\parallel}$ (12B) shows a relatively stiffer volumetric strain curve after dilation and less strain in each direction than $S_{l\perp}$ (25A), indicating this Mancos Shale is more ductile perpendicular to bedding. Both samples demonstrate increased strain to failure with a stress peak followed by a small stress drop, compared to the 45 MPa mean stress tests. With constant mean stresses of 200 and 160 MPa for $S_{l\parallel}$ and $S_{l\perp}$, respectively (Figure 8D), $S_{l\parallel}$ (14B) shows a response similar to $S_{l\parallel}$ (12B) at 100 MPa mean stress with a peak followed by a small drop in the stress-strain curve. However, $S_{l\perp}$ (22A) shows no peak and drop behavior, and the response is simply a "roll over" into a near-constant stress plateau. This sample formed a much lower angle of shear band from the horizontal direction than the rest of the samples (see Table 4), indicating that at this mean stress the samples are very close to switching from a dilatant to compactive failure regime.

Samples 14A ($S_{l\parallel}$) and 29A ($S_{l\perp}$) were tested hydrostatically over a range of stress conditions (Figure 8E). These samples showed no signs of compactive failure up to the maximum applied stress, indicating that a higher mean stress needs to be applied to achieve pore collapse or even shear-enhanced compaction. Thus, all samples tested fall into the so-called brittle regime.

The loci of peak stresses, along with results of indirect tensile testing, together form failure surfaces applicable to parallel or perpendicular loading as shown in Figure 9A. At low mean stresses the two surfaces coincide, deviating at mean stresses above 50 MPa. Testing results of Weatherford (2010; solid symbols in Figure 9A) show that Davis Federal 3 No.15 core lithofacies, and in particular the LMS lithofacies, are slightly stronger than the quarry block LMS lithofacies. It is likely that uplift and weathering of the quarry block sample has weakened it slightly, and this is most likely evident from the microfractures observed in the block in Figure 5D.

Evolution of elastic moduli along stress paths up to failure, determined from unload-reload loops, is shown in Figures 9B-D. Young's modulus and Poisson's ratio measured directly from the two unconfined tests is presented in Figure 9B. In both directions with respect to bedding, Young's modulus increases with increasing stress with $S_{l\parallel}$ samples showing a slightly larger Young's modulus than $S_{l\perp}$. Poisson's ratio for the material also varies depending on sample layer directions, ranging from 0.18 to 0.4 for $S_{l\perp}$ and 0.15 to 0.22 for $S_{l\parallel}$. Figure 9C shows bulk moduli increase as a function of mean stress for both bedding orientations, with slightly larger increases perpendicular to bedding. Shear moduli increase slightly with mean stress, and may decrease slightly with increasing plastic strain, especially at tests run at higher mean stresses, although we do not quantify this effect here (Figure 9D).

Characterization of Fractures from ASC Testing

Fracture morphology of shear bands produced during failure of samples 12B ($S_{l\parallel}$) and 22A ($S_{l\perp}$) are shown in Figure 10 both by μCT (Figure 10A-B) and white-light profilometry (Figure 10C-D). μCT reconstructed image of fractures for sample 22A (Figure 10A) shows a major through-going, roughly planar, shear fracture from upper right to lower left, along with several smaller conjugate shear fractures at roughly 30 to 40 degrees from the main fracture. In contrast, sample 12B, deformed parallel to bedding, shows only a single, roughly planar, through-going fracture. The differences in fracture morphology can be seen by comparing Figure 10C and D: Figure 10C (sample 22A) displays much more fracture roughness and ancillary fractures (blue inset) at relatively high angle from the main fracture plane, compared to Figure 10D (sample 12B) which shows ancillary fractures sub-parallel to the main fracture plane (blue inset).

Thin section images (samples 15B for $S_{l\parallel}$ and 28A for $S_{l\perp}$ with mean stress of 45 MPa from Figure 8B) link microscale fracture patterns to micro-lithofacies distributions (Figure 11). For each sample, two thin sections were analyzed with one through the central horizontal plane, crosscutting the main shear fracture, and the other through the vertical plane, aligned with the main fracture. For the 15B $S_{l\parallel}$ sample, the horizontal thin section through the central portion of the core sample shows one primary fracture and two secondary fractures. Regions of interest (ROI) 1 and 2 show fracture intersection and bifurcation, with small-aperture microfractures crosscutting micro-lithofacies. Larger, sub-laminae parallel fractures tend to follow boundaries between sandier and more clay-rich micro-lithofacies. ROI 3 and the accompanying blow-up show that microfractures propagate in between quartz grains, but through clay-rich micro-lithofacies. ROI 4 and 5 in the vertical thin section show that microfracture splays off of the main fracture, where displacement is accommodated by several bifurcations in between quartz silt grains and across organic and clay-rich portions.

For sample 28 A ($S_{l\perp}$), the horizontal thin section reveals that the through-going main fracture is curved, with ROI 1 and 2 displaying similar microfracture patterns splaying in between quartz grains. ROI 3 in the vertical thin section shows a microfracture cross cutting the fM micro-lithofacies into a scM micro-lithofacies, with decreasing aperture. In the sandier layer, the opening displacement is accommodated by multiple microfractures with smaller apertures compared to the single fracture in the clay- and organic rich fM micro-lithofacies. ROI 4 shows a similar pattern with a single microfracture in the fM bifurcating into two smaller aperture microfractures in the scM.

Indirect Tensile Testing

Four indirect tensile strength tests (commonly known as Brazilian tests) were performed with two samples cored parallel and two cored perpendicular to bedding, to measure indirect tensile strength and to observe effects of micro-lithofacies on crack initiation and propagation. The two samples cored perpendicular to bedding were cored from two different lithologies. Sample 14 was cored from mM with some mS lenses. Sample 18 was cored in the mM, smM and mS/scM lithofacies. Cored parallel to bedding, sample 24 contains scM/mS and mM and sample 25 contains the scM macro-lithofacies. Figure 12A shows thin section images of each sample post-testing, with corresponding mapped micro-lithofacies. Sample 14, loaded at a 45° angle to lamination direction, experienced failure at the lowest stress (2.6 MPa) and low displacement (0.0037 mm) relative to the other samples. Sample 18, with laminations perpendicular to the loading direction, experienced an intermediate failure stress (4.5 MPa) and high displacement (0.00054) compared to the other samples. Sample 24, with laminations parallel to the vertical loading direction, resulted in moderate failure stress (4.7 MPa) and low displacement (0.00035) compared to the other samples. Sample 25, with laminations parallel to the loading direction, experienced relatively higher failure stress (6.5 MPa) and low displacement (0.00039) compared to the other samples tested. These tests produced comparable results as observed in the ASC tests in that the sample loaded perpendicular to laminations experienced the most displacement prior to failure, and the samples loaded parallel to laminations failed at higher stresses.

Figure 12B shows the mineralogical distribution of thin core sample polished by ion-milling using the MAPS, strain patterns imaged using digital image correlation (DIC), and an example of phase field modeling results. The detailed description of the experiments, digital image correlation, and phase field modeling results was reported in Na et al. (2017). The thin section image shows tensile strain occurring near the loading points (top area filled with a pink epoxy) and then along the boundary between clay-rich micro-lithofacies and sandy micro-lithofacies. This is shown in the mineralogy mapping with clay-rich layers (mostly illite and illite-smectite). A transition area from fracturing in the clay-rich to the vertical crack is highlighted in back scattered electron image and mineralogy mapping at 1-micron resolution. Based on digital image correlation and numerical modeling results, fractures initially develop near the loading points on top and bottom, but propagated along the interface of fine-grained (fM) and coarse-grained layer (mS) in the upper region. On this particular facet, a vertical crack originating from the lower region merged with an inclined crack before failure. The other thin section of this sample shows the inclined crack developed to the boundary of core sample along the interface between fine-grained and coarse-grained layers without the fully developed vertical crack. As discussed by Na et al. (2017), millimeter scale features such as layer orientation, thickness, volume fraction and defects influence the onset, propagation and coalescence of fractures. In addition, spatial heterogeneity and material anisotropy highly affected crack patterns and effective fracture toughness, and the elastic contrast of the two constituents significantly alters the effective toughness.

Nanoindentation Testing

To augment the associations between fracture propagation behavior and micro-lithofacies distributions, we performed nanoindentation testing along two vertical traverses at differing resolutions on an ion milled sample containing fM, mM, cM, smM, scM, and mS micro-lithofacies (Figure 13A); the yellow rectangle outlines a region analyzed at 20-micron resolution, and the red rectangle outlines a region analyzed at 2-micron resolution using MAPS (Figure 13B). Based on mineralogy mapping, nanoindentation testing corresponding to a peak loading of 10 mN was performed to directly link compositional heterogeneity to mechanical properties (Figure 13 C&D). The elastic properties of indentation results over two 5x5 grid areas in mM micro-lithofacies are shown in Figure 13 E&F. Two commonly used mixture models (Voigt and Reuss) have been used to estimate the upper and lower bounds of elastic modulus values weighted by the area of each mineral observed over the plastic zone area computed from Eqn. (3). This comparison demonstrates that mineralogical information itself is not enough to estimate the elastic properties influenced by local mineralogical and texture heterogeneity. Instead of bulk compositions, indentation results are separated into three diverse groups: quartz/feldspars/pyrite (QFP), carbonates, and clay-rich mineral mixture areas. As shown in Figure 13F, measured moduli have a broad range for QFP, moderately for carbonates, and narrowly for clay mixtures.

This also shows that the stiffness and hardness has clear relationships as a function of major constituents of the mineralogical composition. Previous works on coupled nanoindentation and EDS analysis of clay and kerogen rich shales (e.g., Abedi et al., 2016; Deirieh et al., 2012) also reveal that mechanical properties estimated using statistical clustering can be characterized with clay and kerogen fractions. Although the number of indentation is small in our work, our analysis can shed light on the stiffness and hardness relationship in the form of QCC commonly used in the classification scheme.

Figure 14 shows high resolution SEM images of individual nanoindentation impressions (locations) for three different mineral groups along with measured modulus and hardness values. For QFP the measured strength is predominantly influenced by impurities over the indentation area. The measured modulus values from the center of large quartz grains with small inclusions are similar to the value from pure quartz, while moduli near grain boundaries (seen as dark contrast in the high-resolution SEM image) and around mixture of other minerals were less. For carbonates this trend is similar, but certainly different carbonate minerals with different moduli (i.e. calcite and dolomite) contribute to the moduli variability. Regions where multiple minerals are present show quite different residual indentation impressions depending on texture and mineral compositions over the indentation area. Interestingly, hardness values for the multiple mineral areas show a narrower distribution. This can be attributed to the relatively large plastic zone volume (see Eq. 3) of the indents in the regions of mixed composition. This larger volume will make it more likely that a major defect is probed and therefore normalize the measurement. The variations in moduli for mixture areas can be attributed to different mineral compositions and exact locations of the indenter tip. Overall, mechanical properties obtained from nanoindentation testing in mM micro-lithofacies show that the mineralogical and textural heterogeneity significantly contribute to the heterogeneous distribution of mechanical properties. This micro-heterogeneity can influence local micro-fracture features observed in thin-sections and SEM images (Figures 11-12).

Discussion and Conclusions

Characterizing and predicting mechanical behavior of shale and mudstone formations is challenging in part due to heterogeneity at all scales and poor recovery of core. In our study we combine description and analysis of a remarkably intact core through the Mancos Shale (El Vado Formation, Tocito Formation-equivalent and upper Carlile Shale) from the eastern San Juan Basin with a detailed analysis of a major lithofacies obtained from a quarry block sample from the Ferron Tongue member. In part, we follow the "pore-to-regional" workflow for characterizing shale proposed by Slatt et al. (2012).

P- and S-wave velocity measurements made on core samples in unconfined benchtop environments do not vary appreciably between bulk lithofacies types and show a large scatter, but appear to increase with confining pressure. Velocities are larger in magnitude when measured parallel to bedding and lamination direction, and this is consistent with measurements of other shale types around the world (Sone and Zoback, 2013a, b; Sondergeld and Rai, 2011; Vernik and Liu, 1997). The perpendicular measurements from the core that were largest in slowness magnitude correlate with sonic well logs when adjusted for depth, and this, together with the quasi-static measurements presented herein, could be used to predict static and dynamic rock mechanical measurements across the regional San Juan Basin.

The LMS lithofacies identified in the core was further investigated by use of a quarry block sample, which avoided typical problems with mechanical characterization of core (i.e. small volumes and poor recovery). We show that the bulk LMS lithofacies is in fact composed of nested macro- and micro-lithofacies, each bearing slightly differing mineralogical content and mechanical responses. The distribution of these influences the eccentricity of propagating fractures, whereas fractures propagating across laminations will have differing morphology to those propagating parallel to laminations, commensurate with ranges of interpreted fracture toughness values. Failure strengths of LMS in both bedding-parallel and bedding-perpendicular orientations increase non-linearly with increasing mean stress. Quarry block samples appear to be slightly weaker than similar lithofacies from the core samples, and this may be due to near-surface weathering, or unloading fractures associated with uplift and erosion of the quarry rocks.

Nanoindentation measurements taken across the micro-lithofacies show a range in responses. In clay-bearing regions, measured hardness and elastic modulus values vary over a narrow range compared to carbonate and quartz+feldspar+pyrite (QFP) values, and appear to be consistent regardless of micro-lithofacies. In contrast, QFP and carbonate nanoindentation hardness and modulus values show a much larger range. For carbonates, this is due in part to different carbonate minerals encountered.

Ultrasonic velocities in the Davis Federal 15 No. 3 core in clay-rich lithofacies are consistent with the nanoindentation experiments and the analysis of quarry block failure experiments. The relative uniformity of velocity both parallel and perpendicular to bedding in clay-rich parts of the core implies that moduli of clay-rich lithofacies fall into a narrow range at centimeter and decimeter scales suggesting that observations of nanoindentation hold at larger scales. Additionally, the greater range of slowness and velocities in sand-rich facies may not only be due to the relative amounts of sand. Rather, it may also be related to the systematic variation of moduli of sands and grain contact welding plus or minus quartz cement. This could be caused by either depositional style or sediment provenance but requires additional research.

Unequivocally, however, carbonate cementation and its mineralogy does influence velocity magnitudes of the core. This core is located in a fractured oil pool in the eastern San Juan Basin (Fassett and Jentgen, 1978) that has been subjected to heating and uplift during the Laramide orogeny (Emmendorfer, 1989). This led first to extensive carbonate cementation of the shale followed by the extensive vertical fracturing that aids in this interval as an oil and gas producer. The pervasive cementation may play a role in the good agreement between the sonic log and ultrasonic slowness, and the overall low variation in velocities.

The previously observed differences in velocity between perpendicular and parallel measurements, with parallel-to-bedding measurements having higher velocities (lower slowness) with a relatively small uncertainty, and perpendicular-to-bedding measurements having lower velocities (larger slowness) and greater internal variance. Consistent with previous theory and observations, we interpret this as the focusing of ultrasonic waves along stiff, fast bedding leading to more consistent, greater velocities. Perpendicular-to-bedding velocities are more variable and slower, as individual lamina are not bypassed, leading to a net lower velocity (greater attenuation and slowness), and greater variability within a sample interval. This explanation is additionally supported by the higher V_p/V_s ratio of the perpendicular-to-bedding samples than in the parallel-to-bedding samples. V_p/V_s has been used to quantify the degree of fracturing or pore-space in reservoirs at seismic frequencies. Here, at ultrasonic frequencies, we find that the greater V_p/V_s ratio also can represent a more heterogeneous ray path, crossing more and larger pores or other low shear velocity media (i.e., clays).

The above interpretation of the difference between parallel- and perpendicular-to-bedding ultrasonic velocities directly parallels our interpretation of the quarry block failure data. In the quarry block samples, we hypothesize that failure parallel-to-bedding is initiated in stiff, quartz-rich micro-lithofacies, leading to more brittle styles of failure and greater overall strengths in the parallel-to-bedding samples than in the perpendicular-to-bedding samples at the same mean stress. The perpendicular-to-bedding samples have failure initiated in weaker, less stiff micro-lithofacies. The greater velocities in the parallel-to-bedding than in the perpendicular-to-bedding samples correlate to this hypothesis—parallel-to-bedding has fast (i.e., stiff) pathways that would be preferentially loaded parallel-to-bedding, causing failure in these beds. The greater Vp/Vs ratios of the perpendicular-to-bedding samples leads to more support for failure initiation in the less stiff layers. Because greater Vp/Vs implies greater porosity, discontinuity/defects along different bedding layers, or at least media less able to bear shear stress, this implies that, for the shear failures induced, the failure should occur in the less stiff layers even if peak strengths of all micro-lithofacies were equal.

Both XRD and MAPS mineralogical data show that the Mancos LMS bulk composition, and macro- and micro-lithofacies, plot in the “brittle” regime as determined by Ulmer-Scholle et al., (2014), although the more clay-rich samples plot very close to the “brittle-ductile” transition as defined by these authors. In terms of mechanical behavior, the LMS and other lithofacies show deformational behavior that is truly brittle in the rock mechanics sense, with little evidence of pore collapse. The LMS bulk composition plots near the boundary of “brittle shales” and “sealing shales” as defined by Bourg (2015), and the macro- and micro-lithofacies define a trend toward the more quartzose end-member composition. This would suggest that the LMS lithofacies of the Mancos Shale is better suited to hydrocarbon extraction, rather than for CO_2 or radioactive waste storage (Bourg, 2015). However, although we have not addressed this rigorously here, it appears that the more clay-rich bulk lithofacies of the Mancos Shale, abundant just above and below the Niobrara-Carlisle unconformity (Figure 2 and 3 herein), should plot in the "ductile" regions of such schemes. Certainly, the evidence in the San Juan Basin and other Mancos Shale-dominated basins would support the sandier portions of the Mancos Shale as better suited to hydrocarbon production (Ridgley, 2000; Broadhead, 2015; and Hawkins et al., 2016). Could the Mancos thus be a "dual-use" shale, with the lower portions more suited to storage uses and the upper better suited for energy extraction?

Acknowledgements

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under contract DE-SC0006883. Dana Ulmer-Scholle provided invaluable help with the core descriptions. We thank Jennifer Wilson and Charles Choens for help with the microscopy and profilometry measurements. Ohtark Kwon re-evaluated XRD analysis of the quarry block. Charles Bryan designed the constant humidity system used for ASC testing. Nanoindentation work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

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Figure Captions

Figure 1. **A.** Geological map of San Juan Basin and location of Davis Federal 3 No. 15 (after Lorentz and Cooper, 2003) and **B.** stratigraphic nomenclature and gamma ray-resistivity log of the Mancos Shale in the Davis-Federal No. 3-15 core. The El Vado Sandstone Member is separated into Niobrara zones (A, B, & C). Adapted from Emmendorfer (1992) and Rosandick (2014).

Figure 2. **A.** Sections of the Davis Federal No. 3-15 that are representative of main lithofacies types observed in the core. Sand content of the lithofacies increases from left to right in the figure.

(Adapted from Rosandick, 2014). **B.** Distribution of lithofacies in the core compared to sonic, caliper, and gamma ray logs.

Figure 3. Refined velocity measurements taken perpendicular and parallel to bedding and compared to the electric logs and lithology. Brackets identify ranges calculated from precision measurements with the corresponding dot representing the median. Black arrows represent sequences identified by Jim Rine (Personal Communication, 2014). Red arrows represent our interpretation of sequences from core analysis. Dominant facies and mechanical facies are shown left of the gamma log, with the Niobrara-Carlile unconformity represented by the wavy line.

Figure 4. Compressional (V_P) and shear (V_S) velocities of Mancos Shale lithofacies measured at room conditions. **A.** Mancos core velocities by interpreted lithofacies, measured perpendicular to lamination or bedding direction. **B.** Same as (**A**), but measured parallel to lamination or bedding direction. **C.** V_p and V_s measured in one-inch core plugs of Mancos Shale LMS lithofacies sampled from the large Mancos block (see Figure 5). For the "parallel" results, the angle is referred to the lamination direction. For the "perpendicular" results, the angle is referred to an arbitrary plane.

Figure 5. A. All samples cut from the Mancos Shale Formation quarry block used in this study: macroscopic description (blocks), XRD (Slice 2), microscopic description (Slice 1 and 2), and geomechanical testing (Core and Large Blocks). **B.** Macro-lithofacies interpretations (solid colors) and locations of XRD samples taken from Slice 2, cut 'A', separated along interpreted macro-facies boundaries (yellow lines). Sample 10 is fracture-fill. The bulk rock XRD sample (11) is derived from cut 'B'. Interpreted sedimentary structures and bioturbation features in Slice 2. **C**. Enhanced scan of Slice 2 used for macro-lithofacies interpretations from petrographic analysis of Grigg (2016). **D**. Interpreted fractures in slice 2. **E**. Approximate core locations on the Large Block (as shown in **A**) of axisymmetric compressive test samples (red and violet makers) and indirect tensile test samples (blue and violet makers). The upper macro-lithofacies map of the side view of the Large Block and the lower scan image of the side view of the Large Block. Sample locations cored perpendicular to bedding is shown in **A**.

Figure 6. A. A ternary diagram (classification from Ulmer-Scholle et al., 2014) showing the normalized quartz, carbonate and clay values from XRD analysis (Table 2). **B**. Ternary diagram of grain size (after Folk, 1974; and Lazar et al., 2015a) with the micro-lithofacies classifications,

including sandstone (S), muddy sandstone (mS), sandy coarse mudstone (scM), sandy medium mudstone (smM), sandy fine mudstone (sfM), coarse mudstone (cM), medium mudstone (mM), and fine mudstone (fM). **C**. MAPS data of QFPs (quartz, Feldspars, pyrite), carbonates (calcite, dolomite, ankerite), and clay/micrite phases over an A5 thin section (Figure 7). Data points are identified by micro-lithofacies. The classification scheme is modified from Ulmer-Scholle et al. (2014).

Figure 7. A. Thin section A5 (left) with an overlay micro-lithofacies color-coded map (right). Most common sedimentary structures are labeled on the map. **B.** Photo micrographs demonstrating intra- and inter-micro-lithofacies heterogeneity. Photographed micro-lithofacies include fM (a-c), mM (d-f), smM (g-i), scM (j-l), and mS (m-o).

Figure 8. Results of ASC and hydrostatic testing of Mancos Shale quarry block samples loaded parallel (left) and perpendicular (right) to lamination direction or bedding. Red curves plot axial stress versus axial strain; dark blue and black curves plot axial stress versus lateral strain 1 and 2, respectively; green curves plot axial stress versus volumetric strain; and light blue curves plot shear stress versus axial strain. For samples loaded parallel to bedding, lateral strain 1 is measured in the plane of bedding, while lateral strain 2 is measured perpendicular to bedding. **A.** Samples tested under unconfined conditions. **B.** Samples tested at 45 MPa constant mean stress. **C.** Samples tested at 100 MPa constant mean stress**. D.** Samples tested at 200 MPa constant mean stress (14B) and 160 MPa constant mean stress (22A). **E.** Samples tested hydrostatically. Sample core locations within the quarry block are shown in Figure 5.

Figure 9. **A.** Failure surfaces in shear stress-mean stress for quarry block LMS lithofacies samples loaded both parallel and perpendicular to bedding direction, and for core samples of different lithofacies loaded parallel to bedding. Also plotted are results from indirect tension testing of quarry block samples (diamonds). **B**. Evolution of Young's modulus (circles) and Poisson's Ratio (squares) during testing of unconfined samples. Both increase with increasing axial stress, both parallel (16B) and perpendicular (32A) to bedding. **C**. Evolution of bulk modulus during hydrostatic loading experiments (shown in Figure 8E). **D**. Evolution of shear modulus during constant mean stress loading portions of experiments in Figure 8.

Figure 10. **A**. X-ray micro-Computed Tomography (μCT) of sample 22A, deformed perpendicular to bedding, showing a major, roughly planar, through-going shear fracture from upper right to lower left, along with several smaller conjugate shear fractures. **B**. X-ray micro-Computed Tomography (μCT) of sample 12B, deformed parallel to bedding. In this case failure was accomplished by a single through-going shear fracture, with no observed conjugate fractures. Horizontal bands evident in the CT reconstructions are due to ring artifacts in the original images. **C.** White-light profilometry results for sample 22A, including azimuthal direction for off-plane fractures (blue inset). **D.** White-light profilometry results for sample 12B, including azimuthal direction for off-plane fractures (blue inset).

Figure 11. Thin section images of failed samples loaded parallel to bedding (15B, **A**) and perpendicular to bedding (28A, **B**) under 45 MPa confined condition (see Figure 8B for testing results). The circular thin sections were taken through the horizontal plane of central portion of core samples and the rectangular thin sections were taken through the vertical plane of upper portion of core samples. Petrographic microscope images were taken at two different scales to highlight the fractures and cracks. Numbers for microscopic images are corresponding to the box numbers on the thin section.

Figure 12. **A.** Thin section images of the four cylindrical (1-inch diameter and 0.5-inch-thick) samples used in the indirect tensile tests along with the micro-lithofacies color maps of those thin sections. Samples were loaded with different orientations to the bedding plane (Sample 14 at 45°, 18 at 90°, and 24&25 at 0°) and the sample locations are in Figure 5. The most prominent fractures at which the samples failed are marked in red on both the scans and the maps. **B.** The mineralogy mapping and BSE image obtained from the MAPS for sample 14 showing the main tensile crack with the damaged surrounding fractures. A horizontal strain distribution is based on digital image correlation (DIC) during the test with red and blue colors representing high and low strains, respectively. Examples of phase field modeling in different layered cases with two components (dark and light blue for stiff and weak materials) are also shown with colormap of the phase field with the dark red as crack or highly damaged path. DIC results and modeling results in (**B**) are modified from Na et al. (2017).

Figure 13. **A.** Ion-polished Mancos shale 18B (1 inch (2.54cm) diameter). Yellow and red areas for mineralogy mapping at 20 μm and 2 μm resolution, respectively, and BSE images at 2 μm and 0.2 μm resolution, respectively. **B.** Mineralogy mapping at 20 μm resolution. Scale bar is 5000 μm. **C.** SEM image of nano-indentation marks (5x5 grid). **D.** Mineralogy mapping (2 μm resolution) overlapped with BSE image over indentation area. **E.** Estimated modulus based on two mixture theories (Voigt and Reuss) versus measured modulus values. **F.** Measured modulus versus measured hardness for different phases – QFP (quartz, feldspar, and pyrite dominant), carbonate (calcite, dolomite) dominant, and clay-rich (illite, illite-smectite, kaolinite, chlorite). 50 indentation results over two grid indentation areas are shown.

Figure 14. Representative high resolution (7nm) SEM images of nanoindentation impressions over different mineral phases. Measured reduced modulus (Er) and hardness (H) values are listed in each image (all data shown in Figure 13F). Representative minerals are listed on each image. The same scale for all image with the scale bar shown in the last image. NOTE: Q=quartz, F=Feldspar, C=Calcite, Dol=Dolomite, Ank=Ankerite, IL=illite (and smectite), and Org=Organic.