

Scientific Project (PIC1)

CRACKING THE CHOCOLATE

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Abstract

The aim of this study was to investigate the fracture behavior of chocolate and determine the most efficient direction to apply force for breaking it. Through a combination of computer simulations using the software Solid Edge 2023 and experimental tests in a laboratory setting, Toblerone[®] chocolate bars were subjected to loading conditions to analyze their geometry and fracture characteristics. The simulations allowed for the exploration of different force application directions, while the laboratory tests utilized the 4 bending test method and a hydraulic press to measure force versus displacement and obtain valuable data. The results revealed important insights into the fracture patterns and mechanisms of chocolate, highlighting the significance of geometry in determining the ease of breaking. The findings indicated that certain force application directions led to more favorable fracture outcomes, with lower forces required to achieve complete breakage.

I. INTRODUCTION

A. "Andas em física, devias saber isso!..."

Chocolate, with its enticing aroma and delightful taste, has captivated the palates of people around the world for centuries. Beyond its culinary allure, understanding the mechanical behavior of chocolate presents an intriguing avenue of exploration, providing valuable insights into typical fracture characteristics and potential applications across diverse industries.

A common topic of debate among connoisseurs and casual consumers alike, the question of the easiest way to break chocolate has long intrigued both amateurs and experts. Motivated by an anecdote involving a familial dispute over chocolate-breaking techniques, our exploration was sparked by the persistent claim of a family member that their preferred method of breaking chocolate was superior. Thus, we embarked on this research endeavor to uncover the scientific principles governing chocolate fracture and to provide evidence-based insights into the most effective approach.

B. Overview of a Fracture

Fracture is a phenomenon that occurs when a material breaks in response to an applied stress. This rupture mainly occurs due to the cracking and breaking of atomic or molecular bonds within the material [1]. The fracture process of materials happens when the stress exerted on them exceeds their elastic limit.

Stress is a physical quantity that describes forces present during deformation [2]. When an object is subjected to external forces that pull it apart, such as stretching an elastic band, it experiences tensile stress, resulting in elongation. On the other hand, when an object is compressed, like a crumpled

sponge being pressed together, it undergoes compressive stress, causing it to shorten.

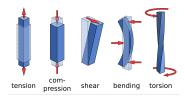


Figure 1: Types of Mechanical Stress [2]

Stress is frequently represented by a lowercase Greek letter sigma (σ) and can be expressed simply as:

$$\sigma = \frac{F}{A} \tag{1}$$

where **F** represents the total force applied and **A** is the total area over which the force is distributed. This representation is applicable when considering simple scenarios with a uniform stress distribution, such as in isotropic materials under uniaxial loading. In such cases, the stress is equal in magnitude and direction in all orientations, resulting in no variation across the material.

However, it's important to note that stress is generally treated as a tensor quantity. In three-dimensional space, stress is represented by a stress tensor, consisting of nine components:

$$\sigma = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix}$$

This tensorial representation captures not only the magnitude of stress but also its directionality and variation across different planes within the material.

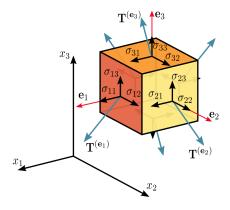


Figure 2: Tensor Representation of Stress [3]

Strain represents the measure of deformation in a material resulting from applied forces or displacements [4]. It measures the material's response to stress and is expressed as:

$$\epsilon = \frac{\Delta L}{L} \tag{2}$$

where L represents the original length and ΔL the change in length.

In a continuous body¹, the presence of applied forces or changes in temperature gives rise to a stress field, which in turn leads to a deformation field. The relationship between stress and strain is described by constitutive equations, such as Hooke's law for linear elastic materials. When a stress field is applied and subsequently removed, deformations that completely recover the body's original configuration are referred to as **elastic deformations**.

On the other hand, certain deformations persist even after the removal of stresses. These irreversible deformations are known as **plastic deformations** [4][6]. They occur in material bodies when the applied stresses exceed a certain threshold called the elastic limit or **yield stress**. Plastic deformations are attributed to atomic-level mechanisms, such as slip or dislocation, and they cause permanent changes in the material's shape.

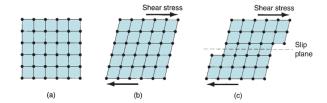


Figure 3: «Deformation of a crystal structure: (a) original lattice; (b)elastic deformation, with no permanent change in positions of atoms; and (c) plastic deformation, in which atoms in the lattice are forced to move to new "homes."»[7]

The Stress-Strain graphs show the relationship between applied stress and resulting deformation, revealing important properties like yield strength, ultimate strength (maximum stress the material can withstand), and toughness (ability to absorb energy before fracture).

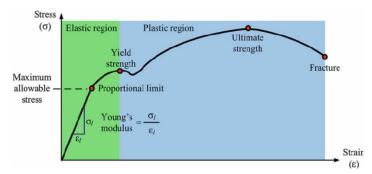


Figure 4: Conventional Stress vs Strain Graph [8]

While in the plastic region, stress and strain are usually proportional, with its proportionality constant being called **Young's Modulus** (represented by the letter **E**) and given naturally as:

$$E = \frac{\sigma}{\epsilon} \tag{3}$$

By this point, it becomes crucial to distinguish types of fractures and materials. Fractures can be classified into **ductile** and **brittle**, depending on the material's response to stress. Ductile fractures are characterized by significant plastic deformation before failure, while brittle fractures occur with minimal plastic deformation. Just like so, materials that exhibit a significant ability to undergo plastic deformation are referred to as ductile, whereas materials that fracture with minimal plastic deformation are considered brittle [4].

¹In the context of mechanics and materials science, a continuous body refers to a physical entity or material that is considered to have a continuous and uninterrupted structure throughout its entirety, exhibiting homogeneous properties and behavior. It is characterized by the absence of voids, gaps, or discontinuities at macroscopic scales. [5]

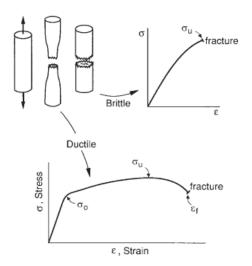


Figure 5: Types of materials and their strain-stress graphs [4]

Chocolate exhibits both brittle and ductile behavior due to its unique composition and structure. The brittleness is influenced by the semi-crystalline fat network formed by cocoa butter, where the liquid portion is trapped within. The van der Waal's forces contribute to the formation of interactions between fat molecules in cocoa butter, affecting the overall brittleness of chocolate [9].

The ductility arises from the presence of non-fat solid particles suspended in the fat network. Interactions between these particles, as well as particle-fat interactions, contribute to the chocolate's ductile properties. Additionally, **hydrogen bonding** between polar particles further influences its ductility [9].

Ductile materials can also become brittle due to temperature change, like chocolate, for example. As the temperature decreases, the fatty acids in cocoa butter start to solidify and form crystal structures, enhancing its brittle characteristics.

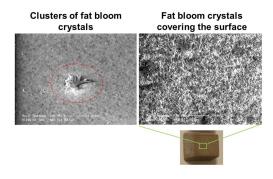


Figure 6: Fat Crystals on Chocolate [10]

C. Stress Raisers

Notches are intentional or unintentional discontinuities in a material that can significantly affect its strength and fracture behavior. The presence of a notch causes stress concentration, resulting in higher stresses at the notch tip compared to the surrounding material. This localized concentration of stress can significantly affect the material's strength and fracture behavior.

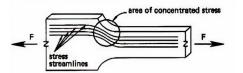


Figure 7: Streamline analogy to stress concentrations [11]

The Stress Concentration Factor (K_t) is a dimensionless parameter that quantifies the amplification of stress at the discontinuity compared to the stress in the unnotched region. It is defined as the ratio of the maximum stress at the notch or hole to the nominal stress² in the material without the discontinuity:

$$K_t = \frac{\sigma_{\text{max}}}{\sigma_{\text{nom}}} \ge 1 \tag{4}$$

The maximum stress at the notch can be obtained through numerical analyses, such as finite element simulations. The nominal stress can be given as [12]:

$$\sigma_{\text{nom}} = \frac{3PL}{2Bh^2} \tag{5}$$

with P the applied load, L the span length, B the depth and h the width.

It is worth noting that when comparing identical materials with varying stress concentration factors (K_t) at a specific location, the material with a higher K_t is more susceptible to failure or breakage; because of the bigger amplification of stress, this results in significantly higher local stress levels, when compared to the nominal stress applied to the material.

D. Bending Tests

Bending tests are mechanical tests used to evaluate the behavior and mechanical properties of materials under bending loads. These tests involve ap-

²Nominal stress is the average stress along a specific cutting plane within a structure.

plying a load to a specimen, typically in a threepoint or four-point configuration, to induce bending deformation [13].



Figure 8: 3-point bend test [14]

II. EXPERIMENTAL PROCEDURE

The primary objective of this study is to determine the easier way to break chocolate, whether it is with **Method 1** or **Method 2**.

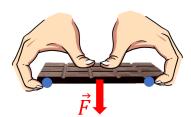


Figure 9: Method 1

In Method 1, the chocolate sample is positioned with the notch or crack facing upwards, and the force is applied perpendicularly downwards.

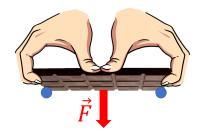


Figure 10: Method 2

In Method 2, the chocolate sample is positioned with the notch or crack facing downwards, and the force is applied perpendicularly downwards as well.

To study the problem, a 4-point bending test was conducted in the laboratory, and numerical simulations were performed.

A. 4-point bend test

The 4-point bending test involved placing the chocolate sample on two supports and applying a load at two points in between, according to C393 standard [13]:

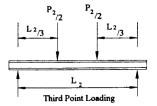


Figure 11: C 393 Standard [13]

It was used two thin plates of aluminium to, depending on the situation, either to disperse the force from the hydraulic press evenly across the fragile vertices of the triangle or to help support the triangle on the base (see figures 12 and 13).

As sample, it was used half of a 100 g Toblerone chocolate bar to each experiment, and depending on the method being tested, it was placed either facing upwards or downwards.



Figure 12: Method 1 Apparatus



Figure 13: Method 2 Apparatus

The sample had the following dimensions, in mm (with an uncertainty of $\frac{1}{20}$ cm):

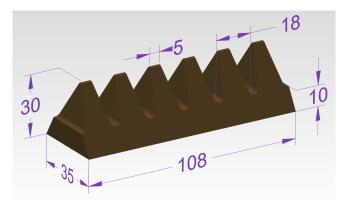


Figure 14: Toblerone 100 g half bar, modeled in Solid Edge 2023.

During the testing process, the hydraulic press (Instron 5566 model) was operated with precision to apply a controlled and gradual load on the chocolate samples. The load was increased at a constant rate of 3 mm/min, allowing sufficient time for the chocolate to deform and fracture. The maximum load force experienced by each sample was recorded, and the average value was calculated to determine the overall strength of the chocolate in each method.

To ensure the reliability of the experimental data, multiple trials were performed for each method, with the uncertainties represented by the standard deviations. This approach allows for a more robust analysis and reduces the impact of random variations in the results.

The temperature registered in a mobile app was $(23 \pm 1)^{\circ}$ C.

B. Numerical simulation

A finite element simulation is a computational method used to analyze and predict the behavior of complex systems or structures. The simulation is based on the discretization of the object or system into smaller, finite elements. These elements represent specific regions or volumes within the object and are interconnected at shared nodes. By applying mathematical equations and numerical techniques, the behavior of each element can be determined, allowing for the overall response of the entire system to be calculated. Since the focus of this work does not involve discussing these models, they will not be elaborated on here. However, it can be found extensive discussions on the matter in the following references [15][16][17].

For the simulation it was used Solid Edge 2023. It was created a new material to recreate chocolate's

mechanical characteristics, with the following properties:

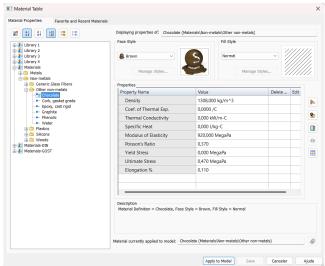


Figure 15: Material Creation in Solid Edge

The properties were taken from [12] Table 1.

It was chosen to simulate both methods in the same way as one would physically break a Toblerone, in order to obtain more meaningful results. The bottom face was fixed, with the force being applied as one would do in real life.

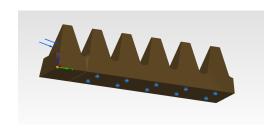


Figure 16: The Toblerone's Equivalent Fracture of Method 1

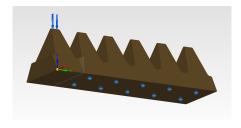


Figure 17: The Toblerone's Equivalent Fracture of Method 2

For the simulation, the following parameters were chosen:

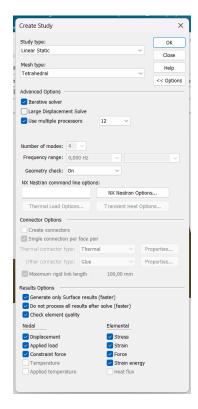


Figure 18: Parameters Chosen

III. RESULTS

A. 4-point bend test

The results for the experimental apparatus are represented in the following Force vs Displacement Graphs.

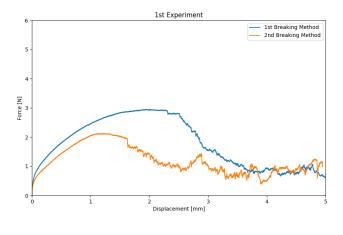


Figure 19

Maximum Load Forces for 1st Experiment

Method 1: 2.9484 ± 0.0001 N Method 2: 2.1238 ± 0.0001 N

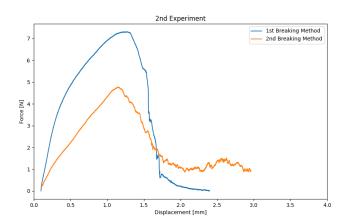


Figure 20

Maximum Load Forces for 2nd Experiment

Method 1: $7.3100 \pm 0.0001 N$ Method 2: $4.7636 \pm 0.0001 N$

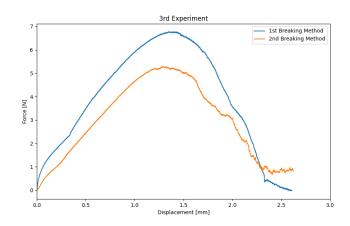


Figure 21

Maximum Load Forces for 3rd Experiment

Method 1: $6.7726 \pm 0.0001 N$ Method 2: $5.2856 \pm 0.0001 N$

The fractures were registered:



Figure 22: Fracture of Method 1



Figure 23: Fracture of Method 2

B. Numerical Simulation

The result of the two simulations were as follows:

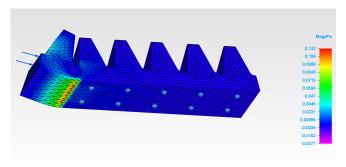


Figure 24: Fracture of Method 1

Max Principal Stress: 0.122 MPA

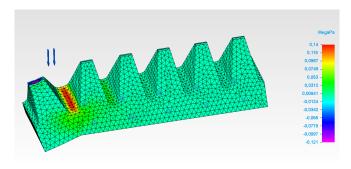


Figure 25: Fracture of Method 2

Max Principal Stress: 0.14 MPA

DATA ANALYSIS AND FINAL **COMMENTS**

The analysis of the graphs reveals the different behavior of chocolate. In the first test, the chocolate was exposed to room temperature for a longer period and was more melted. As a result, its ductile behavior became more evident, which is visible in the graph as it approaches that of a ductile material, unlike the other graphs that exhibit more brittle characteristics. The data from the graphs lead to the conclusion that the second method required less force to break the chocolate compared to the first method: this was observed in all the tests made. If we calculate the averages:

For Method 1

Load Forces: 2.9484 ± 0.0001 N, 7.3100 ± 0.0001 N, 6.7726 ± 0.0001 N

Average Load Force = 5.6767 N

Uncertainty Calculation:

$$\sigma_{\text{average}} = \frac{1}{\sqrt{N}} \sqrt{\sum_{i=1}^{N} \sigma_i^2}$$

$$\begin{split} \sigma_{\text{average}} &= \frac{1}{\sqrt{N}} \sqrt{\sum_{i=1}^N \sigma_i^2} \\ \text{Therefore, the average load force for Method 1 is} \end{split}$$
 5.6767 ± 0.0001 N.

Doing the same steps for Method 2, we get to the conclusion the average load force for Method 2 is 4.0577 ± 0.0001 N.

There's a difference almost of 2N (1.619N) on the difference average of the two methods maximum loading forces.

The significant difference in breaking force between the two methods was expected since the second method involved the use of a notch in the area where the crack is initiated, which acts as a local stress concentrator, as we saw previously. Consequently, less force was needed to initiate fracture compared to the first method. The simulation data also supported this finding by showing higher stress values in the fracture zone for the second method, indicating easier fracture initiation. And although the maximum stress values obtained from the simulations do not directly correspond to the 4-point bending test conditions, they provide qualitative insight into the stress concentration factor. It can be inferred that the stress concentration factor for the second method would be higher than that of the first method, consistent with the previous observations.

In conclusion, the objectives of this study, which aimed to investigate chocolate fracture and determine the easiest way to break it, have been achieved. Through data analysis and theoretical considerations, the second method emerged as the easiest way to fracture the chocolate due to the promoting effect of the notch.

Regarding the specific case of Toblerone, although the fracture analysis and simulation confirmed the easiest method, pulling the triangles inward might be easier from an ergonomic standpoint. This could be attributed to the dexterity of our opposable thumb and the ease of creating inward force compared to prying the thumb and fingers apart. Additionally, the geometry of Toblerone makes it easier to grip and push the triangles forward rather than pulling them backward. Therefore, while mechanical fracture analysis suggests a downward force as the technically easier method, ergonomic factors should also be considered when evaluating what appears to be the easiest approach.

It should be noted that the location of fracture differed between the two methods in the 4-point bending test. In the first method, the fracture occurred at the center of the bar, while in the second method, it occurred near the hydraulic press' cylinder, a common occurrence in such tests [18]. However, for the purposes of this study, the focus was not on the location of fracture but rather on understanding the timing and manner of fracture - and indeed it was observed that the second method exhibited faster fracture and required less force under the same loading and positioning conditions, despite of the fracture position.

Other thing worth to be noted is that chocolate's complex and non-linear behavior, influenced by temperature, moisture content, and microstructure, makes it challenging to accurately capture its fracture process using LEFM's (Linear Elastic Fracture Mechanics) simplified assumptions. Chocolate is a viscoelastic material, exhibiting both elastic and viscous responses under stress. Nevertheless, the 4-point bending test and numerical simulations provided valuable insights into the fracture behavior of chocolate, despite the limitations of the models used.

To overcome these limitations, future studies could explore more advanced fracture mechanics models that incorporate the viscoelastic and non-linear properties of chocolate. These models could consider factors such as strain-rate dependency, moisture content, and microstructural effects to provide a more accurate representation of chocolate fracture behavior.

Different chocolate formulations, sizes, and testing conditions may yield different results. Therefore, further investigations involving a broader range of chocolate samples and testing conditions would contribute to a more comprehensive understanding of chocolate fracture behavior.

REFERENCES

[1] V. Altstädt, J. K. Sandler, and H. Ruckdäschel, "Influence of nanoscale morphology on

- the micro- and macromechanical behaviour of polymers and polymer nanocomposites," Mar 2007.
- [2] W. Contributors, "Stress (mechanics)," Jun 2023.
- [3] W. Contributors, "Cauchy stress tensor," Mar 2023
- [4] N. E. Dowling, M. V. Kral, and S. L. Kampe, Mechanical behavior of materials: engineering methods for deformation, fracture, and fatigue. Hoboken, Nj: Pearson Education, Inc, 2019.
- [5] A. M and A. Guran, Theory of elasticity for scientists and engineers. Boston: Birkhauser, 2000.
- [6] Wikipedia contributors, "Deformation (physics)," Year. Accessed on 16 June, 2023.
- [7] R. S. Molla, "A study on manufacturing of deformed bar (g 60-400w) at elite iron and steel industries," 05 2018.
- [8] C. Engineering, "Stress strain curve || detail explanation," Nov 2018.
- [9] H. Zhao, B. Li, and B. J. James, "Structure-fracture relationships in chocolate systems," LWT, vol. 96, p. 281–287, Oct 2018.
- [10] J. Carson, "The process of fat bloom formation in pralines and its main causes," Jul 2017.
- [11] T. C. Tech, "Machine elements design." http://www.thecartech.com/newsite/subjects/machine_elements_design/note_2.htm.
- [12] F. Gómez, A. Salazar, M. I. Martínez, S. Rana, and J. A. Rodriguez, "Fracture of notched samples of chocolate," vol. 121, p. 103477–103477, Oct 2022.
- [13] J. R. Davis, Tensile testing. Materials Park, Ohio: Asm International, 2004.
- [14] Thwing Albert, "Ta238 3-point bending fixture." https://www.thwingalbert.com/es/producto/ta238-3-point-bending-fixture/, Jul 2022.

- [15] Y. Chen, X. Hu, and B. Liu, "Modelling of bone fracture using the fundamental functional unit osteon," vol. 118, p. 103216–103216, Dec 2021.
- [16] A. M. Ranjbar, A. Izadpanahi, and A. A. Ebrahimi, "Numerical analysis of geomechanical behavior of fractures and faults in a deformable porous medium," vol. 12, p. 2955–2966, Apr 2022.
- [17] J. Chen, L. Zhou, A. I. Chemenda, B. Xia, X. Su, and Z. Shen, "Numerical modeling of fracture process using a new fracture constitutive model with applications to 2d and 3d engineering cases," vol. 8, p. 2628–2647, Mar 2020.
- [18] J. S. Lobo, "Study of four point bending specimen geometry," Master's thesis, IST, Lisbon, October 2020. Thesis to obtain the Master of Science Degree in Mechanical Engineering.

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