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Incomplete Crack Sealing Causes Localization of Fracturing in Hydrothermal Quartz Veins

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Key Points:

- Systematic phase-field study captures elementary steps of the crack-seal process at grain scale
- Incomplete sealing makes a vein weaker than the host rock and localizes a new fracture inside the vein which leads to multi-crack-seal
- Probabilistic simulations show how systems of many microveins and a few thick crack-seal veins form side by side

Supporting Information:

Supporting Information may be found in the online version of this article.

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Abstract

Cyclic microfracturing and epitaxial crystal growth have long been recognized in crack-seal veins, but an understanding of a single crack-seal cycle is still missing. Here we present a phase-field model that includes both fracture mechanics of crack propagation, and epitaxial crystal growth on the fracture walls, repeating this cycle multiple times in a polycrystalline, microporous quartz rock. Our simulations have two end members: If a vein completely seals, it is stronger than the host rock, cracking is delocalized, forming many single-seal microveins. Incomplete sealing makes the vein weaker than the host rock and localizes the new fracture inside the vein, leading to multi-crack-seal. We suggest that the sealing degree is a key parameter in hydrothermal systems and multi-crack-seal veins are long-lived, microporous sites of mechanical weakness. We generalize the phase-field approach to conduct probabilistic simulations in between these two types, and show how systems of microveins and multi-crack-seal veins emerge.

Plain Language Summary

Fluids in the Earth's crust can alter permeability and porosity, precipitate and dissolve minerals, transport material and interact with deformation. This affects the transport and mechanical properties of the rock system and in turn has consequences for example, in subsurface engineering applications. In this work we simulate the processes of fracturing and crystal growth on grain scale in a microporous rock structure and show how different crystal structures form. The basic steps of a crack-seal process and how fracturing and sealing interact are explored. Our results show that if a fracture completely seals a new crack will form in the host rock and many thin microveins form. In contrast, an incomplete sealing makes the vein weaker than the host rock and leads to a new cracking inside the vein, which enlarges the existing structure with each cycle. This implies that the degree of sealing is the cause of this division, where crack-seal veins are microporous sites of mechanical weakness. Additionally, we perform probabilistic simulations which show how many single-seal microveins form side-by-side with a few multi-crack-seal veins. Our studies provide valuable insight in structure-property linkages and enable a better prediction of fracture-sealing.

1. Introduction

Syntaxial crack-seal veins (Ramsay, 1980) are first order structures in deep, hydrothermal and reactive environments where fluids create and moderate permeability and reactions interact with deformation. The coupled processes in crack-seal veins are far from being understood, whereas the recent review of Laubach et al. (2019) points out some of the knowledge gaps.

Understanding of these environments is important in basic geoscience and applied studies: examples are the seismic cycle (Micklethwaite & Cox, 2006; Sibson et al., 1988), evolution of ore deposits (Cox, 2005), the production and injection of fluids from and into the subsurface (Almansour et al., 2020; Dockrill & Shipton, 2010; Knipe, 1993), and the evolution (and interaction) of permeability in fractured geothermal reservoirs (Berkowitz, 2002; Davison et al., 2013; Pyrak-Nolte et al., 1988; Pyrak-Nolte & Morris, 2000; Rutqvist, 2015; Watanabe et al., 2009; Yasuhara et al., 2006).

The vast majority of mineral veins grow epitaxially from both sides of the fracture (syntaxial veins, Passchier and Trouw (2005); Hilgers et al. (2001)) where the vein minerals are usually the same as those of the wall rocks (Becker et al., 2010; Bons et al., 2012). They record the history of effective stress (Bons et al., 2012), while chemical and isotopic analysis of vein cement and fluid inclusions allow inferences on the environmental conditions, fluid flow and (advective or diffusive) mass transfer during vein formation (Becker et al., 2010; Boullier & Robert, 1992; Cox, 2007; Fisher & Brantley, 1992). Individual crack apertures are of the order of micrometers,

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and sealing these forms hairline veins, while multi-crack-seal veins can be up to decimeter thick (Cox et al., 1987; Cox & Etheridge, 1983; Renard et al., 2005) and tens of meters long (Hilgers et al., 2004). A cracking event followed by widening creates local porosity and can increase matrix and fracture permeability, while during the sealing event the growing crystals (partly or fully) fill the crack and restore rock strength over time (Beutner & Diegel, 1985; Cox et al., 1987; Fisher et al., 1995; Labaume et al., 1991; Lee et al., 2015).

In natural systems (Figure 1) thick multi-crack-seal veins (Renard et al., 2005) are frequently found side by side with many thin hairline veins which suggest only one crack-seal cycle: these are named crack-seal and crack-jump veins respectively (Caputo & Hancock, 1998).

Besides the analysis of natural outcrops, core samples and laboratory experiments, numerical simulations have emerged in the last decades to provide a better understanding of vein formation processes (Laubach et al., 2019). Different numerical approaches were used for modelling the formation of syntaxial and antitaxial veins (Bons, 2001; Lander & Laubach, 2015) and fracture formation in subsurface environments (Paluszny et al., 2020; Virgo et al., 2014). However, including both processes of fracturing and sealing at the grain scale has been proven to be difficult. The phase-field method with its diffuse interface approach has been utilized in recent years for modelling fracture formation and crystal growth incorporating crystallographic anisotropies in open fractures in 2D and 3D (Ankit et al., 2015; Wendler et al., 2016). We build on these achievements and computational studies to develop an integrated simulation procedure to depict both, cracking as well as sealing in a consecutive and recurring process.

Even though it is clear from previous studies (Holland & Urai, 2010; Virgo et al., 2014) that if a vein is stronger than the host rock, a new fracture will form in the host (crack-jump) and weak veins lead to localized crack-seal, this transition behavior at the grain scale has not been quantified so far.

Here we show that an incomplete sealing makes a vein weaker than the host rock and leads to localized fracturing, whereas complete sealing causes delocalized fracturing.

2. Results

We present a novel application of the phase-field method, where both the fracture propagation and fracture sealing are computed sequentially on grain scale. We incorporate variable apertures and sealing times and show that the two classes of crack-seal and crack-jump naturally emerge from our simulations. Details of our models with the numerical setup, the simulation procedure of fracture propagation, widening, and sealing with assumptions and supporting figures are given in the Supporting Information S1.

We first generate a microporous host rock comprised of quartz grains (Figure S1 in Supporting Information S1) to simulate extension fracturing which is common in deeply buried sandstones in sedimentary basins (Laubach et al., 2019). Here we compute the fracture propagation in an anisotropic rock structure. After the crack fully propagates through the numerical rock (Figure 2a), the model is manually opened to a fracture aperture a, followed by epitaxial crystal growth on the quartz grains. The aperture a is chosen to be similar to the grain size and scale a by the host rock grain diameter D_m. Therefore, the length scales of our model is defined by D_m and for the time scale we have taken literature from Wendler et al., 2016. Crystal growth velocity of the rough (irrational) surfaces is initially fast (Figure 2a), and drops once facets have formed (Hartman and Perdok (1955)).

During crack sealing, favorably oriented crystal fragments (c-axis perpendicular to crack) bridge shortly after the sealing starts before euhedral termination of c-axis (Lander & Laubach, 2015) (Figure 2a). Crystals with a tilted c-axis reach their euhedral shape and reconnect with a growth velocity that depends on axial tilt and their grain size (Lander & Laubach, 2015). In regions where prism facets appear, sealing is slowest (Figure S2 in Supporting Information S1). After a user-defined sealing time increment t_s a new crack is initiated by extending the model, and the crack-seal cycle is repeated 5 times with constant aperture a, allowing us to capture all essential elements of the process.

The models show that both thin, single-seal and thick, multi-crack seal veins (Figures 1, 2b and 2c) form, depending on the sealing time t_s.

When t_s is sufficiently large, the veins fully seal and the models produce delocalized single-seal vein bundles. Here (Figure 2c) the vein is stronger than the porous host rock because of the absence of pores so that the next

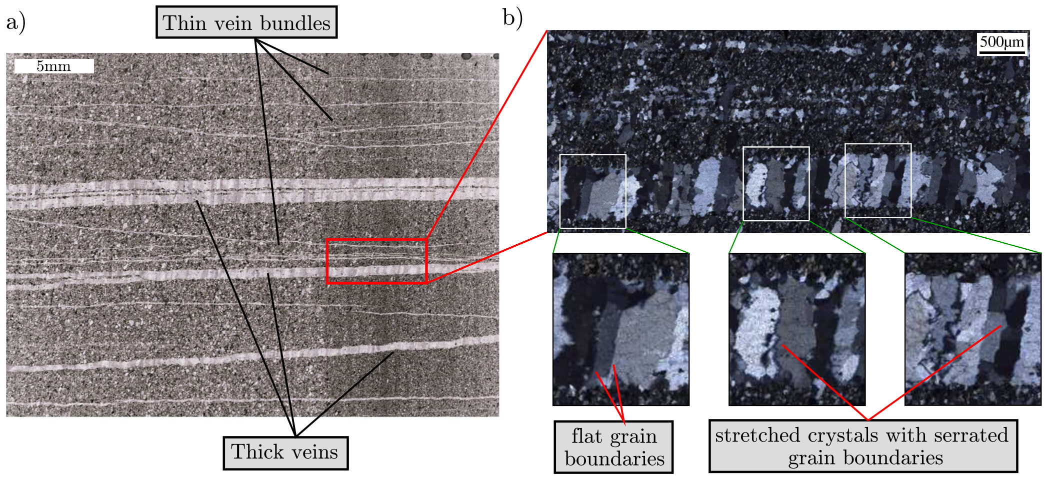

Figure 1. (a) Micrograph under plane polarizers of thick and thin veins in quartz microstructure from Portugal near Carrapateria (Reber et al., 2010; Zulauf et al., 2011). (b) Outcrop from (a) under cross-polarized filter showing small crystals in thin veins and stretched crystals with radiator(-fin) structures and flat grain boundaries in thick veins.

crack initiates in the host rock: crack-jump. When t_s is shorter, multi-crack-seal veins form, because pores in the incompletely sealed vein form asperities (Figure 2b): the vein is weaker than the surroundings. In these multi-crack-seal veins the new crack event enlarges the remaining pore space in the vein. This process increases the time required to fully seal the crack and initiates the next crack in the host rock. As long as the local conditions do not change, a re-fractured vein will have the tendency to remain in multi-crack-seal mode (Figure S3

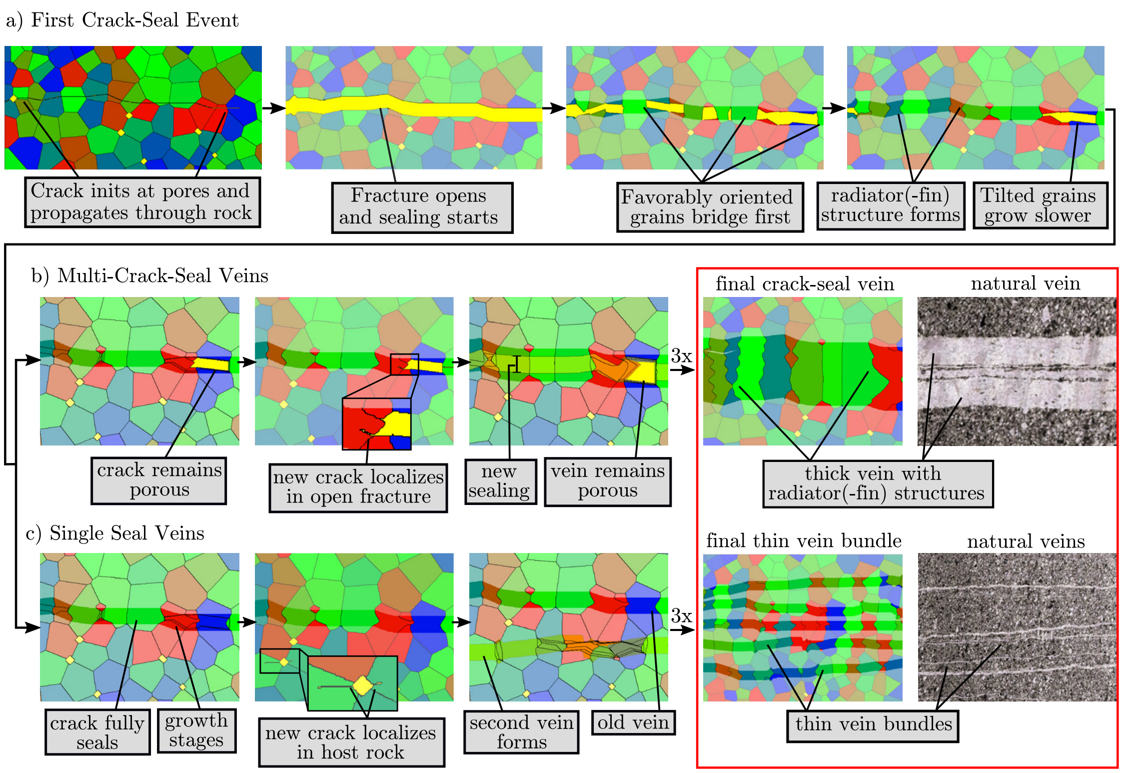

Figure 2. Formation of different vein types in representative out-crops: (a) First crack-seal event with cracking (left) and crystal growth in opened fracture. Crystals reconnect during sealing with their fractured fragment. The aperture is 0.8 D_m. (b) Multi-crack-seal and (c) single-seal veins form due to different sealing times. The numerical rock fractures either at host rock pores (when previous vein is sealed) or in partially open vein. Initial host rock is marked in light gray, the fluid in the vein in yellow. Intermediate growth stages are highlighted with black isolines. On right: Comparison of final numerical veins to natural veins from Figure 1.

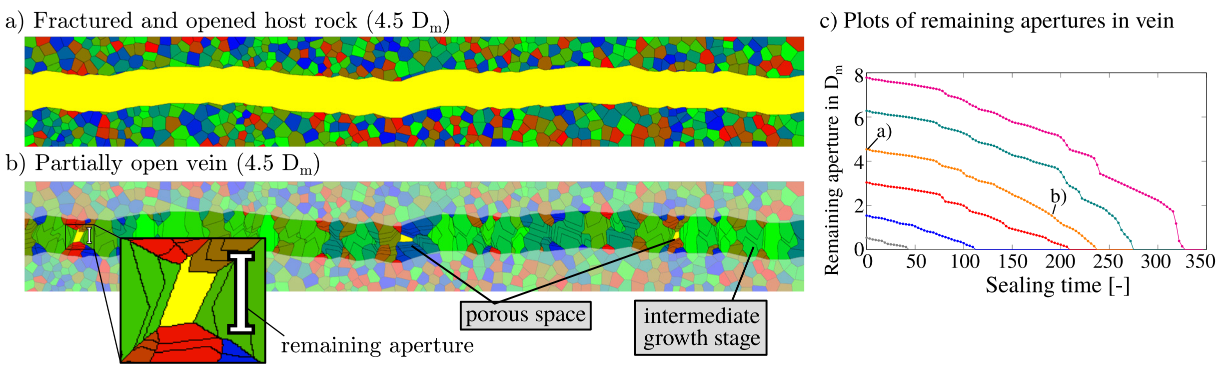

Figure 3. Single-seal veins in larger setup: (a) Opened fracture. (b) Partially sealed vein. Inset shows remaining aperture, which is used for probabilistic simulations. Black lines indicate intermediate growth stages, host rock is highlighted in light gray. (c) Plots of remaining aperture in veins with different apertures.

in Supporting Information S1). (In more detail, the remaining porosity in the vein does not need to be zero for delocalized cracking, this transition occurs at a critical remaining pore size p*).

The new microstructure models do not only reproduce the crack-seal and crack-jump processes, but also many other microstructures observed in syntaxial quartz veins. If the sealing time is even shorter than in the case of multi-crack-seal veins, a new fracturing event starts when only isolated crystal bridges are present (e.g., Lander & Laubach (2015)), these have a high volumetric crystal growth rate, tending to stabilize the crystal bridges. In the multi-crack-seal vein models serrated grain boundaries form which are well known in nature as radiator(-fin) structures (in Cox et al. (1987); Bons et al. (2012); Ankit et al. (2015); Lander & Laubach (2015); Späth et al. (2022b)). These are formed by the different relative orientation of a crystal and its neighbors in relation to the location of the fracture (Figures 2b and 2c). The fractured crystal fragments are in growth competition with their neighboring crystals and each new crack-seal event produces a new radiator-fin or extends an already existing one. In multi-crack-seal veins the models produce wider quartz crystals by growth competition, while grains in delocalized crack-jump veins, have a grainsize similar to the host rock (Figure S3 in Supporting Information S1).

A simulation series with a smaller fracture aperture (half aperture used in Figure 2) shows the same vein types (thick veins vs. thin vein bundles) as before. As expected, the sealing time t_s of multi-crack-sealing veins decreases for smaller apertures. In these simulations, the radiator(-fin) structures are less pronounced and growth competition is less strong for small apertures (Figure S5 in Supporting Information S1).

The next level of complexity in our models considers the variability of t_s and a in natural systems. Because of the high computational cost, the consideration of theses quantities requires the following simplification. We run simulations of single-seal veins with different apertures a in a model which is sufficiently large to contain all grain orientations and which captures the variability in local sealing rates discussed above. In all these models we compute the remaining aperture as a function of time until complete sealing (Figure 3). This is used in probabilistic crack-seal vein simulations with the criterion found in our initial models: A new fracture will reactivate an existing vein when $p > p^*$, otherwise the new fracture will form in the host rock (for details see Supporting Information S1). This allows probabilistic simulations with a few thousand crack-seal events for selected distributions of t_s and a. We assumed normal distributions for both parameters, with a cutoff at zero.

Results show three different domains. As in the full phase-field simulations we obtain bundles of single-seal veins when the sealing times are long (higher median value) and one thick multi-crack-seal vein when the sealing time is short (low median value; Figure 4). In the transition between these two domains, more complex combined grain structures can be observed. We (somewhat loosely) define a non-dimensional number R as the ratio between average opening velocity and average sealing velocity in a crack-seal system (Hilgers et al., 2001). When $R \gg 1$, the veins will be dominated by euhedral crystals growing in a free fluid, and for $R > 1$ multi-crack-seal veins form, (Figure 4). When $R < 1$ bundles of single-seal veins will be dominant. For values of R close to 1, both single-seal crack-jump veins and multi-crack seal veins will develop, producing the structures shown in Figure 4. The ratio between opened volume to the precipitated volume of one crack-seal event is denoted by χ and defines another non-dimensional microstructural quantity which provides a measure for classifying vein types. If $\chi = 1$ the pore

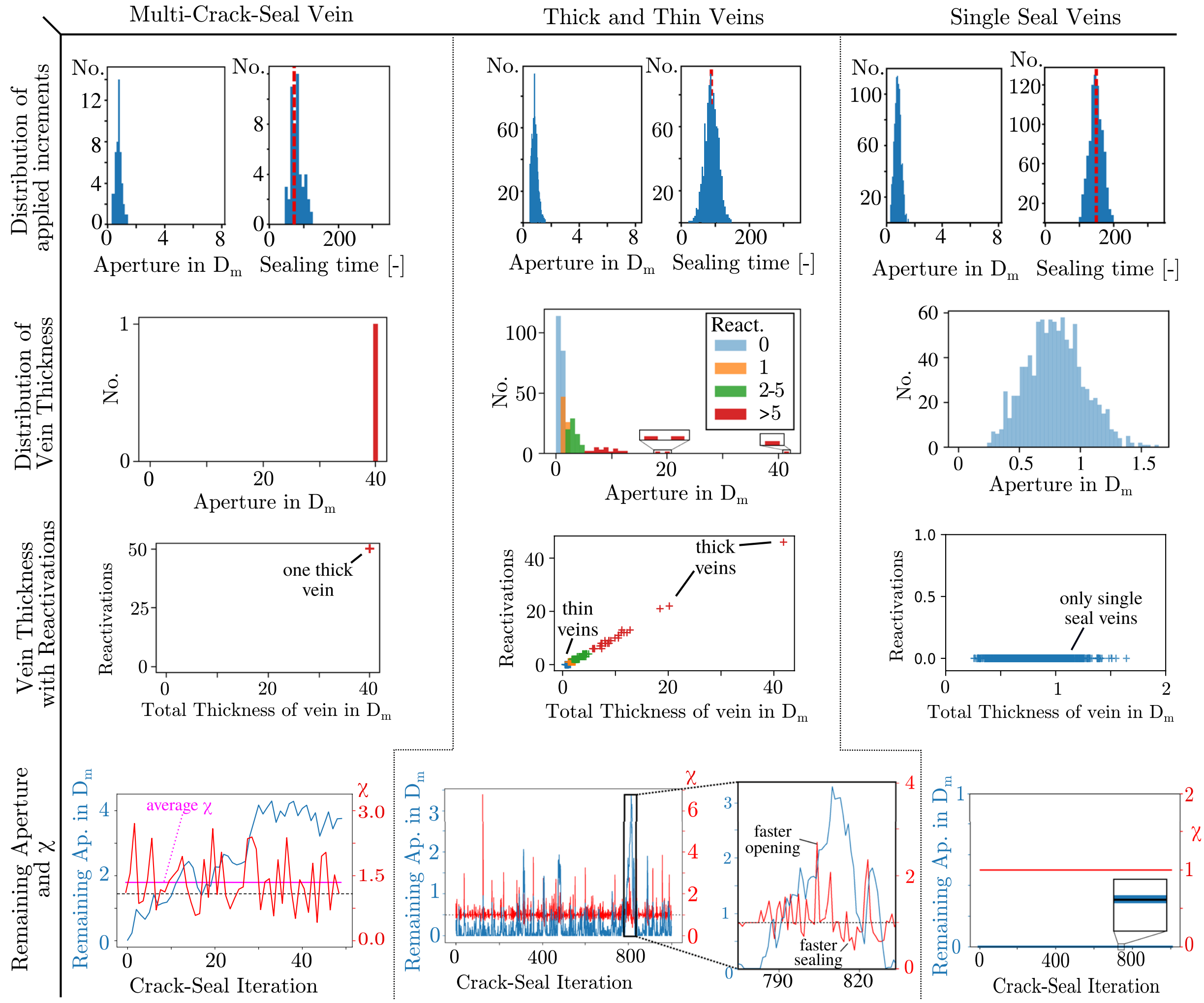

Figure 4. Probabilistic simulations: Three cases with normal distributed values for opening and sealing time increment. The median value of sealing time increment (red dotted line in top row) increases from left to right. On Left: Short sealing time results in thick vein (always reactivated). Vein stays porous (bottom row) and the average χ is greater than one. On Right: Long sealing time results in full vein sealing and new fractures form delocalized ($\chi = 1$). Middle Column: Sealing time is in between and results in thick and thin veins. When $\chi > 1$ vein opens. When $\chi < 1$ vein closes.

space in the open vein between two crack-seal events does not change, whereas for $\chi < 1$ or $\chi > 1$ the vein pore volume closes or increases respectively. For the thin vein bundles the average χ (and in each iteration) always equals one, for pure multi-crack-seal veins the average $\chi > 1$ (Figure 4).

Additional simulations with an increasing background extension rate over time (Poissonian process like) show also the occurrence of both single-seal vein bundles and a thick multi-crack-seal vein (Figure 5).

3. Discussion

Natural veins in sandstone show a wide range of aperture size distribution (Hooker et al., 2014) and can contain purer quartz (no pores, no other weak minerals) with bigger crystals than the host rock. Our results suggest that if sealing is complete in nature ($R < 1$) the stronger veins would result in ubiquitous crack-jump veins. When the sealing is incomplete the veins are weaker and get reactivated to form multi-crack-seal veins or crystal bridges. Moreover, the simulations indicate that common multi-crack-sealing creates a porous and permeable polycrystalline vein structure during the formation.

Even though we simplified the mechanics of fracture formation (Mode I loading) and opening (prescribed aperture) and only performed simulations with a specific porous host rock composition and comparatively large

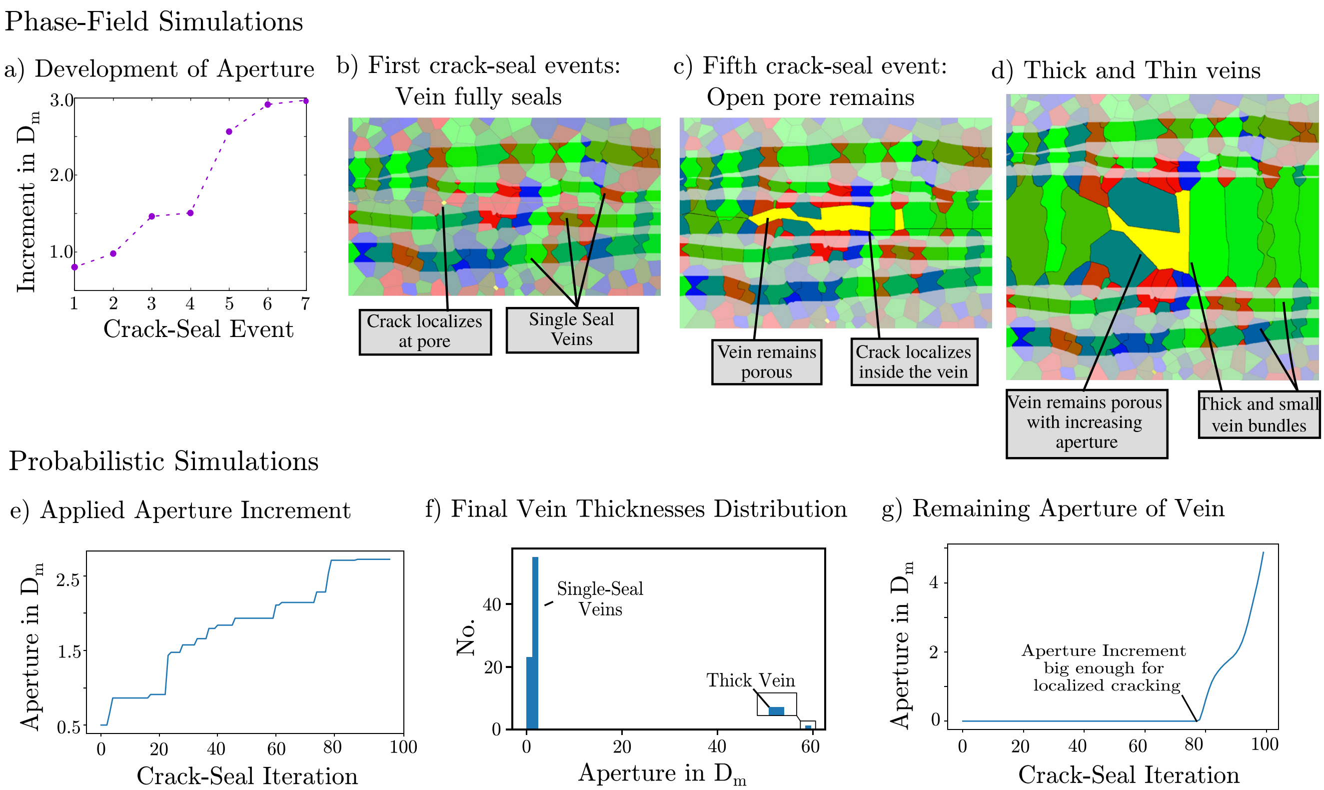

Figure 5. Stress heterogeneities in the crust are modelled by applying a Poissonian-process like aperture (constant recurrence time with increasing background extension): Phase-field (top; 7 crack-seal events) and probabilistic approach (bottom, 100 events). (a and e) Opening increment follows Poisson process (constant sealing time increment). The sealing time is longer as in Figure 2 and chosen as 1.75xAverage time until full sealing (in a)-d)) and in (e–g) 2xTime for single-seal veins in Figure 4b) Delocalized cracking in first events. (c and d) Vein stays porous and fracturing remains localized. (f) Final vein distribution with single-seal veins and big multi-crack-seal vein. (g) Vein remains porous after the applied aperture (in d) is large enough. Continuously, the remaining aperture further increases due to the increasing applied aperture increment.

apertures (Hooker et al., 2014), we expect the same archetypes of veins (crack-seal vs. crack-jump) would still form in rocks with different porosities (e.g., less compacted sandstones) or smaller apertures, because the detected and quantified growth characteristics are the result of fundamental evolution mechanisms (localized vs. delocalized cracking). Based on the findings, the computations allow the prediction that a more porous host rock tends to show more delocalized cracking for the same sealing time. Furthermore, additional parameters as temperatures, rock types, and fracture opening rates impact the evolution of these archetypes (Laubach et al., 2019).

In natural veins the crack-seal structure and the location of a new microfracture (Hooker et al., 2014, 2018) can depend on the host rock composition (Laubach et al., 2016). New fractures can initiate at inhomogeneities in the rock structure such as micropores, second phases or weak grain boundaries, especially in rocks with low porosity and many mechanical heterogeneities. We expect that a host rock with more inhomogeneities (e.g., more porous or more accessory minerals) shows an earlier tendency for delocalized fracturing, whereas in strong monomineralic sandstones with low porosity multi-crack-seal veins are more common.

In the present work we simplify a complex natural rock system to a microporous rock model and perform the simulations in 2D to reduce computational costs for the modelling of multiple crack-seal events in a polycrystalline rock system. A constant supersaturation over time during crystal growth and the same loading direction in all simulations are applied. With these assumptions, natural microstructures with serrated grain boundaries (radiators-fin structures) in thick veins and their transition to delocalized fracturing with thin vein bundles are recreated in the computations. However, an extension to 3D is necessary if information about permeability or fluid connectivity during the vein sealing is required (Kling et al., 2017; Spruženiece et al., 2021). Furthermore, the studies can be extended with complex loading conditions (e.g., shearing) or a time dependent varying supersaturation once data from natural systems are available. We emphasize that the modelling methods as well as the simulation framework PACE3D are directly capable to study 3D microstructure evolution and complex strain states. In contrast to natural systems we do not observe fragments of the host rock in our simulations. We suspect however they would occur with a more complex and time varying stress state and in models including more details of host rock microstructure.

Once a vein is mostly sealed the permeability and fluid connectivity reduces in the open fracture, if there is no matrix porosity to provide the supersaturated fluid. Therefore, the critical porosity in the vein for delocalized cracking should be reached more slowly in natural systems and would make the occurrence of thin vein bundles even more unfavorable.

We utilize a comparatively small polycrystalline rock system for simulating multiple crack-seal events in order to enable simulation studies at reasonable computing times. In these models the sealing time which is required for delocalized cracking is variable, since the grain structure may not contain slow growing regions and therefore results are different for the same t_s and a (Figure S3 in Supporting Information S1). In larger, more representative domains, where slow growing grains are always present (responsible for localized cracking) we expect a sharper transition from localized to delocalized cracking as in the probabilistic simulations.

We generalize the model results for probabilistic simulations in the domain between the end members, and show how systems of many microveins with a few thick crack-seal veins emerge. The probabilistic simulations extend the work of Clark et al. (1995) and Hooker et al. (2012). In the work of Clark et al. (1995) veins are chosen to be reactivated randomly and not by a mechanistic reasoned criterion, whereas in the work of Hooker et al. (2012) veins are reactivated on diagenetic and mechanical considerations. Based on the observations of the presented full phase-field simulations we include a mechanical criterion for the reactivation of a vein (based on the porosity) and obtain (similarly as Clark et al. (1995) and Hooker et al. (2012)) a power-law distribution between the number of veins and their thickness, when normally distributed values for aperture and sealing time increments are applied. Even though we chose a normal distribution for the two variables, we anticipate that when other probability distributions are chosen (e.g., power law) thick and thin vein bundles would still form.

The probabilistic vein simulations use a data set, generated from simulations with only one crack-seal event. When a vein fractures multiple times, unfavorably oriented grains can be overgrown and the growth competition leads to faster sealing. However, as a is small in our simulations, we infer that this does not significantly affect our results.

In this study we capture the elementary step of the crack-seal process at the grain scale. Our coupled models explain why a few thick crack-seal and many single-seal veins may form in the same rock in nature by quantifying the feedback between fracturing and sealing processes. The models reproduce many aspects of syntaxial veins, like radiator(-fin) structures and growth competition and propose that the ubiquitous multi-crack-seal veins in sandstones deformed in hydrothermal systems retain some porosity and permeability during their evolution. We expect that the conclusions are also applicable to vein development in many other rock types which show syntaxial vein development. The models can be extended to include second phase minerals and to simulate fluid flow in 3D, providing a platform for further study (e.g., mechanical, hydraulic, residual aperture (fracture collapse), fabric orientation (Jiang et al., 2020), mineralization-distribution (Lang et al., 2015, 2016) affecting permeability and stiffness (Pyrak-Nolte & Nolte, 2016)).

Data Availability Statement

The software package PACE3D version 2.5.1 was used for the generation of the simulation data sets. The software license can be purchased at Steinbeis Network (www.steinbeis.de) in the management of Britta Nestler and Michael Selzer under the subject area "Material Simulation and Process Optimization." The complete data set, on which this research article is based, can be accessed in the open-access repository at Späth et al. (2022a) (https://doi.org/10.5281/zenodo.6337652).

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