The relationship between the proportion of microboudinaged columnar grains and far-field differential stress: A numerical model for analyzing paleodifferential stress

Tarojiro Matsumura*, Tatsu Kuwatani** and Toshiaki Masuda***

*Graduate School of Science and Technology, Educational Division, Shizuoka University, Shizuoka 422-8529, Japan
**Department of Solid Earth Geochemistry, Japan Agency for Marine–Earth Science and Technology, 2-15 Natsushima-cho, Yokosuka 237-0061, Japan
***Institute of Geoscience, Shizuoka University, Shizuoka 422-8529, Japan

Microboudin paleopiezometry is an intensive endeavor that involves measurement of several hundred grains per sample to produce reliable estimations of far-field differential stress. This procedure is particularly time-consuming when conducting stress analysis for a large number of samples within a metamorphic belt. To improve and expedite the stress estimation procedure, we propose a numerical model that uses grain-shape data to calculate the relationship between the proportion of microboudinaged columnar grains \( p \) and the far-field differential stress \( \sigma_0 \). Our model combines the weakest link theory and the shear-lag model. The weakest link theory is used to derive the fracture strength of grains, whereas the shear-lag model is used to determine the relationship between the differential stress within a grain \( \sigma \) and \( \sigma_0 \). An intact grain becomes a microboudinaged grain when \( \sigma \) is higher than its fracture strength at a specific point within the grain. Here, we make calculations of \( p \) for all intact grains under increasing \( \sigma_0 \) from 0 to 20 MPa. Our calculations show that the modeled and observed distributions of \( p \) and the aspect ratio have similar patterns for both intact and microboudinaged grains. The value of \( p \) increases with increasing \( \sigma_0 \), with 70% of the grains being microboudinaged when \( \sigma_0 = 20 \) MPa. These results suggest that our model is capable of reproducing observed data for microboudinaged columnar grains and that the relationship between \( p \) and \( \sigma_0 \) can be used to estimate the magnitude of differential stress without the need to measure grain-size data for several hundred grains with a wide range of aspect ratios.

Keywords: Numerical simulation, Microboudinage structure, Proportion of microboudinaged grains, Far-field differential stress, Paleopiezometer

INTRODUCTION

Microboudinage structures within columnar grains such as tourmaline, piemontite, and glaucophane (Fig. 1a) provide information regarding the paleodifferential stress that occurred during rock deformation (Masuda and Kuriyama, 1988; Passchier and Trouw, 2005). The microboudinage of an intact columnar grain into two separate segments takes place in three stages (Masuda and Kimura, 2004): (1) before fracturing, (2) during fracturing, and (3) after fracturing. By studying Stages 1 and 2 of microboudinage, Masuda et al. (1989, 2003) and Kimura et al. (2006, 2010) developed a paleopiezometer based on the microboudinage structures developed within columnar mineral grains. The microboudin paleopiezometer is superior to other widely used paleopiezometers, such as those based on recrystallized grain size (e.g., Stipp and Tullis, 2003) and calcite twinning (e.g., Lacombe, 2007), because it can reveal trends in differential stress with increasing plastic strain (Masuda et al., 2011). Although this paleopiezometer makes it possible to estimate the magnitude of differential stress during microboudinage in the crust (e.g., Masuda et al., 2011), the procedure requires the measurement of 300-500 columnar grains across a wide range of aspect ratios \( r \) (1–10) for each sample. Therefore, this method is timeconsuming, labor intensive, and unsuitable for applying to the large numbers of samples necessary to reveal regional variations in
differential stress within a metamorphic belt.

In this study, we focus on the proportion of microboudinaged columnar grains ($p$), the value of which is defined as the ratio of the number of microboudinaged grains to the total number of grains (microboudinaged + intact grains). A microboudinaged grain is occasionally separated into several segments. The relationship between $p$ and the far-field differential stress ($\sigma_0$) enables rapid analysis of paleostress (Masuda et al., 1995, 2004). However, this relationship has remained unclear because change in the value of $p$ with respect to $\sigma_0$ cannot be observed from a sample. Therefore, in the present study, we propose a numerical model to investigate this relationship based on the weakest link theory and the shear-lag model. The former theory describes grain fracture strength based on the Weibull distribution, whereas the latter theory describes the distribution of differential stress $\sigma$ that develops along grains as a result of $\sigma_0$.

Our numerical model calculates values of $p$, which are then used to estimate values of $\sigma_0$ for data collected from columnar grains within a sample. As an initial application of this model, we estimate paleodifferential stress from tourmaline grains embedded in a quartz matrix based on the relationship between $p$ and $\sigma_0$. This estimate is then used to infer the magnitude of the differential stress that occurred during the microboudinage event. Our numerical model can be used as a paleopiezometer, utilizing observed grain-shape data obtained from a rock sample.

### BASIC THEORY

#### Weakest link theory

Masuda et al. (1989) used the weakest link theory (e.g., Paterson and Wong, 2005) to represent the probability of fracture strength in columnar grains, $g(r,s)$, as a function of aspect ratio ($r$) and fracture strength ($s$), as follows:

$$g(r,s) = \left(\frac{m-1}{S^*}\right)^m r s^{m-1} \exp\left[-\frac{m-1}{m} r \left(\frac{s}{S^*}\right)^m\right]$$ (1),

where $m$ is the Weibull parameter and $S^*$ is the grain fracture strength. Kimura et al. (2006) and Masuda et al. (2008) expressed $S^*$ as

$$S^* = S_{0*}^* K_0 K_C \left(\frac{1}{\bar{w}}\right)^{1/2}$$ (2),

where $S_{0*}^*$ is the instantaneous fracture strength, $r$ is the grain aspect ratio, $\bar{w}$ is the grain geometric mean width, $1/\bar{w}$ is a non-dimensional term, and $K_0$ and $K_C$ are the stress intensity factors, with $K_0$ being the subcritical crack-growth limit and $K_C$ representing the fracture toughness. Masuda et al. (2008) introduced $K_0$ and $K_C$ to incorporate the influence of time on the fracture strength of minerals and assumed a value of $K_0/K_C = 0.1$. Kimura et al. (2006) reported values of $m = 2$ and $S_{0*}^* = 39$ MPa for tourmaline.

#### Shear-lag model

The shear-lag model (Zhao and Ji, 1997) determines the relationship between the far-field differential stress ($\sigma_0$) and the differential stress ($\sigma$) transferred to the elastic fiber embedded within an elastic matrix at position $x$, as follows:
\[ \sigma = \frac{E_f}{E_q} \sigma_0 \left[ 1 - \frac{1 - \frac{E_f}{E_q}}{1 + \frac{E_f}{E_q}} \cosh (\beta p) \right] \cosh (\beta l) \]

where

\[ \beta = \frac{r}{l} A_0 \]

and \( l \) is the half-length of grains; \( v_{\text{mm}} \) is the Poisson’s ratio of the matrix; \( R_0 \) and \( r_0 \) are the radii of the unit cell and fiber, respectively (see also Masuda et al., 2003 and Zhao and Ji, 1997); and \( E_q \) and \( E_f \) are the elastic constants of the matrix and the columnar grains, respectively. The variable \( \beta \) can be rewritten with the constant \( A_0 \) as

\[ \beta = \frac{r}{l} A_0 \]

Columnar tourmaline grains embedded within a quartz matrix have constant \( E_q/E_f \) and \( A_0 \) values of 2 and 0.4, respectively (Kimura et al., 2006, 2010).

**NUMERICAL MODEL**

Our numerical model calculates values of \( p \) corresponding to values of \( \sigma_0 \) using a given dataset collected from columnar mineral grains within a sample. This dataset is inputted into the numerical model as the initial conditions. The numerical model calculates the fracture strength of each grain based on the weakest link theory (Eq. 1) using the inverse transform method, which is an established method for generating sample numbers at random based on a given probability distribution (Chapter 11.1.1 in Bishop, 2006; Chapter 2.1.2 in Robert and Casella, 2010). When fracturing occurs in a grain, two new grains are generated, and in this model, their fracture strength values are also calculated using Equation 1. Assuming that grain fracturing occurs at the weakest points throughout a grain, the fracture strength values of new grains must be higher than the value of the original grain prior to microboudinage. The yield stress along a columnar grain (\( \sigma \)) is also calculated from the shear-lag model (Eq. 3). The maximum value of \( \sigma \) occurs at the center of the grain, but the value of \( \sigma \) around the central three-quarters of the grain is almost equivalent to the maximum value (see also Zhao and Ji, 1997; Kimura et al., 2010).

We define a microboudinaged grain in terms of the distribution of points in an intact grain where the fracture strength is less than \( \sigma \). These points in each grain can be calculated from fracturing point data in the initial conditions, and we assume that the distribution of such points can be represented by the Beta distribution. The numerical model computes such points for all intact grains for each value of \( \sigma_0 \). These calculations are performed with a continuously increasing \( \sigma_0 \) from 0 to 20 MPa because the paleodifferential stress magnitude was previously estimated to be within this range based on microboudin paleopiezometry (Masuda et al., 2008, 2011). Our model provides values of \( p \) with respect to the aspect ratio \( r \) (\( p_r \)) and defines the relationship between \( p \) and \( \sigma_0 \).

**DATASET USED FOR THE CALCULATIONS**

We obtained the grain–shape dataset from tourmaline grains embedded within a quartz matrix of metachert from the Warrawoona greenstone belt in the East Pilbara Terrane, Western Australia. This greenstone belt has been affected by contact metamorphism (Van Kranendonk et al., 2002). Details of the geological setting and observations of this area are provided by Collins et al. (1998) and Van Kranendonk et al. (2002). The metachert is composed of quartz, tourmaline, muscovite, chlorite, and kyanite. Collins and Van Kranendonk (1999) proposed that the kyanite-containing rocks must have reached amphibolite–facies conditions during the contact metamorphism. The arrangement of muscovite grains defines the foliation, which consists of millimeter-scale compositional banding of muscovite-rich and quartz-rich layers (Fig. 1b). The lineation is defined by the alignment of tourmaline long axes upon the foliation, based on the method of Masuda et al. (1999). We selected tourmaline grains with long axes within \( \pm 15^\circ \) of the mineral lineation on the foliation surface in accordance with the procedure described by Masuda et al. (2011). We measured the widths and lengths of tourmaline grains and microboudinage gap distances for a total of 1432 tourmaline grains (Fig. 1c). These measurements reveal that 35% of the tourmaline grains have microboudinage structures (\( p = 0.35 \)). The dataset was reconstructed for the model calculation using the strain-reversal method (Ferguson, 1981). The distribution of the fracturing points of the measured microboudinaged tourmaline grains (Fig. 2) shows that more than 95% of such grains are fractured within the central three-quarters of the grain, and the best-fit curve of the Beta distribution shows an excellent fit to the measured data. Thus, for the calculation, we generated the specific points of fracturing at random based on the Beta distribution (Fig. 2).

**RESULTS**

Knowledge of the relationship between \( p \) and \( \sigma_0 \) is needed to conduct rapid analysis of paleodifferential stress.
Our numerical model allows the variations in $p_r$ and $p$ with increasing $\sigma_0$ to be established based on a single sample. Figure 3 shows the value of $p_r$ for each $\sigma_0$. The solid black line represents the best–fit curve of the theoretical function of microboudinage $G(r, \lambda)$, which represents the probability of grain fracturing with respect to the aspect ratio of the grain ($r$) and the non–dimensional stress parameter ($\lambda$). The best–fit curve of $G(r, \lambda)$ is determined using the least–squares method with weighting for the total number of measured grains at each aspect ratio (see also Masuda et al., 2003, 2011). Most grains are intact under lower differential stress (0–5 MPa), although very weak grains become microboudinaged. Because grains with high aspect ratios ($r > 10$) are likely to possess lower fracture strengths compared to grains with low aspect ratios, according to the weakest link theory (Eq. 1), most grains with high aspect ratios are microboudinaged under moderate differential stress (5–10 MPa). The values of $p_r$ for these grains are much larger than predicted by $G(r, \lambda)$ because in each case, the number of measured grains used to generate these values is quite small (<10 grains); these values of $p_r$ are therefore very sensitive to increasing $\sigma_0$. Grains with low aspect ratios are rarely microboudinaged under higher differential stress (15–20 MPa), whereas grains with high aspect ratios are commonly microboudinaged (Fig. 3). Figure 4 shows the value of $p_r$ and the frequency distribution of microboudinaged grains, which represents the number of microboudinaged grains (gray bars) and intact grains (white bars) according to grain aspect ratio, for the same stress parameter $\lambda$ of $G(r, \lambda)$ in the modeled and observed data. The modeled data are distributed similarly to the observed microboudinage structures of tourmaline grains (Fig. 4).

The calculations outlined above were repeated 1000 times with the generated initial fracture strengths and fracturing points using the same dataset for the aspect ratios of the tourmaline grains. Because the fracture strength and fracturing point of a grain vary for each calculation, the relationship between $p$ and $\lambda$ is variable. Repeating the calculation 1000 times revealed that the $p$–values are positively correlated with the far–field differential stress (Fig. 5). The calculated values of $p$ for each value of $\sigma_0$ lie within a range of approximately ±3% (Fig. 5). According to these results, the value of $p$ increases continuously with increasing $\sigma_0$ (Fig. 5). Approximately 70% of grains have
microboudinage structures when \( \sigma_0 = 20 \text{ MPa} \). The relationship depicted in Fig. 5 suggests that \( p \) can be used to provide a reasonable assessment of the variation in \( \sigma_0 \).

DISCUSSION AND IMPLICATIONS

Our numerical model is based on the weakest link theory and the shear–lag model, and it provides data to clarify the relationship between \( p \) and \( \sigma_0 \). The model is able to reproduce an observed dataset of microboudinaged columnar mineral grains (Fig. 4), although model verification is still needed. The \( p_x \) value for grains with high aspect ratios (\( r > 10 \)) is higher than that predicted from \( G(r, \lambda) \) (Fig. 4). Because the number of grains with high aspect ratios is relatively small, these deviating \( p_x \) values affect the calculations very little. The model provides a theoretical curve to represent the relationship between \( p \) and \( \sigma_0 \) (Fig. 5), which is represented empirically by the cumulative distribution function of the Weibull distribution, as follows:

\[
\sigma_0 = \mu \left\{ -\ln\left(1 - p\right) \right\}^\frac{1}{\kappa}
\]  

(7).

Equation (7) can be used to estimate \( \sigma_0 \) from values of \( p \), similar to Masuda et al.’s (1995) method for rapidly estimating the dimensionless parameter related to \( \sigma_0 \) from the proportion of microboudinaged columnar grains. The relationship established in the present study indicates that a \( p \)-value of 0.35 corresponds to a \( \sigma_0 \) value of 11.3 MPa (Fig. 5). Given that the microboudinage is considered to have occurred immediately before the rock entered the brittle–plastic transition from the plastic realm (e.g., Masuda et al., 2007, 2011), the estimated value should reflect the state of differential stress corresponding to the last stage of plastic deformation.

The relationship defined above is applicable only to the sample used in this study because the curves derived from Equation 6 depend on the dataset of the distribution of the aspect ratios of columnar grains. Therefore, a dataset must be obtained for each sample of interest. However, the proposed procedure can reduce the time consumed measuring grains for two reasons. First, the dataset need not cover the wide range of aspect ratio values empirically required to cover more than five data points of \( p_x \) for the reliable estimation of \( \lambda \). Our calculations can be conducted without this range of aspect ratios. Secondly, we can obtain a reliable value of \( \sigma_0 \) from the \( p \)-value for only \( \sim 100 \) grains per sample, given that Masuda et al. (1995) reported that the confidence interval for
$p$ becomes $< \pm 0.1$ with 100 grains measured (see also Fig. 1 of Masuda et al., 1995).

Given that the numerical model was applied only to the tourmaline-quartz system in a single sample, the applicability and validity of the model must still be assessed. Therefore, further investigation is required by, for example, applying this model to samples from the piemontite-quartz (Masuda et al., 2004) and glauco- phosphate-calcite (Masuda et al., 2011) systems. We emphasize that our numerical model is a reliable paleopiezometer that can be rapidly applied for the large number of samples necessary to identify differential stress variations over a wide area of a metamorphic belt.

ACKNOWLEDGMENTS

We thank Atsushi Okamoto and an anonymous reviewer for improving the manuscript and Koichiro Fujimoto for kindly editing the manuscript. The authors are grateful to Hideki Mori for preparing thin sections and Kenta Yosida for encouragement in writing this paper. This study was supported by the Joint Usage/Research Center Program No. 2015-B-04 from the Earthquake Research Institute, University of Tokyo and by JSPS KAKENHI Grants No. 25120005, No. 25280090 and No. 15K20864.

REFERENCES


Masuda, T., Nakayama, S., Kimura, N. and Okamoto, A. (2008) Magnitude of $\sigma_1$, $\sigma_2$ and $\sigma_3$ at mid-crustal levels in an orogenic belt: microboudin method applied to an impure metachert from Turkey. Tectonophysics, 460, 230–236.


Manuscript received July 11, 2016
Manuscript accepted November 4, 2016

Manuscript handled by Koichiro Fujimoto