



Research Article

The Conundrum of the Crack Initiation Stress of Rock Type Material – II. The Second Derivative Method

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Received: 18 July 2025

Revised: 7 August 2025

Accepted: 8 August 2025

Published date: 9 August 2025

Doi: 10.70425/rml.202503.22



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Abstract: In part II of this study, a second method for the prediction of the crack initiation stress was suggested. The new technique is based on an elementary mathematical calculus theory. Particularly, the one that supports that the points where the second derivative of a function is equal to zero can be considered as possible inflection points of the function. The proposed Second Derivative method fulfilled all the necessary criteria, that were mentioned in part I, so that it can further advance the research field. The method was applied to ten rock specimens, specifically eight marbles and two vesicular basalts, that were subjected to uniaxial compressive tests. The predicted crack initiation stresses from the new method were compared with those obtained from the established techniques of the existing literature. The new method had very close results with all other utilized methods for the marbles, thus meaning that the proposed Second Derivative technique can accurately and consistently determine the onset of stable crack growth for that rock type. On the contrary, the new method displayed a poor correlation with the other techniques for the two basalts, hence indicating that further tests need to be conducted in the future for that rock type.

Keywords: Crack initiation; Crack damage; Uniaxial compressive tests; Brittle fracture

1. Introduction

In the second part of this study one more method will be suggested for the determination of the onset of stable crack growth. It has generally been accepted amongst researchers that the latter threshold can serve as a more realistic indicator of the in-situ spalling strength of the rock mass [1-3]. The new method is based on an elementary mathematical calculus theory and specifically the one that supports that the values where the second derivative of a function are equal to zero can be regarded as potential points of inflection of the function. The physical explanation of the aforementioned Second Derivative (SD) method will be thoroughly provided in the next section.

Likewise with part I of the study, the SD method will be applied, and subsequently validated, using ten rock specimens, particularly eight marbles and two vesicular basalts, which were subjected to uniaxial compressive tests. These two different rock types were selected in an attempt to test rocks of both high (vesicular basalts) and low (marbles) porosity, since for the most part previous studies that have dealt with the onset of stable crack growth of rocks have neglected high porosity rock type material and mainly focused on low porosity rocks. The physical properties (i.e. the dry density and the porosity), as well as the dimensions of the aforesaid samples are given in part I. Additionally, the laboratory set-up that was used during the ten compressive tests is also presented in part I. Moreover, in the previous part the mechanical properties of the samples, i.e. the compressive strength, Young's modulus, and Poisson's ratio, are also provided. For reference, the mean Uniaxial Compressive Strength (UCS) of the eight marble specimens was approximately 111.10 MPa, with a computed standard deviation of around 18 MPa. Moreover, the mean value of Young's modulus for the same rock samples was close to 44.78 GPa, with a standard deviation of 3.94 GPa. Furthermore, the mean value of Poisson's ratio was approximately 0.33, with a standard deviation of just 0.068. As for the two vesicular basalts, their mean UCS was approximately 69.71 MPa, with a calculated standard deviation of about 15.47 MPa. The mean values of the two elastic constants, i.e. Young's modulus and Poisson's ratio, were 16.07 GPa and 0.155, respectively. Their standard deviations were around 5.49 GPa (Young's modulus) and 0.007 (Poisson's ratio). It is worth noting that in part I a brief literature review is also carried out, where the majority of the existing empirical techniques capable of identifying the onset of stable crack growth are showcased. The aim of the review was mainly to mention the main criticism that each method has received over the years.

Finally, the results of the SD method were compared with those obtained from the established techniques of the existing literature. The newly suggested method displayed exceptionally close results with the other applied techniques for the eight marble specimens, thus meaning that the SD method can accurately determine the onset of stable crack growth for that rock type. However, the SD technique had a poor correlation with the other methods for the two basalts. As a result, more specimens from the latter rock type need to be tested in the future, in order to safely determine whether the newly proposed technique can consistently determine the Crack Initiation (CI) stress for the aforesaid rock type.

2. Second Derivative Method

As it was clearly stated in part I of this study: “... it is easily comprehended that any new methods that are suggested for the determination of the CI threshold must fill some specific criteria, in order to advance the research field. Particularly, new techniques must totally exclude subjective errors, possess a robust and clear physical explanation, while also combine easy implementation from the user. ...”. Consequently, having the aforesaid necessary requirements in mind a new technique was developed that essentially utilizes an elementary mathematical calculus theorem. Subsequently, the new method mainly relies on the approximation that the points where the second derivative of a function are zero can be considered as possible inflection points of the function.

Overall, the main steps of the SD technique can be summarized as follows. Firstly, theoretically the method can be applied using either the lateral or the volumetric strain curves. However, the author strongly suggests utilizing the lateral strain curve, because it has generally been accepted that the latter is more sensitive to the propagation of cracks, before the onset of unstable crack growth [3-6]. Additionally, the choice of the lateral strain curve is strongly influenced by one more factor that will be thoroughly discussed and mentioned below. Ultimately, the first step of the method involves applying a third-order polynomial fitting to the axial stress-lateral strain data, up until the onset of unstable crack growth. The third-order polynomial combines a very high value for the coefficient of determination (R^2), and it also eliminates the possibility of overfitting. Hence, the aforesaid factor for the choice of the lateral strain curve, rather than the volumetric, lies in the fact that the latter curve cannot be adequately fitted using a polynomial of the third-order, mainly due to the unique shape of the volumetric curve (i.e. its characteristic reversal

point). Consequently, a higher order polynomial is needed that is very vulnerable to overfitting. It is worth noting that the mean coefficient of determination that was achieved from the third-order polynomial fitting for the eight marble specimens and the two basalts was around 0.9971 and 0.9988, respectively. In Figure 1a below the application of a third-order polynomial fitting is showcased. In order to assure a comprehensive coverage the fitted lateral strain data for the ten rock specimens of the study are illustrated in the Appendix. In this way, the equation of the lateral strain curve is produced. As long as the axial stress is displayed on the y-axis and the lateral strain on the x-axis, respectively, the equation should have the following general form:

$$\sigma(\varepsilon_l) = \alpha_1 \varepsilon_l^3 + \alpha_2 \varepsilon_l^2 + \alpha_3 \varepsilon_l \quad (1)$$

where, $\sigma(\varepsilon_l)$: denotes the axial stress equation as a function of the lateral strain, ε_l : symbolizes the lateral strain, and $\alpha_1, \alpha_2, \alpha_3$: represent the coefficients that are determined from the third-order polynomial fitting. The next step requires solving the following equation:

$$\frac{d^2 \sigma(\varepsilon_l)}{d\varepsilon_l^2} = 0 \quad (2)$$

where, the operator $\frac{d^2}{d\varepsilon_l^2}$: denotes the second derivative of a function in terms of the lateral strain. The solution of the previous equation essentially represents the point where the second derivative of the fitted lateral strain curve is zero, i.e. its possible inflection point. By taking into account Equation (1), the previous equation can be expanded, and subsequently written as:

$$6\alpha_1 \varepsilon_l + 2\alpha_2 = 0 \quad (3)$$

The previous linear polynomial equation can be easily solved analytically, and yield the following obvious solution:

$$\varepsilon_l^1 = -\frac{1}{3} \frac{\alpha_2}{\alpha_1} \quad (4)$$

where ε_l^1 : denotes the solution of the linear polynomial equation. The previous real solution holds when the following condition is met:

$$\varepsilon_l^1 < 0 \quad (5)$$

Which by taking Equation (4) into account the previous equation can be expanded as follows:

$$\frac{\alpha_2}{\alpha_1} > 0 \quad (6)$$

Meaning that for the condition of Equation (5) to hold it must be that either:

$$\alpha_2 > 0; \alpha_1 > 0 \quad (6)$$

or

$$\alpha_2 < 0; \alpha_1 < 0 \quad (7)$$

The aforesaid condition of Equation (6) is solely dependent on the coefficients that are obtained from the fitting. Consequently, it is clearly

revealed why a high coefficient of determination is necessary. If the previous condition is not satisfied the linear equation (i.e. Equation (3)) produces a positive solution, and as a result higher-order polynomial fitting is required, more specifically a fourth-order. However this was only needed for one of the eight marble samples, specifically M5. Regardless of the order of polynomial fitting the explained procedure so far for the application of the SD method is exactly the same. The only difference that arises from the fourth-order polynomial fitting lies in the fact that the resulting equation that must be solved for the determination of the inflection points is a quadratic elementary polynomial equation that can yield two real solution, thus two inflection points.

Moreover, once the inflection point is derived from Equation (4), it can be easily observed from the shape of the lateral strain curve that this should correspond to the CI stress. This inflection point is clearly visualized in Figure 1b below. The latter claim is justified since researchers have agreed that the onset of stable crack growth corresponds to the point of departure from linearity of the lateral strain curve [3-6]. After the deviation from linearity a characteristic concave segment of the curve commences that eventually reaches a plateau as the UCS is achieved. Overall, the point where the concave part is initiated (i.e. the deviation from linearity) can be considered as the sole inflection point of the curve, up until the Crack Damage (CD) stress. Ultimately, following the aforesaid explanation it can be safely assumed that the inflection point that is yielded from Equation (3) is considered to be the CI stress.

To sum up, the steps of the suggested SD technique can be condensed as follows. Fit the axial stress-lateral strain data with preferably a third-order polynomial. Validate that the condition of Equation (5) is met. If yes, then proceed to solve the simple linear equation (i.e. Equation (3)). If not, then apply a fourth-order polynomial fitting to the axial stress-lateral strain data and subsequently solve the resulting quadratic polynomial equation that is produced from the expansion of the general Equation (2). The solution of Equation (3) is presented in Equation (4). This is the possible inflection point of the curve, and can be ultimately considered as the CI stress. Similarly, in the case of the usage of a fourth-order polynomial fitting, two real solutions should be yielded from Equation (2), the smallest of the two can be considered as the onset of stable crack growth.

3. Application and Validation of the Second Derivative Method

In this section of the paper the SD method will be applied to determine the onset of stable crack growth of the ten rocks. These results will then be compared with those produced by the most frequently utilized methods of the existing literature, such as the Lateral Strain Response (LSR) [3], the Lateral Strain Interval Response (LSIR) [6], the Volumetric Strain Response (VSR) [7], and the Crack Volumetric Strain (CVS) [8] methods. As it has already been stated in part I of this study, methods that were not objective (e.g. [4,9-13]) were totally excluded. Additionally, the Axial Crack Strain (ACS) method [14] could not be applied. Furthermore, the CVS method was inappropriate for the two basalts. Moreover, the Relative Compressive Strain Response (RCSR) method [5] yielded the same results as the LSR technique, thus only the last was utilized and not the latter. Finally, no AE monitoring methods were applied. For more information on the previous points it is strongly suggested to read section 6 of part I.

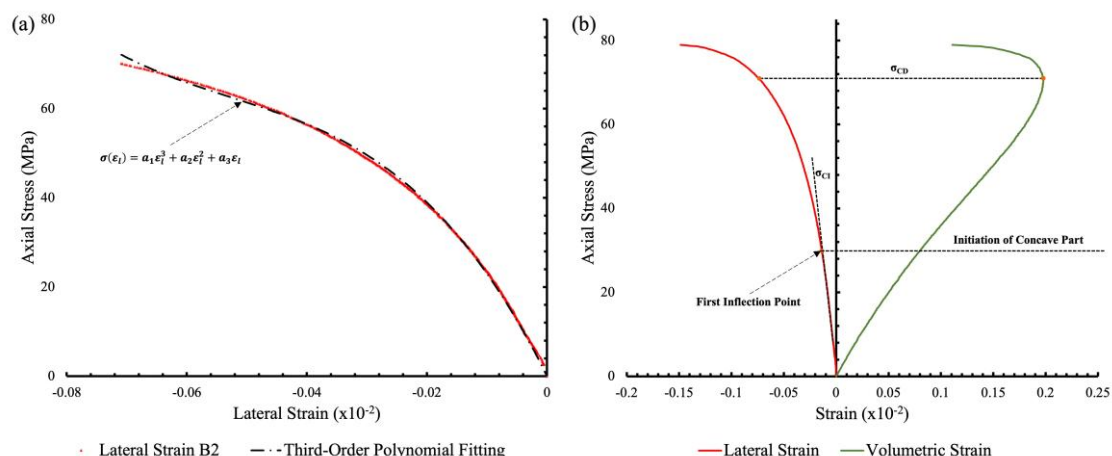


Figure 1. (a) Fitting of the lateral strain data via a third-order polynomial; (b) the sole inflection point of the lateral strain curve, up until the CD stress.

Similarlry, to part I the difference in CI to UCS ratio value between the SD method and the other aforesaid techniques was calculated. These differences, along with the CI stress threshold that was determined from the new SD method for each specimen is presented in Table 1 below. The mean computed difference between the SD and the LSR method for the eight marbles and two basalts was around 5.84 % and 23.03 %, respectively. In addition, the mean difference between the new method and the LSIR technique for the same rock samples was close to 3.31 % and 45.05%. As for the mean difference between the SD and the VSR technique it was calculated to approximately 6.57 % for the marbles, and 5.25 % for the basalts. Finally, the mean difference between the SD and the CVS method was close to 3.49 % for the eight marble samples. From the aforementioned differences it is made clear that the newly suggested SD method yielded close results with all other utilized empirical techniques for the eight marble specimens, and relatively poor results with all methods apart from the VSR technique for the two vesicular basalts. Finally, in Table 1 the standard deviation for the two rock types is thoroughly presented.

4. Discussion

From the simple statistical analysis of the previous section, it was evidently apparent that the SD technique had very close results with the LSR, the LSIR, the VSR, and the CVS methods for the eight marble specimens. As a result, it can be safely assumed that the newly proposed method can accurately and consistently predict the onset of stable crack growth of marbles. However, an especially poor correlation was observed between the SD method and the LSR and LSIR techniques for two basalts. While the new mathematical method displayed close results with the VSR method for the same rock type. Consequently, it is questionable at best if the SD method can accurately determine the onset of stable crack growth for the current rock type.

As it was extensively analyzed in part I the VSR method was rendered inappropriate for the prediction of the CI stress threshold for the two basalts, due to the unique shape of the volumetric strain curves that the latter two samples displayed. Particularly, owing to their shape the maximum difference between the reference line and the volumetric strain curve does not correspond to the deviation from linearity (i.e. the CI stress), but rather to a point very close to the CD stress. Subsequently, the fact that the SD method has very close results with the VSR method, which is known to have erroneous CI thresholds, for the vesicular basalts, ultimately reveals that the latter method cannot accurately determine the onset of stable crack growth for the given two specimens. Additionally, another factor that justifies the previous claim is that the LSR technique should supposedly predict the CI stress accurately, because the stiffness of the elastic part of the lateral strain curve was greater than the slope of the reference line for both specimens. Hence, the large differences between the SD and the LSR methods further highlights the inability of the new technique to predict the CI stress correctly for the two vesicular basalts.

However, as it was explicitly stated in part I the other frequently utilized techniques, such as the LSR, the LSIR, and the VSR methods, were applied and subsequently validated using rocks of low porosity. Particularly, for the LSR method diorites were tested, for the LSIR technique marbles, granites, and sandstones were utilized, and for the VSR method limestone samples were studied. Consequently, none of the frequently applied techniques of the existing literature tested rocks of high

porosity, and specifically vesicular basalts, thus possibly meaning that they may produce inconsistent results for the latter rock type. The previous claim can be easily observed by the very large dispersion of values for the CI stress predicted by the above stated methods. Particularlry, the mean values of the CI stress for basaltic specimens B1 and B2 were approximately 37.56 MPa and 48.70 MPa, respectively. The computed standard deviations were exceedingly high with B1 having around 11.89 MPa, while B2 had close to 16.52 MPa. Therefore, some serious questions arise as to which method ultimately determines the onset of stable crack growth of the previous rock type correctly. As a result, in future research efforts more vesicular basalts need to be tested, in order to fully acknowledge which of the available techniques, including the newly suggested SD method, can accurately predict the CI stress for the latter rock type, because in the present paper only a small number of specimens were available.

Although the SD method had very close results with the other empirical techniques for the marble samples it has a notable limitation. Specifically, its accuracy is heavily influenced by the precision of the polynomial fitting of the lateral strain data, and particularlry the coefficient of determination. This issue is mostly combatted by applying a third-order polynomial fitting that combines a high value for the coefficient of determination, and also excludes the possibility of overfitting. In only one case, a higher-order polynomial, a fourth-order, was necessary in order to satisfy a condition between the coefficients determined from the fitting. Third-order and fourth-order polynomials have been previously used in the literature for the fitting of the curves that have been obtained by compressive tests (e.g. [15,16]), as a means to secure a high value for the coefficient of determination.

5. Conclusions

In part II of this study, a new method for the determination of the onset of stable crack growth was suggested using an elementary mathematical calculus theory. Particularly, the new Second Derivative (SD) method was based on the theorem that states that the points where the second derivative of a function are equal to zero, can be considered as possible inflection points of the function. Generally, the SD technique firstly involved fitting the axial stress (y-axis)-lateral strain (x-axis) data, up until the CD stress, with a third-order polynomial that combined an adequate coefficient of determination and eliminated the possibility of overfitting. Once the function of the lateral strain curve is obtained it must be validated that the condition of Equation (5) does indeed hold. This equation is solely dependent on the coefficients that are produced from the fitting, hence it is of the utmost importance to utilize a reliable software for the third-order polynomial fitting, e.g. MATLAB's curve fitter tool; CurveExpert Professional [17]. If the condition is met, the real solution of Equation (2) is given by Equation (4). If not, a fourth-order polynomial fitting should be applied to the lateral strain data, and Equation (2) must be solved using the new function. The resulting equation from the expansion of Equation (2) is a quadratic polynomial equation that should produce two real solutions. The aforesaid solution, or solutions, of Equation (2), regardless of the order of polynomial fitting, are the possible inflection points of the function. Finally, by observing the form of the lateral strain curve is can be clearly seen that the only inflection point of the curve, prior to the onset of unstable crack growth, is the point from deviation from linearity, hence the CI stress.

Table 1. The predicted CI stress threshold using different methods.

Rock Specimen	CD	SD	LSR		LSIR		VSR		CVS	
	(MPa)	CI (MPa)	CI (MPa)	Difference (%)	CI (MPa)	Difference (%)	CI (MPa)	Difference (%)	CI (MPa)	Difference (%)
M1	28.20	22.00	19.34	2.25	19.34	2.25	9.54	10.54	19.34	2.25
M2	29.33	21.99	8.57	12.13	23.75	1.59	9.38	11.40	19.58	2.18
M3	26.13	19.34	9.12	8.35	18.06	1.05	9.04	8.41	18.06	1.05
M4	24.69	13.34	5.70	9.04	5.70	9.04	7.36	7.07	15.82	2.93
M5	31.35	5.40	12.46	4.95	19.54	9.92	9.42	2.82	17.42	8.43
M6	18.73	9.43	9.43	0.00	8.11	1.27	8.13	1.25	12.53	2.97
M7	23.94	17.74	9.32	9.09	17.34	0.43	8.32	10.17	15.43	2.49
M8	15.90	7.01	8.05	0.92	8.05	0.92	5.99	0.90	13.36	5.59
B1	54.08	48.59	34.42	24.11	22.17	44.95	45.05	6.02	-	-
B2	70.18	63.13	45.43	21.95	26.72	45.15	59.52	4.48	-	-
Mean Marbles	24.78	12.36	10.25	5.84	14.99	3.31	8.40	6.57	16.44	3.49
Mean Basalts	62.13	55.86	39.93	23.03	24.45	45.05	52.29	5.25	-	-
SD Marbles	5.26	6.51	4.12	4.45	6.69	3.85	1.24	4.31	2.62	2.38

SD Basalts	11.38	10.28	7.79	1.53	3.22	0.13	10.23	1.09	-	-
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The SD technique was utilized to determine the CI stress of eight marbles and two vesicular basalts. Its results were also compared with those obtained from the established empirical methods of the existing literature, i.e. the LSR, the LSIR, the VSR, and the CVS methods. Particularly, the results between the SD and all the aforesaid methods were exceptionally close for the eight marble samples with the overall calculated mean difference across all the methods being approximately 4.80 %. Hence, it was made clear that new mathematical-based technique could accurately determine the onset of stable crack growth of that rock type. On the other hand, the SD method showcased very augmented differences with all the other methods, apart from the VSR technique, for the two basalts. Consequently, the fact that the SD and the VSR methods had similar results ultimately revealed that the latter did not predict the CI threshold correctly, because it was extensively analyzed in part I that the VSR method produced erroneous results, due to the unique shape of the volumetric strain curves of the specimens. Moreover, the inaccurate CI stress thresholds that the SD technique produced for the two basalts were also apparent due to very large differences that it displayed with the LSR technique. The LSR method should theoretically determine the previously mentioned threshold correctly, since the stiffness of the elastic part of the lateral strain curve was greater than the slope of the reference line for both samples. Therefore, the SD technique failed to flawlessly determine the onset of stable crack growth of the vesicular basalts. In future research efforts more vesicular basalts should be tested, in order to safely come to the conclusion whether the newly suggested method can consistently determine the CI stress of that rock type or not.

Overall, the CI stress value has a tremendous practical importance for underground works, such as tunnels, shafts etc, since researchers have concluded that it can serve as a much more realistic threshold for the in-situ spalling strength of the rock mass. Consequently, its accurate prediction from laboratory data can serve as a very powerful tool both in the preliminary stages of the project's planning and also during its main excavation and construction phase, because the down-times due to extended failures of the surrounding rock mass will be for the most part diminished. Over the past six decades researchers have proposed a great variety of empirical techniques that can predict the CI threshold with each showcasing its unique strengths and weaknesses. For reference, these were briefly analyzed in part I of this study. As a result, the aforementioned plethora of methods that are available in the literature can sometimes cause confusion as to which method is more appropriate for a certain rock type, loading condition (i.e. uniaxial, biaxial, triaxial conditions), and physical properties of the rock, such as porosity. To sum up, the author strongly agrees with the following statement of Nicksiar and Martin [3]: "... Given the importance of establishing laboratory testing procedures that can be used for estimating in situ strength, it is proposed that the ISRM Suggested Methods develop standardized procedures for establishing crack initiation from laboratory stress-strain data. ...". The previous suggestion was published approximately 13 years ago, to the author's knowledge no steps have been made to fulfil this very accurate proposal.

Acknowledgments

No funding was received to assist with the preparation of this manuscript. The author would like to acknowledge S. Markopoulou and M.A. Marouli for their help in language editing of this paper.

Conflicts of Interest

All the authors claim that the manuscript is completely original. The authors also declare no conflict of interest.

Data availability

All relevant data related to this manuscript are available and can be provided upon reasonable request.

Appendix A1

In Figure 2 below the fitted lateral strain data, along with their respective polynomial functions and their coefficients of determination, are presented for the ten tested rock samples. It should be noted that the fittings were carried out using the CurveExpert Professional [17] software.

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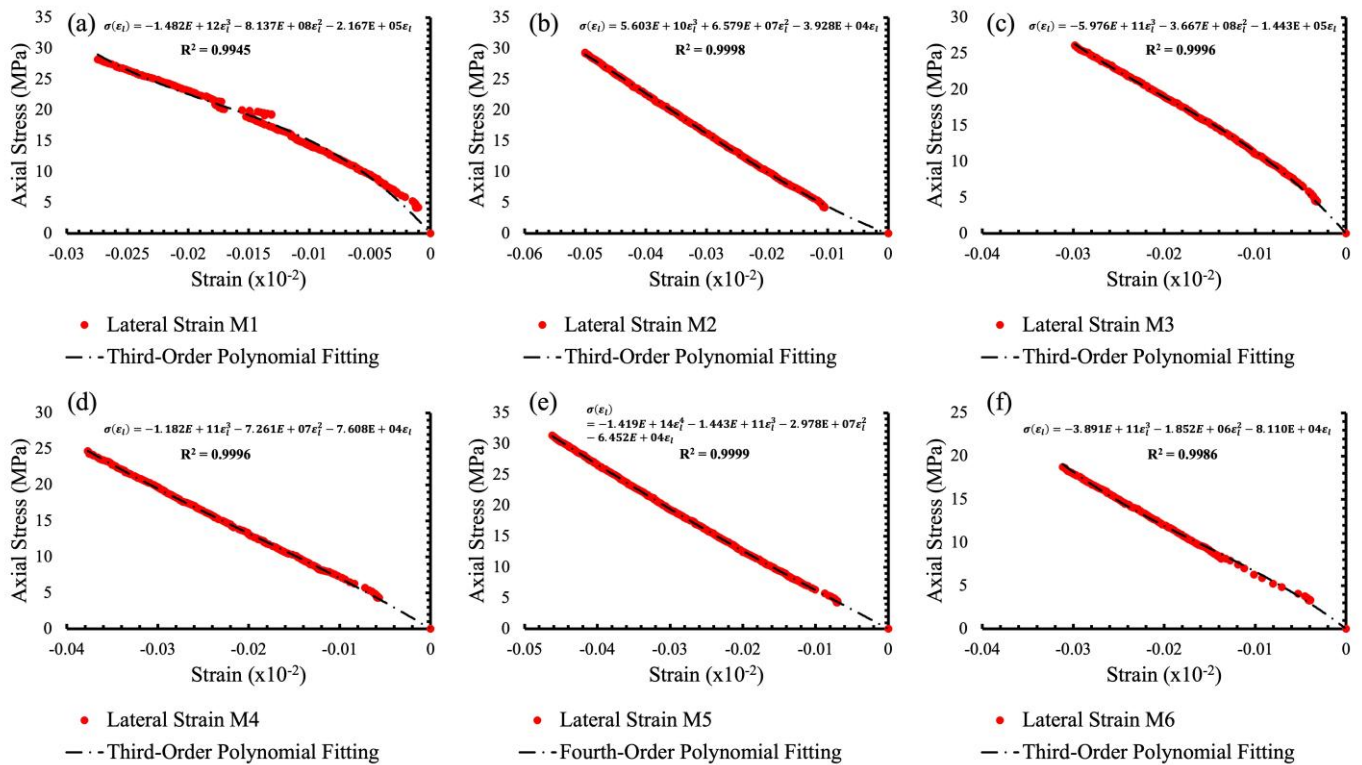


Figure 2. Fitted lateral strain curves of (a) M1; (b) M2; (c) M3; (d) M4; (e) M5; (f) M6.

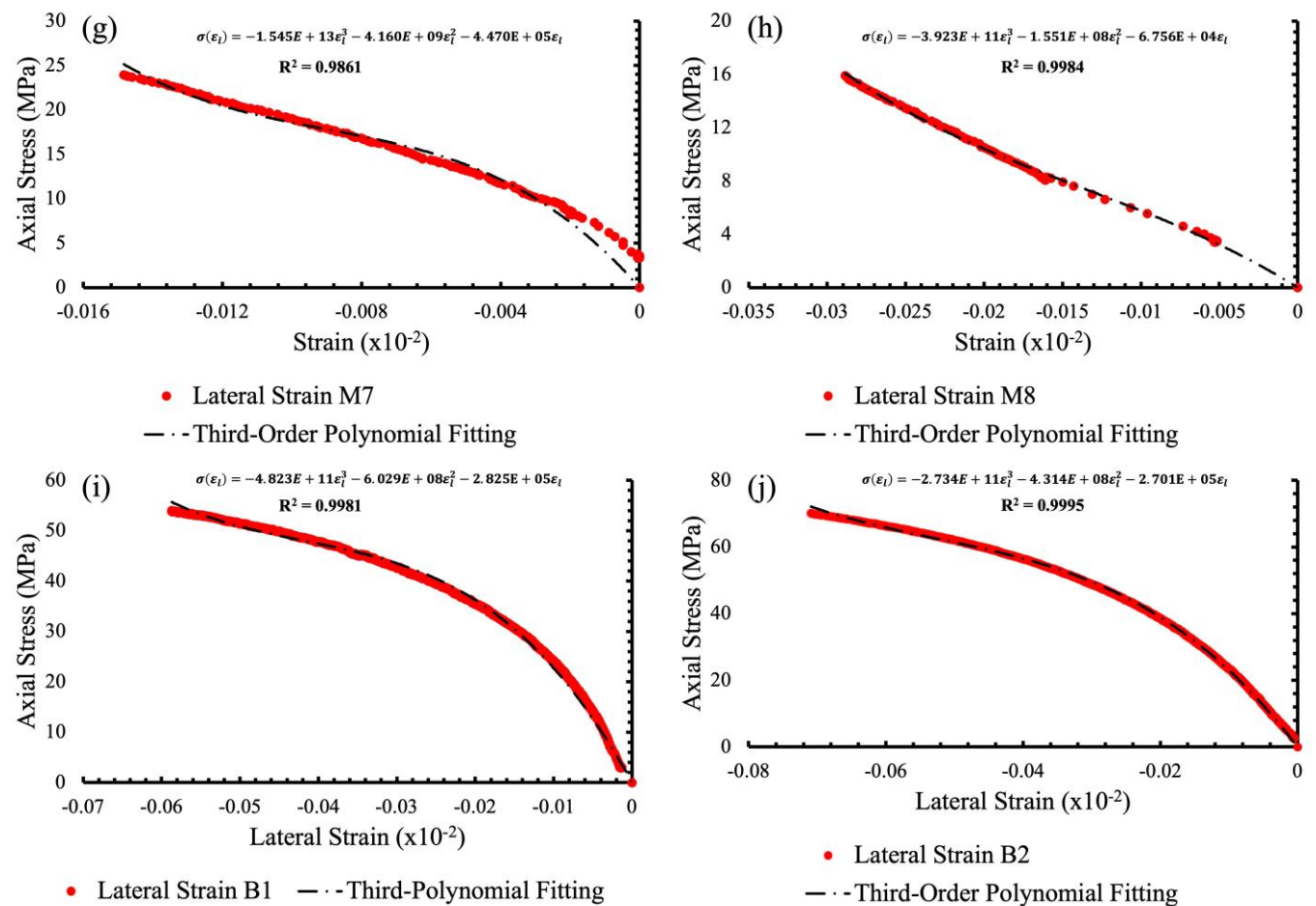


Figure 2. (continued) (g) M7; (h) M8; (i) B1; (j) B2.