

COMPUTATIONAL MECHANICS OF COMBINED PLANAR DEFECTS: EXTRINSIC + INTRINSIC FAULTING IN 3C CLOSE PACKED CRYSTAL STRUCTURES

MECÁNICA COMPUTACIONAL DE DEFECTOS PLANARES COMBINADOS: FALLAS EXTRÍNSECA + INTRÍNSECA EN ESTRUCTURAS CRISTALINAS COMPACTAS DEL TIPO 3C

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Recently, extrinsic faulting has been discussed within the framework of computational mechanics allowing to derive expressions for the statistical complexity, entropy density and excess entropy as a function of faulting probability. In this contribution the analysis is extended to consider the combined presence of two planar faults type within the random faulting model. Extrinsic+intrinsic faults are considered. The ϵ -machine description of the faulting dynamics is presented. Entropic magnitudes are derived as well as expressions for the hexagonality and the probability of consecutive symbols in the Hägg coding. The analysis continues the study started with individual faulting types under the computational mechanics approach.

Recientemente, la mecánica computacional ha sido utilizada para discutir defectos cristalinos extrínsecos en estructuras compactas, en esta contribución el análisis es extendido para incluir la presencia simultánea de defectos intrínsecos. Ambos tipos de defectos cristalinos (extrínsecos+intrínsecos) se asumen dentro del modelo de defectos aleatorios no interactuantes. La descripción está basada en la construcción de la máquina de ϵ , ello permite introducir medidas entrópicas, así como la expresión para la hexagonalidad. El análisis continúa el estudio ya comenzado sobre defectos individuales desde el punto de vista de la mecánica computacional.

PACS: Stacking faults and other planar or extended defects (Fallas de apilado y otros defectos planares o extendidos), 61.72.Nn; time series analysis (análisis de series temporales), 05.45.Tp

I. INTRODUCTION

Computational mechanics aims at treating complexity in dynamical systems by looking at it as a computational device capable of performing physical computation, that is, to store and process information [1]. The approach, as pioneered by Crutchfield et al [2], aims at building the less powerful computational device that can optimally describe the system behavior. Optimality means that any other computing model will be at most, as good in its description capability as the less powerful model. This optimal computing model is called an ϵ -machine. Once the ϵ -machine is found, it is possible to characterize the system by several entropic measures.

The use of computational mechanics in the study of planar faulting have been pioneered by Varn *et al.* [3–6], and Estevez-Rams et al, [7–10]. The approach starts by coding the stacking sequence in close packed structures (CPS) by using some binary code (e.g. Hägg notation or Jagodzinski notation) and then building an optimal Hidden Markov Model (HMM) description of the faulting dynamics. From there it is possible to capture the occurrence of pattern, the amount and nature of disorder and the correlation among features in the stacking arrangement [5, 11]. The HMM approach is general enough to be used beyond the faulting model to describe disorder and polytypism [8,9].

Close packed structures are crystal structures resulting from the stacking of identical periodic layers. They can be treated, once a layer motif is defined, as a one dimensional problem. From the crystallographic perspective they are order-disorder (OD) structures built by stacking hexagonal layers [12]. The constrain that reduces the number of possibilities is that two consecutive layers are not allowed to have the same lateral displacement. The most common CPS are the cubic close packed or 3C (Bravais lattice of type *cF*) and the hexagonal close packed or 2H (Bravais lattice of type *hP*). These two are also the simplest types of polytypes, as each layer is crystallographically equivalent to any other layer (they have the same spatial environment). It is common that periodicity in the stacking arrangement of CPS is not perfect. The disruption of stacking periodicity is known as planar disorder or stacking faults. The model that considers that a single occurrence of planar faulting is an independent event is called the Random Faulting Model (RFM). Within this model, faulting is reduced to certain types: intrinsic (removal of a layer from the sequence), extrinsic (addition of a layer to the sequence) and twinning (change of orientation in the sequence). In the RFM, a constant probability can be assigned to each type of stacking faults [13–15].

RFM is too simple to describe heavy faulting density in solids. The main limitation comes from neglecting any

interaction between defects. Besides such assumption it also considers that no other type of defects happens in the crystal. This assumption implies that faults go through the whole crystal, avoiding the need to account for the appearance of partial dislocations. Finally, planar faulting are taken to occur along only one stacking direction independently of the fact that crystallographic symmetry may imply several possible stacking directions in the crystal (e.g. face centered cubic crystal can be described by several stacking directions all belonging to the $\langle 111 \rangle$ family of equivalent directions).

In spite of its simplicity, the RFM is still interesting as a reference model. It is a good starting point for more sophisticated calculations [16].

In the past, intrinsic and twin faulting in CPS have been studied under the approach of computational mechanics [7]. This study has been followed more recently to include single extrinsic faulting [10]. What has not yet been reported are models that account for the simultaneous occurrence of extrinsic faulting and the other types of defect. The purpose of this paper is to report such analysis for extrinsic+ intrinsic fault model.

In this contribution, the same procedure described in the analysis of extrinsic faulting as explained in [10] will be followed. It will be clear that allowing two type of defects adds several complications to the analysis. Several analytical expressions for disorder will be reported. We have tried to make the article as much as self contained as possible.

II. STACKING FAULTS IN CLOSE PACKED ARRANGEMENTS.

In close packed structures such as face centered cubic (FCC), layers can be stacked in three positions according to their lateral displacement with respect to a common origin. This positions are usually labeled A , B and C [12]. The FCC structure stacking order is then described by $ABCABC\dots$, while the hexagonal compact structure has a stacking described as $ABABAB\dots$ [17]. The close packed constrain then means that in the stacking arrangement the same letter can not happen consecutively.

Hägg devised a less redundant coding [18]. When a pair of layers are of the types AB , BC or CA a plus (or 1) code is assigned, a minus (or 0) otherwise. The close packed constrain is built into the Hägg notation [19]. An interesting feature of the Hägg notation is that the stacking arrangement is now a binary string instead of a three symbols sequence.

Every time that the periodic arrangement is interrupted it is considered a fault. The most simple faults that can be considered are (1) the missing of a layer, or intrinsic fault, for example in the FCC structure could be $ABCA|CABC$, where the $|$ stands for where the fault has occurred. As second type of fault and somehow opposite to the previous one is the (2) extrinsic fault, which is the insertion of a layer in the periodic sequence. In the FCC structure could be $ABC|B|ABC$, where an extraneous B layer has been added to the ideal sequence. Finally a third type is the (3) twin fault which is a reversion of

the stacking ordering. Again, in the FCC structure could be $ABCABC|BACBAC$. In what follows, the probability for the occurrence of a deformation fault will be denoted by α , and of an extrinsic fault by γ .

Using the Hägg code, the different faulting dynamics can be described by a finite-state automaton or machine which is equivalent to a Hidden Markov Model (HMM). A HMM will be defined by an alphabet, in our case the binary alphabet $\{0, 1\}$, a numerable set of states \mathcal{S} , and the transition probabilities between states. The set of transition probabilities defines the transition matrices $\mathcal{T}^{[v]}$, where each entry $t_{ij}^{(v)}$ represents the probability of jumping from state i to state j , while emitting the symbol $v \in \{0, 1\}$ [3-7]. The stochastic transition matrix is defined as $\mathcal{T} = \mathcal{T}^{[0]} + \mathcal{T}^{[1]}$.

According to the HMM description a particular stacking arrangement can be seen as a realization of the finite-state automaton. The system starts at some predefine state and, as it performs transitions with a given probability from one state to another, it outputs a symbols $v \in \{0, 1\}$. In this way, from the HMM perspective, a sequential dynamical system has been defined, statistically equivalent to the stacking arrangement. Care must be taken not to consider the dynamical system as a model of the actual physical or chemical process that lead to the stacking arrangement in the solid. The HMM is just a convenient mathematical device that allows to capture the relevant features in the stacking ordering.

The output of the HMM is a bi-infinite string Υ of 0's and 1's. Of all the HMM models describing a given stacking ordering the minimal one is taken as to be optimal, in the sense of using less resources (number of states) to describe the system ordering. If we add the constrain that in this minimal model, given a state, the output symbol determines unambiguously the transition to another state (unifiliar property), then it is called an ϵ -machine [1, 2].

Once the ϵ -machine of the stacking process is found, several measures can be defined. The statistical complexity C_μ is defined as the Shannon entropy [20] over the ϵ -machine states,

$$C_\mu = - \sum_i p_i \log p_i, \quad (1)$$

where p_i is the stationary probability of the i th-state. The sum is over all states probabilities, logarithm is taken in 2 and in what follows base 2. C_μ measures the amount of information the system stores.

If we denote by $\langle \pi |$ the vector of state probabilities p_i , then $\langle \pi |$ can be calculated as the normalized left eigenvector of the transition matrix \mathcal{T} with eigenvalue unity.

$$\langle \pi | = \langle \pi | \mathcal{T}. \quad (2)$$

The Shannon entropy $H(X)$ for an event set X with discrete probabilities distribution $p(X)$ is defined as [20]

$$H(X) = - \sum_i p(x_i) \log p(x_i), \quad (3)$$

where the sum is taken over all the probability distribution. The units of the entropy are bit.

For the set of all strings Υ^N of length N , the Shannon block entropy $H(\Upsilon^N)$ is given by equation (3), where $p(X)$ is taken as the probability of a given string belonging to Υ^N . The entropy density or entropy rate h_μ is defined as

$$h_\mu = \lim_{N \rightarrow \infty} \frac{H(\Upsilon^N)}{N}, \quad (4)$$

when such limit exist. h_μ is a measure of the irreducible disorder in the stacking arrangement [21].

For an ϵ -machine the entropy density is given by [22]

$$h_\mu = - \sum_{k \in \mathcal{S}} P(k) \sum_{x \in \{0,1\}} P(x|k) \log P(x|k), \quad (5)$$

where $P(a|b)$ means the probability of a conditioned on b . The unit of the entropy density is bit/site.

Consider any position in the bi-infinite string Υ , from that point it can be defined the left half infinite string $\overleftarrow{\Upsilon}$, and the right infinite half $\overrightarrow{\Upsilon}$. Excess entropy E is a measure of predictability and it is defined as the mutual information between the left half and the right half in the system output,

$$E = H(\overleftarrow{\Upsilon}) + H(\overrightarrow{\Upsilon}) - H(\Upsilon). \quad (6)$$

Hexagonality is a measure of the fraction of hexagonal environments found in the stacking sequence. A hexagonal environment is one where a layer has the same displaced layer type above and below (ABA , ACA , BCB , BAB , CBC and CAC). Hexagonality can be calculated as the sum of the probability of occurrence of a sequence 01 and a sequence 10 in the Hägg code. The probability of a sequence 01 is given by

$$P(01) = \langle \pi | \mathcal{T}^{[0]} \mathcal{T}^{[1]} | 1 \rangle, \quad (7)$$

correspondingly for a sequence 10

$$P(10) = \langle \pi | \mathcal{T}^{[1]} \mathcal{T}^{[0]} | 1 \rangle. \quad (8)$$

$|1\rangle$ is a vector of 1's.

III. SINGLE FAULTING DESCRIPTION IN THE FACE CENTERED CUBIC STACKING ORDER

The ideal FCC stacking in the Hägg notation is described as a bi-infinite string of 1s or 0s. The HMM description of an intrinsic fault in a 3C stacking arrangement is depicted in Fig. 1a. In what follows it will be considered the ideal 3C structure described by a sequence of 1s, corresponding to the sequence that goes in the direction $A \rightarrow B \rightarrow C$.

The occurrence of an intrinsic fault, governed by a probability α , is reflected as the insertion of a 0. This case was already analyzed in [7]. The HMM description of the intrinsic faulting process has one state and it is equivalent to the flipping of a biased coin.

The HMM description of an extrinsic fault has been analyzed in [10] and it is shown in Fig. 1b. This case is slightly

more involved than the previous one. The occurrence of the extrinsic fault with probability γ is reflected in the Hägg code as the insertion of two consecutive 0s. The ϵ -machine is made of two states. While no faulting occurs the system stays in the f state, but as soon as an extrinsic fault happens, there is a transition to an e state upon emitting a 0, from where the system returns with certainty to the f state emitting another 0. In [8] is discussed how this dynamics is equivalent to a biased even process.

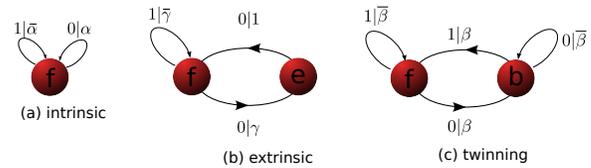


Figure 1. The Hidden Markov Model (HMM) of the (a) intrinsic, (b) extrinsic and (c) twin faults in a 3C structure. The label besides the directed arcs slp must be understood as the symbol emitted with the given probability.

The third type of faulting considered is the twin fault. The probability of occurrence is denoted by the letter β . This faulting has been reported in [7]. The ϵ -machine description is shown in figure 1c. For this type of defect the two possible 3C sequence, one made of 1s and the other of 0s, can happen. The twin fault is nothing else than a jump from one type of sequence to the other.

IV. COMBINED FAULTING IN THE FACE CENTERED CUBIC STACKING ORDER

The HMM description of the stacking arrangement in the presence of combined faulting should be the addition of the HMM for each type of defect. Yet, this is not enough. Additionally, the case of simultaneous occurrence of more than one defect has to be taken into account. Both operations, the direct sum of the isolated HMM and the emergence of new transitions as result of simultaneous defects can result in a non-unifiliar HMM. In such case, the description can not be considered a valid ϵ -machine. In particular it is not well suited for the calculation of the statistical complexity, the entropy density and the excess entropy. A unifiliar representation can be found from the non-unifiliar one by means of mixed states [23].

IV.1. Extrinsic + intrinsic faulting

A possible HMM description for this case is shown in Fig. 2.

The corresponding transition matrix will be given by

$$\begin{aligned} \mathcal{T}^{[1]} &= \begin{pmatrix} \bar{\alpha}\bar{\gamma} + \alpha\gamma & 0 \\ 0 & 0 \end{pmatrix} & \mathcal{T}^{[0]} &= \begin{pmatrix} \alpha\bar{\gamma} & \bar{\alpha}\gamma \\ 1 & 0 \end{pmatrix} \\ \mathcal{T} &= \begin{pmatrix} \bar{\alpha}\bar{\gamma} + \alpha & \bar{\alpha}\gamma \\ 1 & 0 \end{pmatrix} & &= \begin{pmatrix} \alpha\gamma + \bar{\gamma} & \bar{\alpha}\gamma \\ 1 & 0 \end{pmatrix} \end{aligned} \quad (9)$$

where $\bar{\alpha} = 1 - \alpha$ and $\bar{\gamma} = 1 - \gamma$. The stationary probabilities over the recurrent states f and e can be calculated following

equation (2) which results in

$$\langle \pi | = \left(\frac{1}{1 + \bar{\alpha}\gamma}, \frac{\bar{\alpha}\gamma}{1 + \bar{\alpha}\gamma} \right), \quad (10)$$

the first value corresponds to the f state.

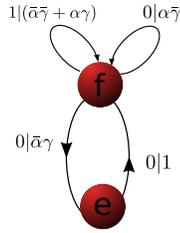


Figure 2. HMM of the 3C system with extrinsic+intrinsic faulting. Labels follow the same description as in Figure 1.

In order to obtain the hexagonality, the probabilities of the sequences 01 and 10 has to be calculated from equations (7) and (8), both expressions turn to be equal and given by

$$P(01) = P(10) = \frac{\alpha\bar{\alpha}(1 - 2\gamma)^2 + \bar{\gamma}\gamma}{1 + \bar{\alpha}\gamma}, \quad (11)$$

from where the hexagonality is given by $2P(01)$. Hexagonality has a maximum value of $1/2$ at $\alpha = 1, \gamma = 1/2$ or $\alpha = 1/2, \gamma = 0$.

The statistical complexity can be considered as given by equation (1). Results are shown in Fig. 3. For a fixed value of γ , increasing value of faulting probabilities results in a decrease of C_μ . For the intrinsic faulting with almost no extrinsic faulting the system is almost all the time in the single state f (Fig. 2). For increasing value of α , extrinsic faulting cancels and the only disorder is given by the intrinsic faulting, correspondingly C_μ decreases (Fig. 3a).

The HMM description used so far can not be considered an ϵ -machine because it does not have the unifilar property. In order to derive the ϵ -machines we need to build a unifilar description from the already found HMM, which results in a mixed state representation. The procedure for doing so can be found in [23]. The result for this case is shown in Fig. 4, where the set of states in the mixed state representation will be denoted by \mathcal{M} .

The first thing to notice is that the unifilar FSA has a numerable but infinite number of states. The starting state is labeled with an S which has a transient character (asymptotically the probability of the system in this state is zero), and the same goes for all states labeled as T_n .

The state labeled as F is recurrent with probability

$$P(F) = \langle \pi | \mathcal{T}^{[1]} | 1 \rangle = \frac{\bar{\alpha} + \gamma(2\alpha - 1)}{1 + \bar{\alpha}\gamma}, \quad (12)$$

for $\gamma = 0, P(F) = \bar{\alpha}$, and for $\alpha = 0, P(F) = \bar{\gamma}/(1 + \gamma)$.

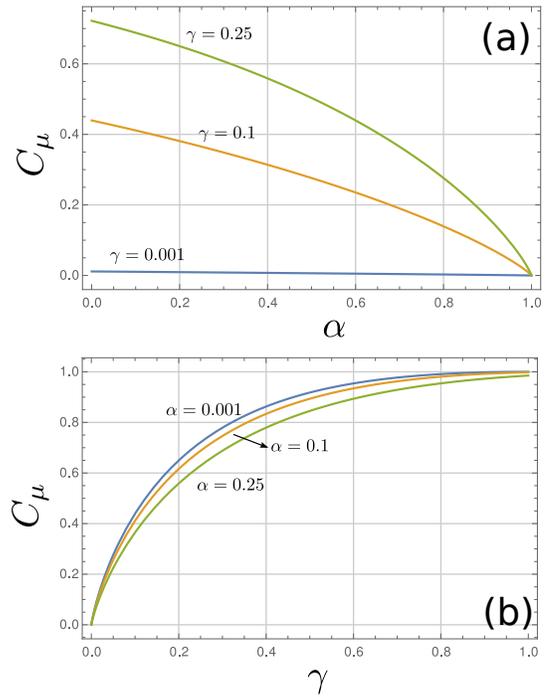


Figure 3. Statistical complexity as a function of (a) the intrinsic fault probability for fixed extrinsic fault probability; (b) the extrinsic fault probability for fixed intrinsic fault probability.

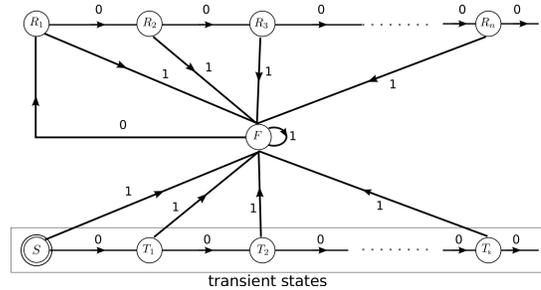


Figure 4. Mixed state representation of the extrinsic+intrinsic faulting. The state labeled as S is the starting state, states labeled as T_i are transient states with stationary probability equal to zero. All other states are recurrent.

The states in the upper line are also recurrent with probability

$$P(R_n) = \langle F | (\mathcal{T}^{[0]})^n | 1 \rangle \quad (13)$$

where

$$\langle F | = (1, 0),$$

and

$$(\mathcal{T}^{[0]})^n = \frac{2^{-n}}{z} \begin{pmatrix} \frac{y^{n+1} - x^{n+1}}{2} & (z - \alpha\bar{\gamma}) \frac{y}{2} \frac{y^n - x^n}{2} \\ y^n - x^n & \frac{z(y^n + x^n) - \alpha\bar{\gamma}(y^n - x^n)}{2} \end{pmatrix}, \quad (14)$$

with

$$z = \sqrt{\alpha^2 \bar{\gamma}^2 + 4\gamma\bar{\alpha}},$$

$$x = \alpha\bar{\gamma} - z, \quad (15)$$

$$y = \alpha\bar{\gamma} + z.$$

Figure 5 shows that the probability of the states R_n drops exponentially with n .

For $\gamma = 0$, $P(R_n) = \alpha^n$, the non-transient part of the mixed representation becomes a redundant, and therefore non-optimal, HMM description of the intrinsic fault process (compare with Fig. 1a). The same goes for $\alpha = 0$, where $P(R_n) = \gamma^{(n+1)/2}$ and the mixed representation is a non-optimal description of the extrinsic faulting.

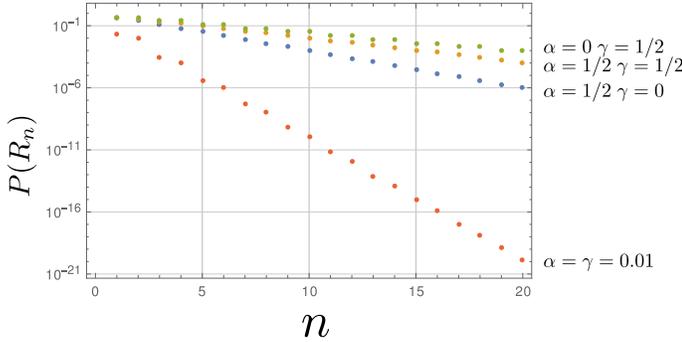


Figure 5. Stationary probability of the recurrent states R_n for given values of faulting probabilities. As n increases, the probability of reaching the state decreases exponentially. Notice the semi-log scale in the plot.

Entropy density can be calculated if we know the transition matrix W of the mixed representation. From the HMM automaton of Figure 4 the transition probabilities are given by

$$\begin{aligned}
 P(0|S) &= \frac{2\gamma\bar{\alpha} + \alpha\bar{\gamma}}{1 + \gamma\bar{\alpha}} \\
 P(1|S) &= 1 - P(0|S) \\
 P(0|F) &= \alpha + \gamma - 2\alpha\gamma, \\
 P(1|F) &= 1 - P(0|F), \\
 P(0|R_n) &= \frac{\langle F | (\mathcal{T}^{[0]})^{n+1} | 1 \rangle}{\langle F | (\mathcal{T}^{[0]})^n | 1 \rangle}, \\
 &= \frac{1}{2} \frac{\alpha(3\gamma-1)(x^{n+1}-y^{n+1}) + (z-2\gamma)x^{n+1} + (z+2\gamma)y^{n+1}}{(3\alpha\gamma - \alpha - 2\gamma)(x^n - y^n) + z(x^n + y^n)}
 \end{aligned} \tag{16}$$

$$P(1|R_n) = 1 - P(0|R_n).$$

The expression for the entropy density calculated from the unifilar representation is given by the expression [22]

$$h_\mu = \langle \pi_W | H(W) \rangle, \tag{17}$$

where π_W and $H(W)$ are the stationary probabilities and the Shannon entropy over the transition probabilities of the mixed states, respectively. The first can be known from an expression similar to (2) using the W transition matrix, the second follows the expression

$$|H(W)\rangle = - \sum_{s \in \mathcal{M}} |\delta_s\rangle \sum_{x \in \{0,1\}} \langle \delta_s | W^{(x)} | 1 \rangle \log \langle \delta_s | W^{(x)} | 1 \rangle \tag{18}$$

δ_i is the distribution with all the probability density on the

i -th mixed state. The reader can refer to [22] for further explanation.

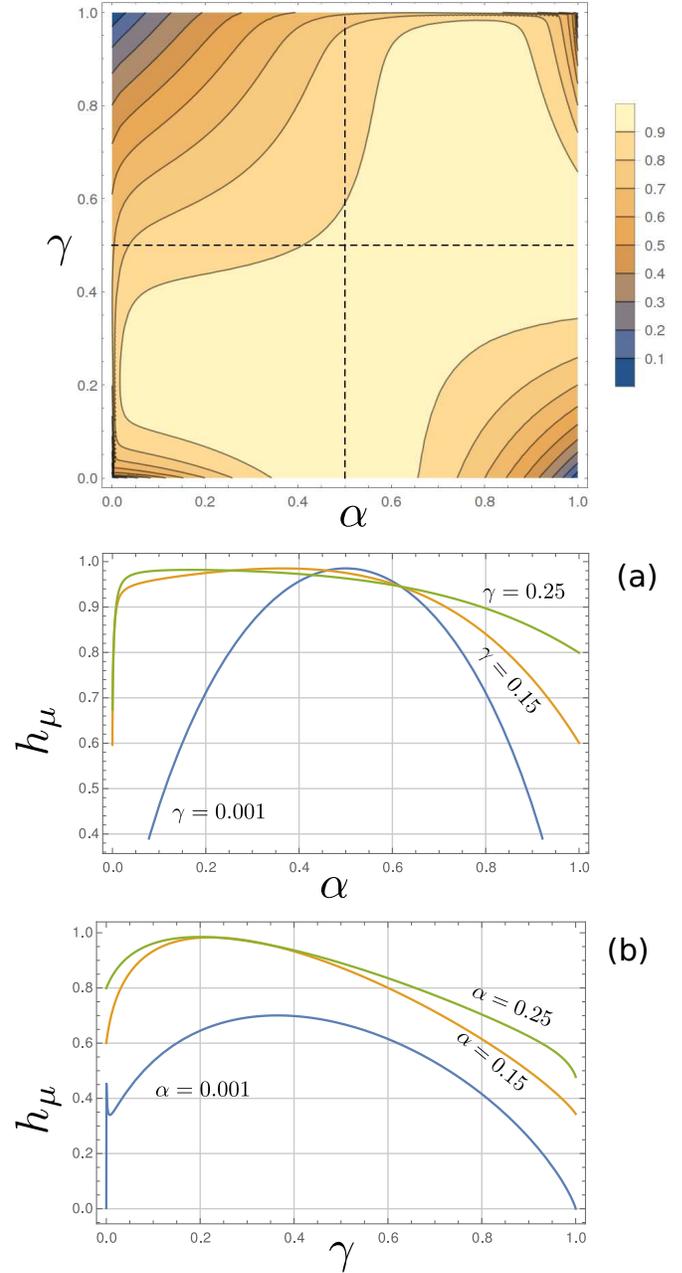


Figure 6. (up) Contour plot of the entropy density h_μ as a function of the faulting probabilities α and γ . (a) h_μ plot as a function of intrinsic fault probability for fixed extrinsic fault probabilities. (b) h_μ plot of entropy density as a function of extrinsic fault probability for fixed values of intrinsic fault probabilities.

In figure 6 at the top, the contour plot of the entropy density as a function of α and γ is shown. The four corners of the plot exhibit zero entropy as should be expected. Again, the symmetry breaking of γ is seen as the graphic is not symmetric with respect to the middle point. The plots in figure 6a further emphasizes this symmetry breaking. The $\gamma = 0.001$ curve is almost symmetrical with respect to $\alpha = 1/2$, a result that recovers the expected behavior for the intrinsic faulted system. This symmetry is clearly broken for larger values of γ as can be seen in the curves for $\gamma = 0.15$ and $\gamma = 0.25$. It is also interesting to notice that for larger values

of extrinsic faulting ($\gamma = 0.25$) the entropy has a jump as soon as intrinsic faulting steps in reaching a maximum, and then it starts to decrease. This can be understood as a result of the opposite effect of both faulting types. While γ and α are small, both faulting happen in isolation and therefore contributes to the disorder of the system. For larger values of faulting probability, if one allows for simultaneous occurrence as it has been done in this model, then each fault cancels itself, which explains the decrease in entropy density. The same reason explains the behavior of the curves in Fig. 6b.

The statistical complexity over the mixed states can be considered, as given by equation (1), using equations (12) and (13) (In the infinite sum, due to the exponential decaying behavior of $P(R_n)$, only a few terms can be considered). Results are shown in Fig. 7. For increasing value of faulting probabilities, C_μ increases. The behavior can be understood by looking at Figure 4 together with Fig. 5. For increasing faulting values the probability of the R_n states increases, which means that more recursive states are significantly involved in the system description. In that sense more resources (memory) are needed to account for the increasing disorder introduced by the faulting.

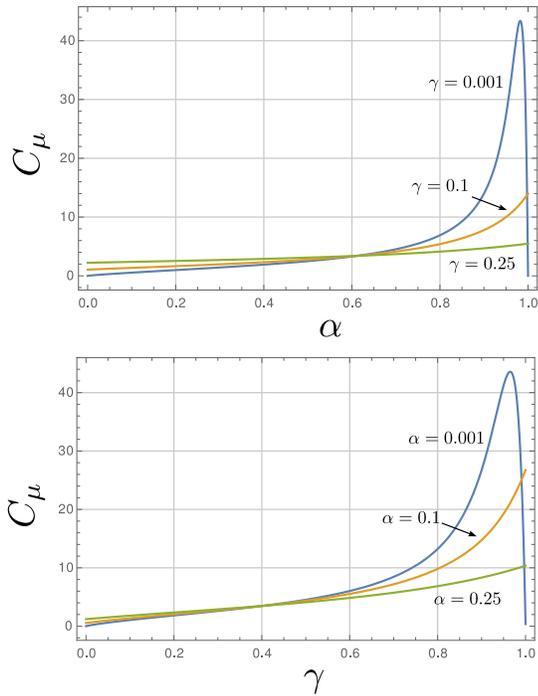


Figure 7. Statistical complexity C_μ as a function of (up) intrinsic fault probability and (down) extrinsic fault probability.

Finally, the probability of a chain of 1's of length n is given by

$$P(1^n) = \langle \pi | (T^{[1]})^n | 1 \rangle \quad (19)$$

From where the average length of blocks of 1's can be calculated

$$\langle L_1 \rangle = \frac{1 - (\alpha\bar{\gamma} + \bar{\alpha}\gamma)}{(1 + \bar{\alpha}\gamma)(\alpha\bar{\gamma} + \bar{\alpha}\gamma)^2}. \quad (20)$$

$$\langle L_0 \rangle = \langle L_1 \rangle \text{ at } \gamma = 0.3623.$$

In Fig. 8 hexagonality as a function of statistical complexity of the HMM (not the mixed representation) and entropy density are shown. There is no functional dependence between hexagonality and both measures. As a tendency, the higher the entropy density is, the higher the hexagonality, which comes as no surprise, as hexagonal neighborhoods are result of faulting events, which in turn implies larger disorder. Yet, the higher the entropy density the larger range of hexagonality the system can accommodate. In both plots of figure 8, the red points corresponds to a system with only extrinsic faulting. It comes immediately that the extrinsic fault curve is the lower bound for the hexagonality vs C_μ plot. The dependence of hexagonality with statistical complexity seems to be functional when only extrinsic fault is present. The introduction of intrinsic faults widens the range of values of hexagonality that a given C_μ can allow. For the dependence with entropy density, the hexagonality for extrinsic faulting alone is a two branch curve, the upper turn being an upper bound (Fig. 8b). The lower red branch happens for an extrinsic fault density γ between 0 and 0.38. The upper branch corresponds to the range $\gamma \in [0.38, 1]$ meaning that above 0.38 "defects" starts prevailing over the ordered underlying sequence.

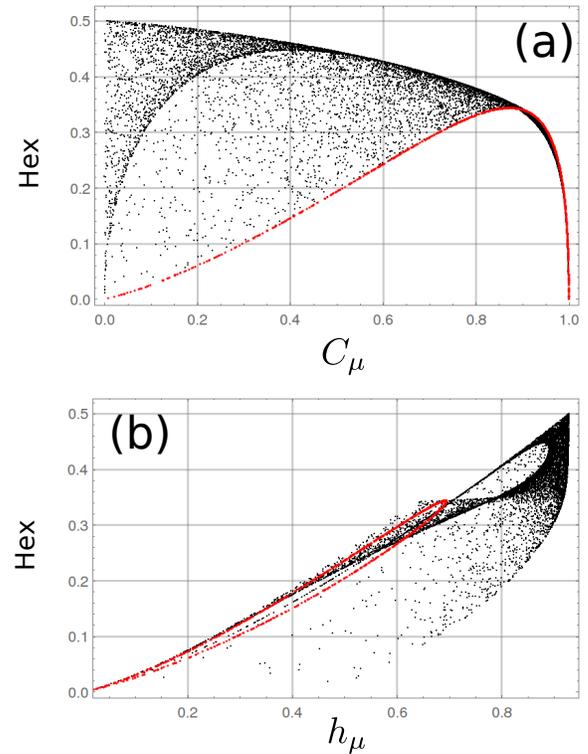


Figure 8. Hexagonality vs (a) statistical complexity and (b) entropy density. Hexagonality is not a function of either measures. Red points correspond to $\alpha = 0$.

V. CONCLUSIONS

The occurrence of intrinsic faults in a system where extrinsic faulting is present breaks the unifilar character of the HMM. The two state description cease to be an e-machine description. As a result, unifilarity must be attained through the mixed state representation resulting in

a HMM description with numerable but infinite number of states. It was already reported that extrinsic faulting leads to a sofic system, and it came as a surprise that such simple system leads to an infinite memory description. Here we find that the addition of intrinsic faulting, still a simple system in terms of the faulting dynamics, has a description with an infinite number of states. Although topologically simple, this fact further emphasizes that even simple physical models can lead to non trivial description in terms of computational mechanics.

Several useful analytical expressions were also derived for different entropic measures, probabilities, and lengths as a function of the faulting probabilities α and γ . Such expressions have not been reported before.

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REFERENCES

- [1] J. P. Crutchfield, L. Lam and V. Narodditsty, Modeling complex phenomena, (Springer, Berlin, Germany, 1992), pp. 66-101 .
- [2] J. P. Crutchfield, Nature **8**, 17 (2012).
- [3] D. P. Varn and G. S. Canright, Acta Cryst. A **57**, 4 (2001).
- [4] D. P. Varn, "Language extraction from zns", Thesis dissertation, The University of Tennessee, U.S., 2001.
- [5] D. P. Varn, G. S. Canright and J. P. Crutchfield, Phys. Rev. B **66**, 174110 (2002).
- [6] D. P. Varn and J. P. Crutchfield, Phys. Lett. A **324**, 299 (2004).
- [7] E. Estevez-Rams, U. Welzel, A. Penton-Madrigal and E. J. Mittemeijer, Acta Cryst. A **64**, 537 (2008).
- [8] E. Rodriguez-Horta, E. Estevez-Rams, R. Neder and R. Lora-Serrano, Acta Cryst. A **73**, 357 (2017).
- [9] E. Rodriguez-Horta, E. Estevez-Rams, R. Neder and R. Lora-Serrano, Acta Cryst. A **73**, 377 (2017).
- [10] E. Estevez-Rams, R. Lora-Serrano, A. P. Madrigal and M. Nespolo, Acta Cryst. A **73**, 449 (2017).
- [11] D. P. Varn, G. S. Canright and J. P. Crutchfield, Acta Cryst. A **69**, 413 (2013).
- [12] S. Đurovič, In Modular Aspect of Minerals, EMU Notes in Mineralogy (Eötvös University Press, Budapest, Hungary, 1997).
- [13] A. J. C. Wilson, Proc. Roy. Soc. A **180**, 277 (1942).
- [14] A. J. C. Wagner, Acta Metall. **5**, 427 (1957).
- [15] B. E. Warren, X-Ray Diffraction (Addison-Wesley, New York, USA, 1969).
- [16] P. Serrano-Alfaro, E. Estevez-Rams, R. L. Serrano and B. Aragon-Fernandez, Submitted for publication (2018).
- [17] A. R. Verma and P. Krishna, Polymorphism and Polytypism in Crystals (Wiley, New York, USA, 1966).
- [18] G. Hagg, Arkiv. Kemi. Mineralogi. Geologi. **16B**, 1 (1943).
- [19] E. Estevez-Rams, C. Azanza-Ricardo, J. Martinez-Garcia and B. Aragon-Fernandez, Acta Cryst. A **61**, 201 (2005).
- [20] C. Arndt, Information measures (Springer Verlag, 2001).
- [21] J. Crutchfield and D. P. Feldman, Chaos **13**, 25 (2003).
- [22] J. P. Crutchfield, C. J. Ellison and P. M. Riechers, ArXiv e-prints (2013).
- [23] D. R. Upper, "Theory and algorithms for hidden markov models and generalized hidden markov models", Thesis dissertation, The University of Rice, U.S., 1989.

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