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Numerical simulations of polycrystal growth in veins

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Abstract

Vein microstructures contain a wealth of information on conditions during vein growth but correct interpretation requires an improved understanding of the processes involved. In this paper we investigate the parameters controlling vein microstructures using numerical simulations of anisotropic crystal growth. We focus on the effects of crystal growth rate anisotropy on growth competition and on the effects of the wall rock on vein microstructure during crack-seal growth.

Growth competition in a free fluid is controlled by the crystallographic orientation and growth anisotropy of the crystals. We discuss the merits and limitations of different algorithms to simulate free growth in veins, based on a detailed study of the crystal facets and grain boundaries produced.

Microstructures in crack-seal veins are influenced by additional parameters, such as the width of individual crack-seal increments and the fracture morphology. We present a detailed study of the transition between free-fluid growth and crack-seal growth as a function of the relative rates of crack opening and crystal growth, to illustrate how this induces the microstructural transition between fibrous and blocky veins.

Keywords: Vein microstructures; Open cavity growth; Crack-seal; Fibrous; Tracking

1. Introduction

Vein microstructures comprise a wide range of crystal habits from dendrites, fibres, elongate-blocky to blocky crystals, depending on the boundary conditions of crystal growth (Ramsay and Huber, 1983; Fisher and Brantley, 1992; Bons and Jessell, 1997) (Fig. 1). Some of the boundary conditions are: *relative time of crystal growth with respect to fracture opening* (syntectonic vs. posttectonic), *fluid properties* (pressure, temperature, flow velocity and supersaturation) (Cox et al., 1986; Knipe and McCaig, 1994), *transport mechanisms* (advection vs. diffusion) (Durney, 1976; McCaig, 1988; Gratier et al., 1994; Jamtveit and Yardley, 1997), *nucleation vs. epitaxial overgrowth*. When the influence of these boundary conditions on the microstructures is sufficiently understood, vein microstructures may be interpreted in order to deduce these boundary conditions of formation (Williams and Urai, 1989; Jessell et al., 1994; Bons, 2000).

Free growth of polycrystals occurs when the crystals grow from the wall rock into an open cavity. The only interference is between the growing crystals. If there is an opposing wall, the distance at which it is located from the growing crystals is sufficiently large to be of no importance. In a syntectonic vein, the growth process is much more complex and depends on the effective stress. Opening events may range from nm to dm. Ramsay (1980) proposed that multiple inclusion bands, parallel to the vein wall, indicate repeated vein growth events, by the so-called crack-seal mechanism.

The space where the crystals grow can be created by the force of crystallization (Correns, 1949; Means and Li, 2001; Wiltschko and Morse, 2001) or by changes in effective stress (Hulin, 1929; Sibson, 1981), and the relative importance of both of these forces is under much discussion (Elburg et al., 2002; Hilgers and Urai, 2002b).

The resulting vein microstructure ranges from blocky

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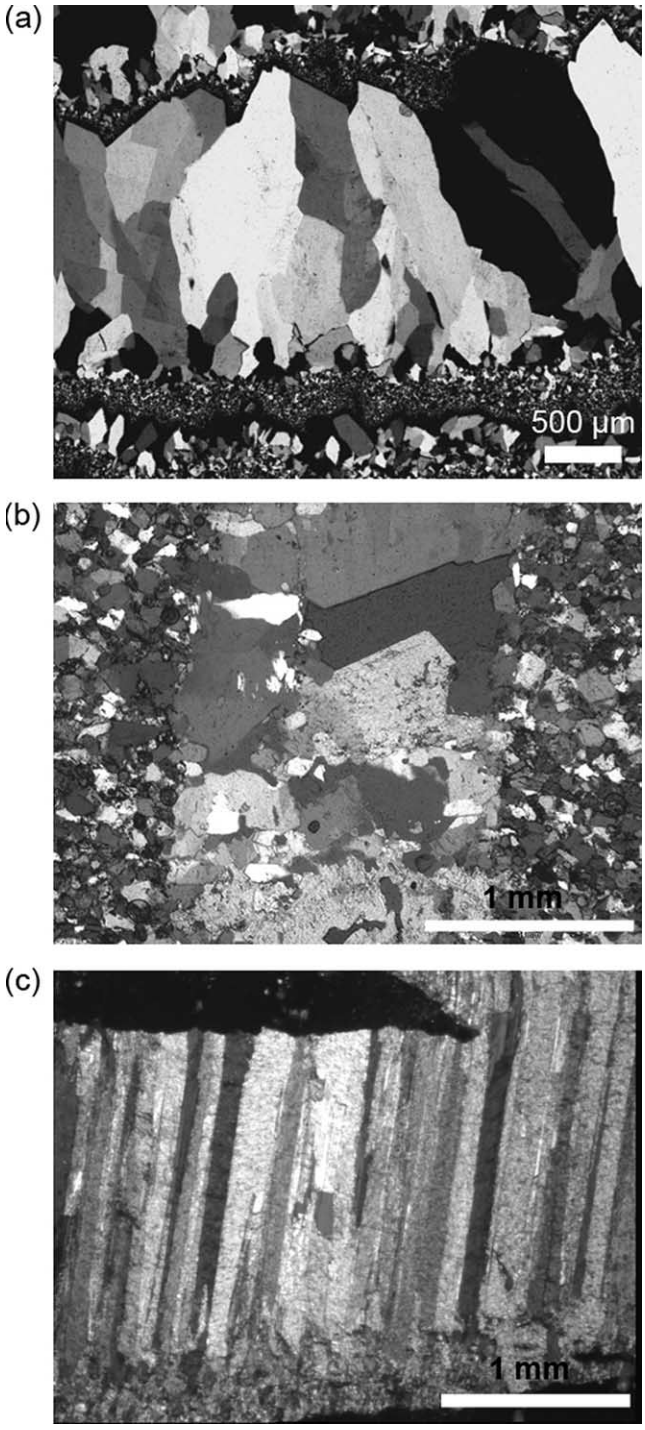


Fig. 1. (a) Example of free growth in a quartz geode with significant growth competition, resulting in a few favourably oriented crystals at the top of the image with an elongate-blocky microstructure. Different generations of seed crystals resulted in different cycles of growth competition. (b) Example of a quartz vein (with minor calcite) in sandstone (German Buntsandstein) showing an elongate-blocky microstructure. (c) Example of fibrous calcite crystals in shale (German Buntsandstein).

with euhedral crystal terminations in free growth, to fibrous crystals, that may or may not track the opening trajectory of the crack when deformation was present (Taber, 1916; Grigor'ev, 1965; Durney and Ramsay, 1973; Bons and Jessell, 1997; Hilgers et al., 2001; Oliver and Bons, 2001) (Fig. 1).

In a free growth microstructure, strong growth competition can be present between the crystals (Fig. 1a,b). Crystals, which have a favourable orientation and position survive, and are able to grow to large crystals. In the example of Fig. 1a, different cycles of nucleation and growth competition are seen. A possible cause is a variation in supersaturation over time, which gave rise to the development of a first growth competition cycle, followed by nucleation of new seed crystals. In a fibrous microstructure, there is no growth competition and crystallographic preferred orientation does not develop (Fig. 1c). The crystals have parallel grain boundaries.

Urai et al. (1991) developed a kinematic model for crystal growth in crack-seal veins and pointed to the importance of the wall rock morphology for the resulting microstructure. They showed that the repeated contact between the crystals and the wall rock has a strong effect on the microstructures. If the crystals have sealed the space available before the next crack event, they loose their facets and assume the morphology of the rough vein wall interface. If opening increments are sufficiently small, the crystals cannot develop crystal facets and grow isotropically (Urai et al., 1991; Hilgers et al., 2001). The result of isotropic growth is that the grain boundaries will grow towards peaks in the wall rock. This control of the grain boundaries by wall irregularities depends on the angle between the incremental opening vector and the local orientation of the crack surface. An important element of the Urai et al. (1991) model was the assumption that the crystal growth kinetics is effectively isotropic if the crack surface is sufficiently rough.

To include anisotropic growth in the model of Urai at al. (1991), the numerical simulation program *Vein Growth* was developed (Bons, 2001). It simulates crystal growth under complex boundary conditions and can simulate crack-seal growth with an incremental opening trajectory. The transition from a faceted crystal to an isotropic growing crystal, due to the interference with the wall rock, can also be simulated with this algorithm.

Simulations with *Vein Growth* produced results consistent with Urai et al. (1991), i.e. fibrous crystals in a vein with the potential to track the opening trajectory of the crack when the wall morphology is rough and the average opening velocity is smaller than the growth velocity of the crystals (Koehn et al., 2000; Bons, 2001; Hilgers et al., 2001; Bons and Bons, 2003). In simulations of a natural microstructure, full tracking was achieved with opening increments smaller than 10 μm (Hilgers et al., 2001), of the same order as the inclusion band spacing in natural crack-seal veins (Ramsay, 1980).

The aim of this paper is to expand previous numerical simulations of polycrystal growth in veins to investigate the details of (1) growth competition in a model that includes the development of facets during growth and (2) crack-seal

growth focusing on the transition from a blocky to a fibrous microstructure.

2. Methods

Vein Growth (Bons, 2001) allows two-dimensional simulations of both anisotropic and isotropic crystal growth in an antitaxial vein. Crystals grow from a substrate towards the wall rock to fill the space that is made available by opening the fracture. The fracture morphology, opening vector and number of crack events can be defined by the user. Seed crystals are defined by their position, width, crystallographic orientation, growth rate and growth anisotropy. Grain boundaries are defined by nodes and the triple junction node movement is calculated as follows: a triple junction is moved to its new position after the calculation of four vectors, two at the segments of the grain-fluid contact and two at the solid–solid contact between two crystals (Fig. 2a) (Bons, 2001). Growth kinetics are defined by different anisotropy functions. The program does not consider mass transport mechanisms (i.e. diffusion and advection) towards the site of precipitation. This means that the supersaturation of the fluid is assumed to be constant everywhere.

The simulation algorithm FACET (Zhang and Adams, 2002) calculates the growth of polycrystals based on the deposition flux of the atoms, incorporating mass transport. The growth algorithm is based on the propagation of low index facets. FACET calculates the movement of triple junction nodes by the vector sum of the growth vectors for each facet neighbouring the triple junction node (Fig. 2b).

In this paper we discuss and compare the different growth algorithms of *Vein Growth* and FACET, their capabilities to simulate vein growth and their effect on the resulting microstructure.

3. Open cavity growth

In naturally growing single crystals, the slowest growing facets survive and the smaller, faster growing facets are eliminated (Mügge, 1925; Mullin, 2001, p. 217). The growth of a polycrystal is more complex, because of the interaction between different oriented facets from all the crystals. Microstructures formed in an open cavity are usually characterized by an increase in grain size and an increasing preferred orientation with euhedral terminations of grains growing away from the substrate towards the open space (Schmidegg, 1928). The morphology of the final microstructure depends on the habit of the crystallised material (Bons and Bons, 2003). The surviving crystals are the ones that have the most successful growth orientation, i.e. most commonly with the fastest growth direction perpendicular to the surface (Thijssen et al., 1992). The orientation of the grain boundary between two different crystals is determined by the orientation of the facets (Schmidegg, 1928; Thijssen et al., 1992; Hilgers and Urai, 2002a). In a polycrystal, one can distinguish two elementary competing processes: (i) facet consumption when a crystal tip line (defined as 'Gratbahn' in Mügge (1925)) crosses a grain boundary line and (ii) crystal consumption when two grain boundary lines (vector sum of the growth vector of two neighbouring facets) cross. Both elementary processes of growth competition are produced in simulations with *Vein Growth*. Simulations were run in *Vein Growth* to investigate the details of growth competition and to test if the model produces natural looking microstructures.

Open cavity growth is simulated in *Vein Growth* if the crystal growth rates are significantly smaller than the average opening velocity. Thus crystals do not touch the opposing wall and crystals with anisotropic growth kinetics will develop facets. This results in growth competition between the seed crystals (Bons, 2001; Bons and Bons, 2003).

The first set of simulations are concerned with anisotropic growth, which is simulated by prescribing the growth rate as a function of the orientation of the crystal surface relative to the crystallographic orientation (Fig. 3). Different anisotropy functions were used in a sensitivity analysis, which causes an originally circular and isolated crystal to develop into a faceted crystal, where the facets depend on the growth rate function. The different anisotropy functions implemented in *Vein Growth* result in the formation of facets and produce a variety of habits (Fig. 3).

To simulate the evolution of a polycrystal, we used 20 seed crystals with random crystallographic orientation and exactly the same width (Fig. 3). In all simulations the same node spacing, seed crystals, growth rate and number of growth increments were used. The substrate, which the crystals grow on in this series, is a straight surface.

The growth rate functions in Fig. 3a–d result in intense growth competition of the polycrystal. Only crystals that are oriented parallel to the final crystallographic preferred orientation survive. The growth rate functions in Fig. 3e–h result in less growth competition. The rate of growth competition is illustrated for each growth rate function by the number of surviving grains as a function of the growth increments (Fig. 4). Crystal anisotropy is an important parameter controlling the microstructure. Strong anisotropy in only a few directions gives rise to intense growth competition.

3.1. Long distance effect on growth competition

The growth competition process has been further investigated in detail at the grain scale using a growth rate function that results in a square morphology

The starting point for the sensitivity analysis is a row of 10 seed crystals, of which two crystals (A and B) have a variable orientation. The term crystallographic orientation refers to the direction of fastest growth (indicated by an

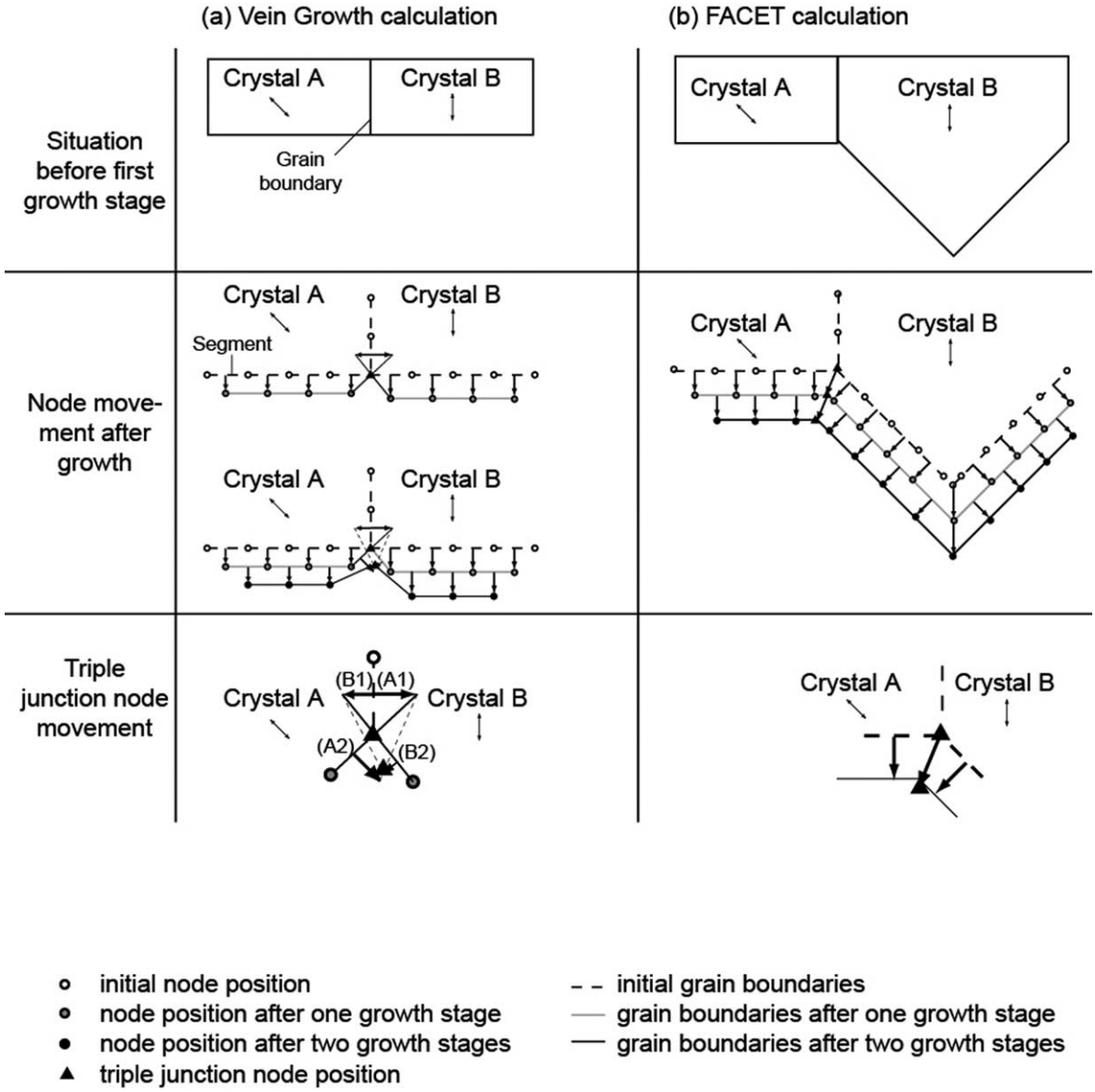
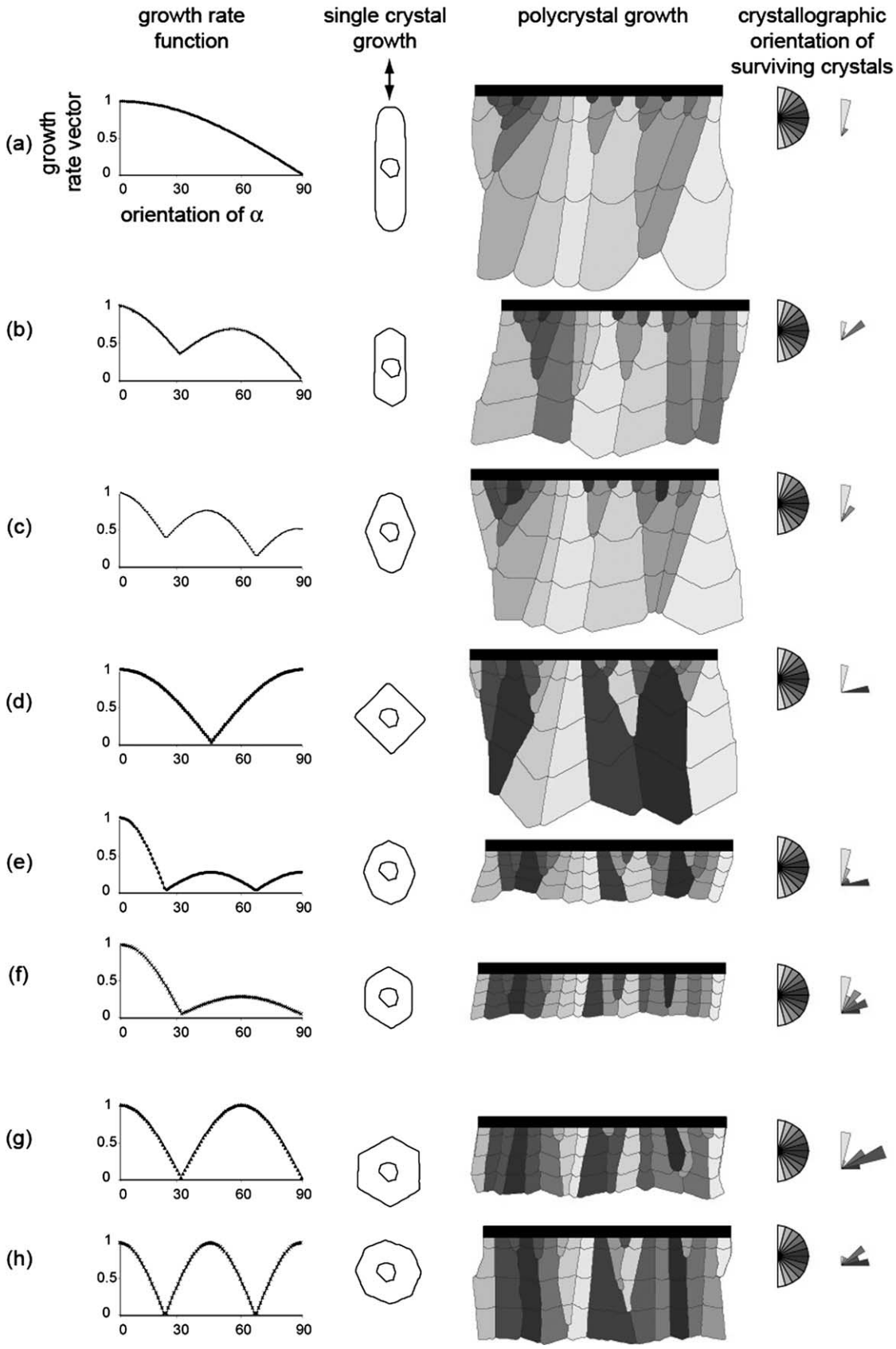


Fig. 2. Schematic illustration of the node movement in (a) *Vein Growth* and (b) FACET, starting with the initial crystals A and B. Grain boundaries of the crystals are defined by the connection of segments, which are connection lines between two nodes. For both simulation codes, two growth stages are sketched. Simulations in *Vein Growth* require a much closer node spacing on the facets than outlined here. The crystallographic orientation of crystals A and B are indicated by an arrow, causing anisotropic growth. This misorientation causes growth competition between neighbouring crystals, where crystal B advances faster downwards than crystal A. In FACET, the preferred facet orientation (and not the crystal's orientation as in *Vein Growth*) can be set. In contrast to *Vein Growth* this results in different crystal morphologies depending on the crystallographic orientation. The movement of the triple junction (black triangle) is calculated after calculation of four vectors, two at the solid–solid contact between two crystals (at the grain boundary): A1 and B1, and two at the segments of the grain fluid contact (at the crystal facets): A2 and B2. In this way, four new node positions are calculated and, for each crystal, the two new nodes are connected. The crossing between these two lines is defined as the new triple junction position. In FACET, the new triple junction node is calculated by the vector sum of the growth vectors for each facet neighbouring the old triple junction node.

arrow) and is calculated based on the input angle of a crystal (Fig. 5a). The crystals located between crystals A and B are oriented at 65°. When crystal A is oriented at 0°, it survives and outgrows its obliquely growing neighbours (Fig. 5b), whereas when A = 25°, the crystal is consumed by its obliquely growing neighbours (Fig. 5c). This indicates that the consumption or survival of a crystal depends on its orientation relative to neighbours. A crystal outgrows its

Fig. 3. Different growth rate functions implemented in *Vein Growth*. Graphs show the growth rate vector value as a function of α (small angle between a crystal segment and crystallographic orientation of the crystal (= input angle)). A single crystal is simulated, starting from an initial random crystal (with crystallographic orientation given by the arrow) and polycrystals are simulated with initially the same, random oriented seed crystals for every growth rate function. The orientations of the surviving grains (= preferred orientation of the growth rate function) in polycrystal growth are displayed as a rose diagram.



The different growth rate functions result in crystals with a specific habit. Notice that the model has wrapping lateral boundaries: the leftmost crystal is a neighbour of the rightmost crystal.

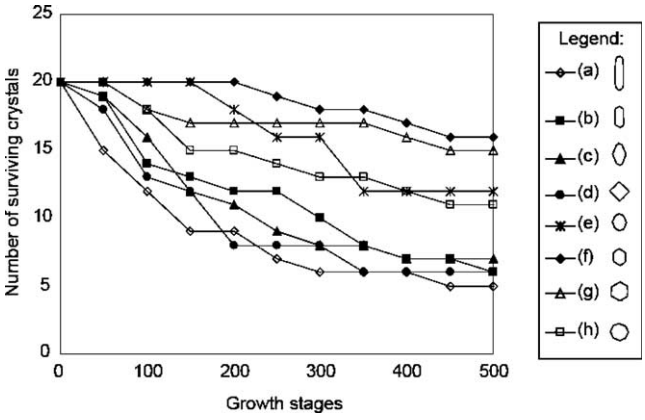


Fig. 4. Number of surviving grains plotted against the number of growth stages for the different growth rate functions used in the simulations in Fig. 3. (a)–(h) as in Fig. 3. Simulations started with 20, initially random oriented grains.

neighbour if its growth vector normal to the substrate is larger than that of its neighbour.

When the orientation of crystal A is 11° and that of crystal B 15°, both crystals survive (Fig. 5d). In contrast to Fig. 5b, crystal B now consumes its neighbours. When A is 10° while crystal B is 15° (Fig. 5e), crystal B is consumed and crystal A survives. Consequently, crystal A influences the survival of non-neighbour crystals. This unexpected long-distance effect on growth competition is further shown when the displacement paths of the tip of both crystals are compared (Fig. 5e). A small difference in orientation of the tip line and in the crystal morphology is observed, which causes a difference in orientation of the grain boundaries. The small difference in the grain boundary's orientation influences the behaviour of crystal B, although there are four crystals between them. A sensitivity analysis of the crystal misorientation showed that randomly oriented crystals at orientations of 64.5–65.5° do not influence the final microstructure. This means that the grain boundaries in the simulations can be seen as subgrains, when compared with natural samples.

The long-distance effect can be explained as follows: when the orientation of one crystal in the polycrystal is changed, the triple junction node between that crystal and its neighbour will also be different (because triple junction nodes are calculated based on the orientation of two neighbouring crystals) (see Fig. 2a). This has two consequences: (1) the segment defined by that triple junction and the neighbouring node has a different orientation, (2) at the next growth stage, the node calculated from this segment is also located at a different position because nodes are moved to a new position by a growth rate vector located at the middle of a segment. The code generates a new segment by adjoining two neighbouring nodes and the segment between that new node and the one next to the new one is then also different. This is caused by the fact that the growth rate vector depends on the orientation of a segment and on the crystallographic orientation.

These simulations show that, although the consumption or survival of a grain in *Vein Growth* depends on its own orientation relative to its neighbours, the orientation of grains further away also has a minor effect on growth competition due to the node movement algorithm and this effect is recognized as a limitation of the calculation algorithm.

The magnitude of this effect is illustrated by mapping the growth behaviour as a function of the crystallographic orientation of crystals A and B (Fig. 6). Three different behaviours can be distinguished: (1) both crystals survive, (2) both crystals are consumed, and (3) one of the two variable crystals is consumed.

It can be seen that boundaries between (1), (2) and (3) are not parallel to the axes of the graph. This is due to the long-distance effect, which causes the survival or overgrowth of a crystal to depend not only on its own orientation with respect to the direct neighbours, but in *Vein Growth* is also dependent on more distant crystals.

3.2. Accuracy of crystal terminations

Another interesting aspect is that when open cavity growth is simulated, the facets of the crystals in the polycrystal do not have the 90° angle according to the square anisotropy that was set. In natural open cavity growth, however, the crystal terminations are always under the same angle (Schmidegg, 1928; Grigor'ev, 1965) and the facets produced in *Vein Growth* simulations are therefore irrational.

When a single crystal is grown in *Vein Growth*, the program produces the facets as expected from the growth anisotropy (Fig. 7a).

A new growth rate function with overall faster growth rate vectors (Fig. 8) was tested in simulations with identical parameters. A single crystal grown with the new growth rate function produces the same squares as before (Fig. 7b). However, polycrystal growth with the new growth rate function results in terminating facets with angles, which are closer to but still not exactly 90° (Fig. 9a,b). Additionally, the crystals grow faster due to the larger growth rate vectors (note the larger spacing between the growth increments), and develop a more isotropic morphology because variation of growth rate vectors is more constant for orientations of about 0–30° and 60–90° (Fig. 8). Although the new growth rate function produces sharper oriented facets, it does not completely overcome the facet problem pointed out above, because the tip of the crystals is now more rounded.

One aspect in the calculation algorithm in *Vein Growth*, which may produce inaccurate euhedral terminations of the crystals, is the calculation of the movement of the grain boundary nodes, as outlined above.

During simulations with polycrystals in *Vein Growth*, the seed crystals originally have an irrational rectangular shape

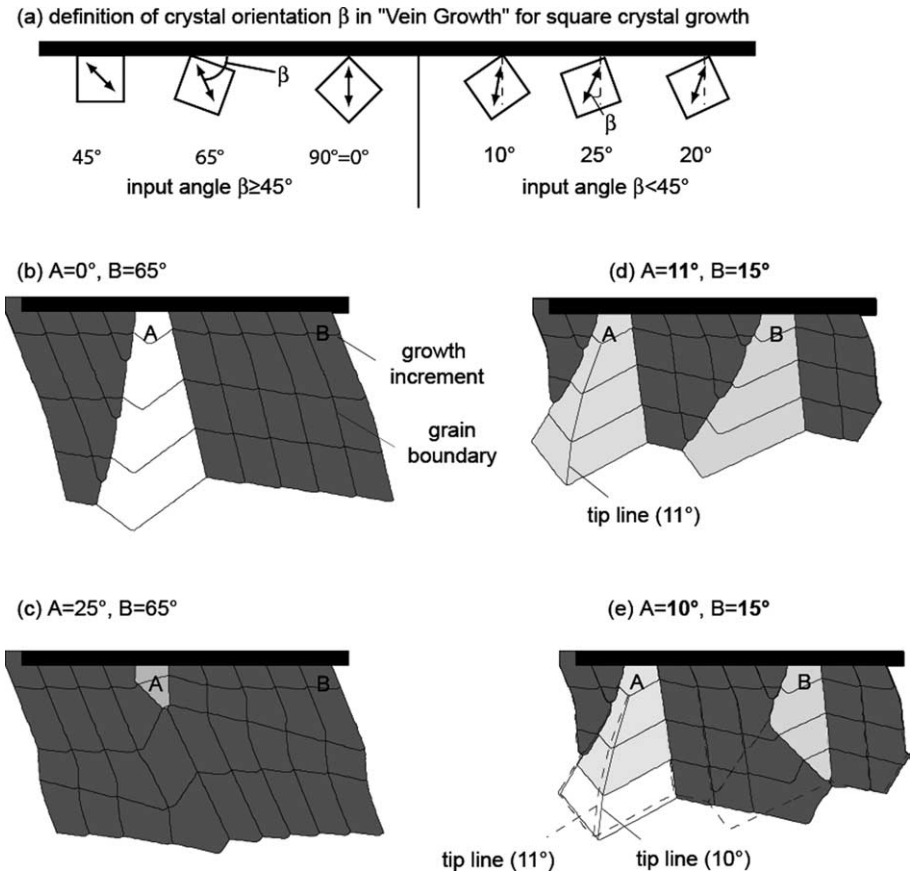


Fig. 5. (a) Sketch illustrating how the crystallographic orientation of a crystal is calculated in *Vein Growth*. The orientation of a crystal is defined by input angle β. If the input angle is $\geqq 45°$, β is calculated clockwise from the horizontal towards the line of fastest growth (indicated by arrow). If the input angle is $<45°$, the code calculates β clockwise from a line oriented perpendicular to the horizontal line. The term crystallographic orientation refers to the arrow in the crystal and to the line of fastest growth for square growth. (b)–(e) Simulations in *Vein Growth* of growth competition phenomena. Crystals A and B have variable crystallographic orientations while the other crystals are oriented at 65° in all simulations. (b) Crystal A = 0°, crystal B = 65°. Crystal A survives and outgrows 65° oriented crystals. (c) Crystal A = 20°, crystal B = 65°. Crystal B is overgrown by the 65° oriented crystals. (d) Crystal A = 11°, grain B = 15°. Both crystals survive. (e) Grain A = 10°, grain B = 15°. Crystal A survives while crystal B is overgrown. The dashed line outlines the microstructure from simulation (d) where crystal A = 11°. Not only crystal A is different, but the grain boundaries of the 65° oriented crystals also grow differently.

and evolve to crystals with facets (Fig. 2a), according to the habit that was set in the first growth stages of the simulations. Due to the calculation routine for the triple junction nodes in the program, the location of the new triple junction, and thus the orientation of a facet, is additionally influenced by the orientation of its neighbouring grain. A neighbouring crystal can therefore 'push' the segment between the triple junction node and the crystal tip or facet to an irrational orientation.

Both the long-distance effect and the crystal terminations that are produced in *Vein Growth* simulations are not observed in natural microstructures and therefore the algorithm should be improved.

We may compare the simulation of a polycrystal under free growth conditions with the results of a simulation in FACET (Zhang and Adams, 2002) (Fig. 9c). In this algorithm, the initial nuclei already have crystallographically correct facets (= *rational facets*) with growth vectors oriented normal to them. By the calculation used in FACET, faster growing facets are outgrown by slower growing facets, resulting in a crystal with crystal terminations without curved grain boundaries but with sharp kinks (Fig. 9c,10). The algorithm correctly describes the propagation of polycrystals and growth competition. However, it is not capable of developing a faceted crystal from a starting material with random morphology as *Vein Growth* can, and crystals cannot fill the open space completely, as happens in natural fracture sealing.

The anisotropic growth rate functions introduced in *Vein Growth* can simulate both isotropic and anisotropic growth. Small opening increments force the crystals to grow isotropically, because of the continuous contact with the opposing wall rock, while growth in an open space results in anisotropically growing crystals that developed facets (Hilgers et al., 2001). Unfortunately, these solutions are at the cost of some inaccuracies in free euhedral growth, and changing the growth rate function in *Vein Growth* cannot completely overcome this problem (Fig. 9a and b).

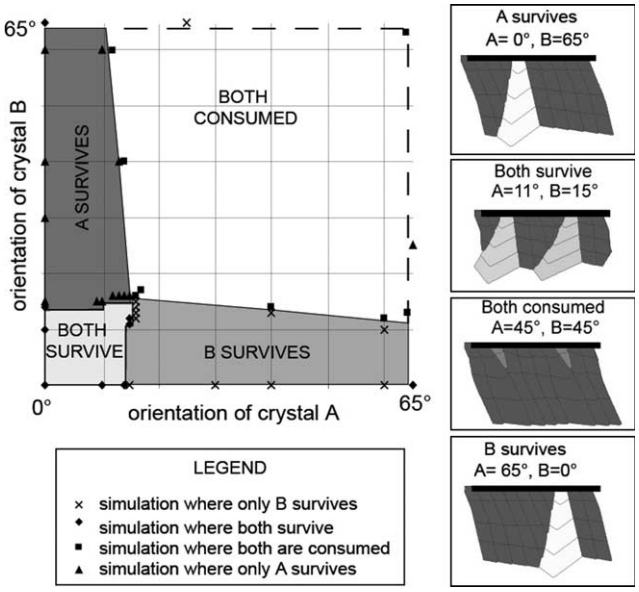


Fig. 6. Numerical simulations in *Vein Growth* plotted on a diagram depending on the orientation of crystals A and B (Fig. 5). The dots represent simulations with a particular orientation for crystal A and for crystal B. Four different areas can be distinguished in the diagram: (1) both crystals survive, (2) both crystals are consumed, (3) crystal A survives and crystal B is consumed, (4) crystal B is consumed and crystal A survives. The border lines between the different areas are not straight lines, which indicates that both crystals influence each others behaviour, due to the long-distance effect. Note that this map is only valid for the situation where the neighbouring crystals are 65°.

4. Crack-seal growth

In previous studies (Koehn et al., 2000; Hilgers et al., 2001), *Vein Growth* has been used to simulate the growth of fibrous crystals in a microstructure. Hilgers et al. (2001) investigated the transitional microstructures between blocky crystals and fibrous crystals in a vein, which depends on the space that is available for the crystals to seal before the next crack event occurs. This study is now expanded by simulating the growth of a polycrystal in a crack-seal environment in *Vein Growth* while only the opening distance in the vertical direction is varied. The size of the crack increment is held constant in each simulation.

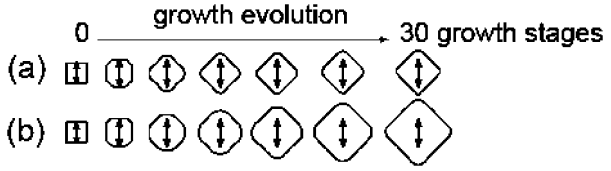


Fig. 7. Comparison of the simulations of a single, initially square crystal, with two different growth rate functions in *Vein Growth*. (a) Simulation with the original growth rate function for square growth in *Vein Growth*. (b) Simulation with the new growth rate function for square growth in *Vein Growth*. In both simulations, crystals are developed with facets oriented according to the crystallographic orientation of the crystals. The angle between the facets is 90° for both crystals. There is no difference in the crystal's shape, but the size is the crystal in (b) is larger, due to the larger growth rate vectors (see Fig. 8).

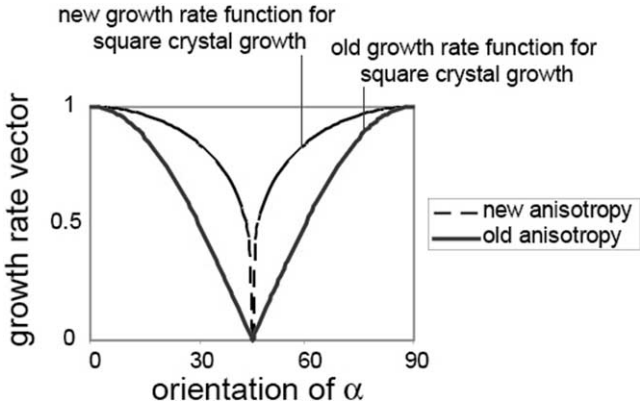


Fig. 8. Growth rate factor plotted against the angle α for two different growth rate functions used in Figs. 7 and 9 that produce square crystal growth in *Vein Growth*. Angle α is the angle between a crystal segment and the crystallographic orientation (=input angle) of the crystal.

Simulations were run with an irregular wall morphology and square anisotropy. The same growth velocity and random oriented seed crystals were used in all the simulations (Fig. 11). We investigated in detail when an irregularity in the simplified wall rock becomes a grain boundary attractor (GBA) (term GBA first used in Hilgers et al. (2001)).

These simulations show that an irregularity in the underlying wall rock acts only as a GBA if the size of the opening increment is lower than the critical value for that amplitude of the irregularity (Fig. 11d). When the opening increment is larger than that critical value, the irregularity is unable to act as a GBA and it does not influence the microstructure, although the grain boundaries were already in contact with the wall (Fig. 11a, b and e) (see also Hilgers et al., 2001). Each irregularity in the simulated wall rock in Fig. 11 has its own critical value as is expected from the relation between the opening distance and the amplitude of the irregularity described in Urai et al. (1991).

The overall microstructure will only be influenced if the growing grain boundaries are at least touching the largest GBA at the end of each sealing event and if this occurs more than once. Grain boundaries that are initially facing a peak survive, while others try to grow towards the peak which gives rise to growth competition and eventually to outgrowing of crystals.

By decreasing the size of opening increments (more frequent contact), the crystal morphology is progressively influenced by the wall rock morphology. However, when the smallest peaks are already touched once, growth competition is still affected by crystallographic orientation effects (Fig. 11e). This can be seen in the rose diagram, representing the orientation of the surviving crystals. These correspond to the preferential crystallographic orientation for the growth anisotropy used. In this simulation, only the largest peaks act as GBAs. The microstructure can still be interpreted as grown in an open cavity, where enough space was available for the crystals to develop rational facets and

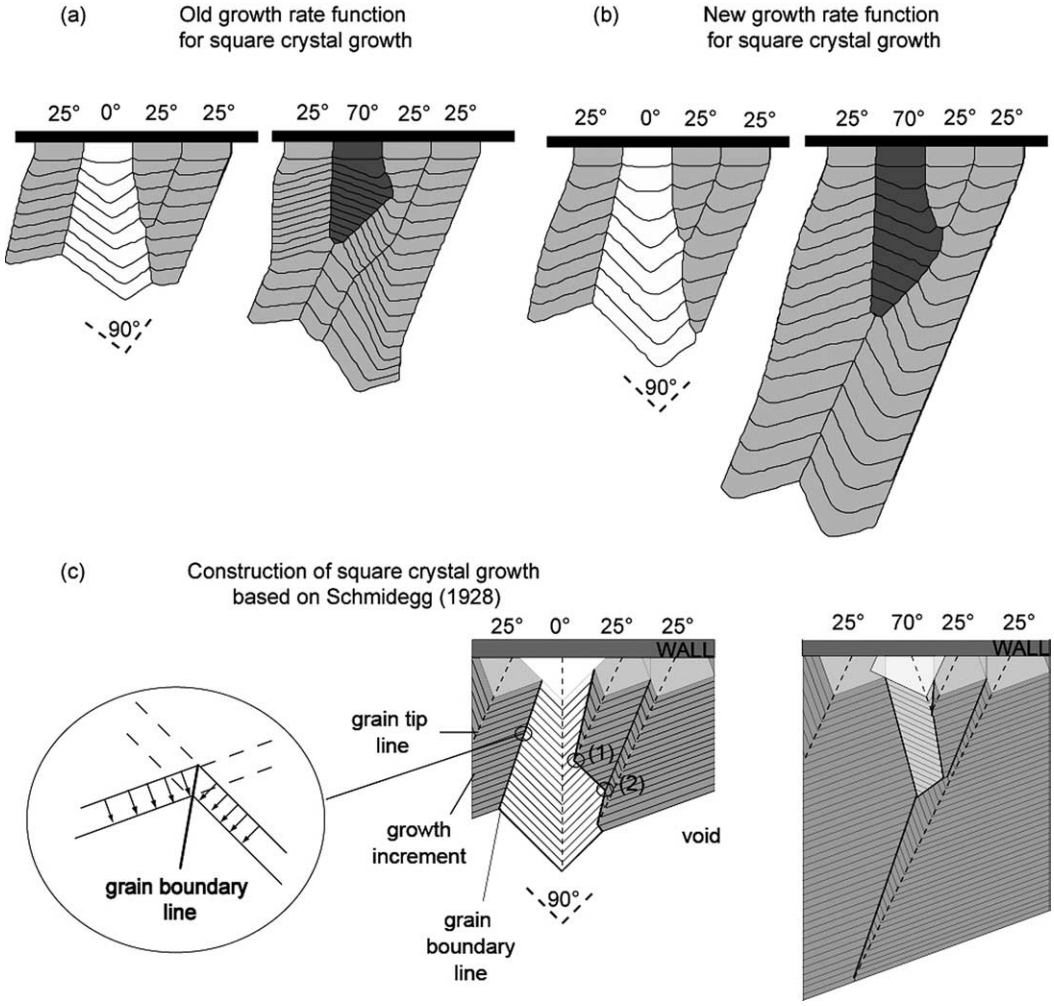


Fig. 9. Simulations of a polycrystal with square anisotropy. The polycrystal contains four crystals. (a) Simulation of the polycrystals with the growth rate function for square growth that was originally implemented in *Vein Growth*. (b) Simulations of the polycrystals with the new growth rate function for square crystal growth in *Vein Growth*. (c) Simulations of the polycrystals with the suggested improved method for the triple junction movement, according to the FACET algorithm. Notice that the facets now make the correct 90° angle for the square crystal model. The same initial settings were used as in (a) and (b). Dashed line for grain tip line; full line for grain boundary line. At growth increment (1), a grain tip line meets a grain boundary line and the result is that one crystal facet disappears and the grain boundary line changes its orientation. At growth increment (2), a grain boundary line meets another grain boundary line and the result is that one grain is overgrown and disappears.

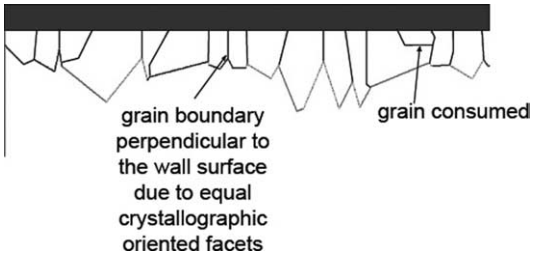


Fig. 10. Simulation of open cavity growth in the program FACET. The initial nuclei have crystallographic correct oriented facets ({100}, {110} and {111}) but the crystals have no individual properties as in *Vein Growth*. The growth vector is for each facet oriented perpendicular to the facet. The location of the moving grain boundaries is defined by the vector sum of both facets, neighbouring the grain boundary. Straight grain boundaries, oriented perpendicular to the wall, are obtained between two facets with identical orientation (e.g. two {100} oriented facets).

to grow anisotropically (Fig. 11e). When the rate of opening is further decreased below the amplitude size of secondary peaks, the competition based on orientation effects decreases (Fig. 11f) and the microstructure has a more fibrous morphology.

With small opening increments (when the opening distance in vertical direction is smaller than the smallest peak amplitude), the resulting microstructure becomes fibrous, without any growth competition or development of crystallographic preferred orientation (Fig. 11g). The crystal growth kinetics changed to isotropic and is irrational due to the regular contact of all crystals and grain boundaries to the wall.

This transition is further illustrated by obliquely opening the crack (Fig. 12). If opening increments are smaller than the smallest peak amplitude, every grain boundary faces its own peak. All grain boundaries have a GBA and the

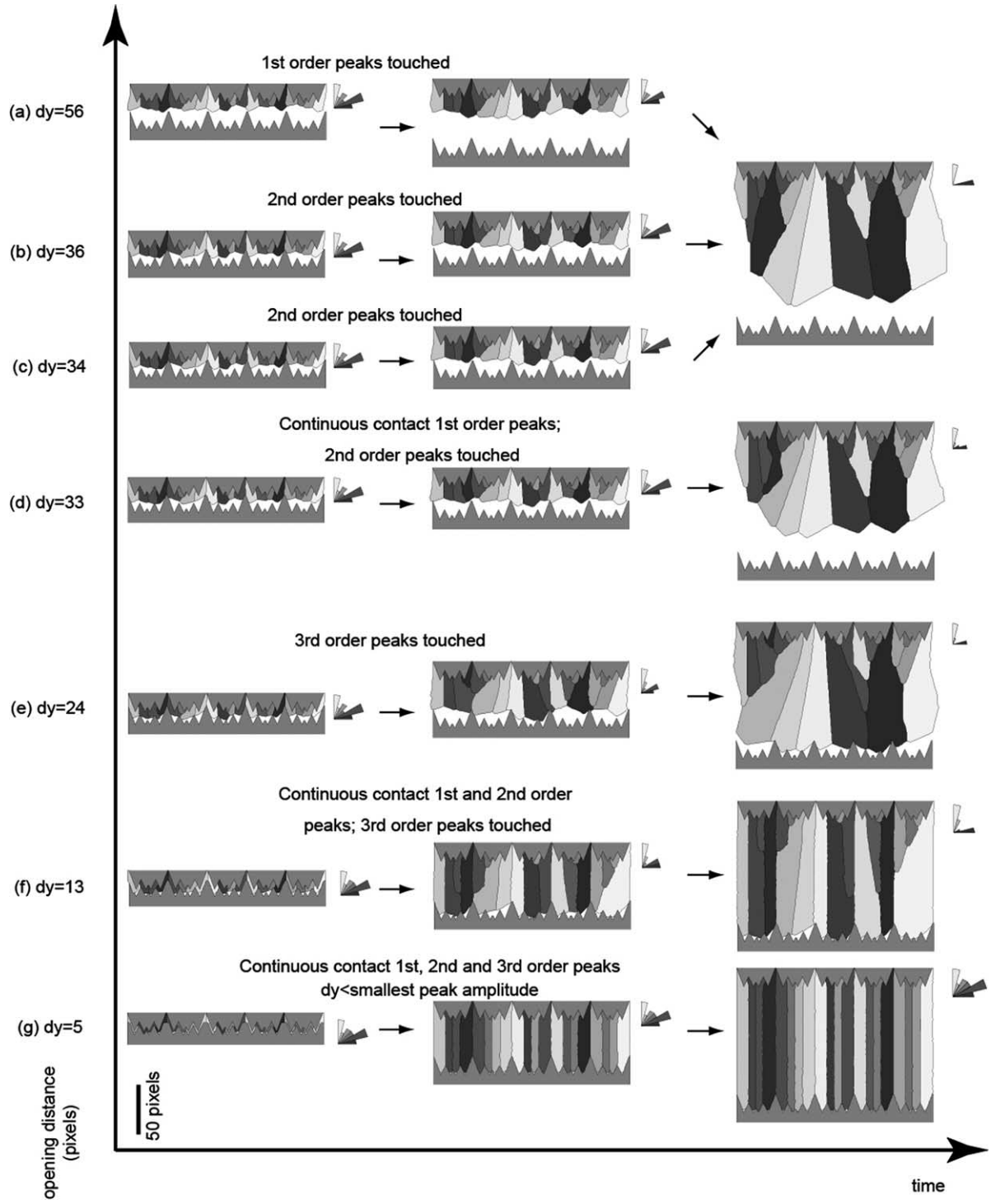


Fig. 11. Overview of numerical simulations with varying opening distances as a function of time in *Vein Growth*. In these simulations, the link between the touching of peaks by the crystals before an opening increment and the magnitude of opening increment was studied. In all simulations, the same wall morphology and seed crystals with the same properties (square anisotropy) were used. The wall rock has peaks with three different amplitudes: 40, 20 and 10 pixels. Magnitude of opening increment is given in the *Y*-axes for each simulation. (a)–(c) show the same final result, the wall morphology has no influence on the growth competition. From simulation (d) on, the wall morphology has influence on the growth competition and the competition effects based on anisotropic growth decreases. In simulation (g), the crystals grow completely isotropically. The orientation of the surviving crystals is given in a rose diagram at the right-hand side of each simulation.

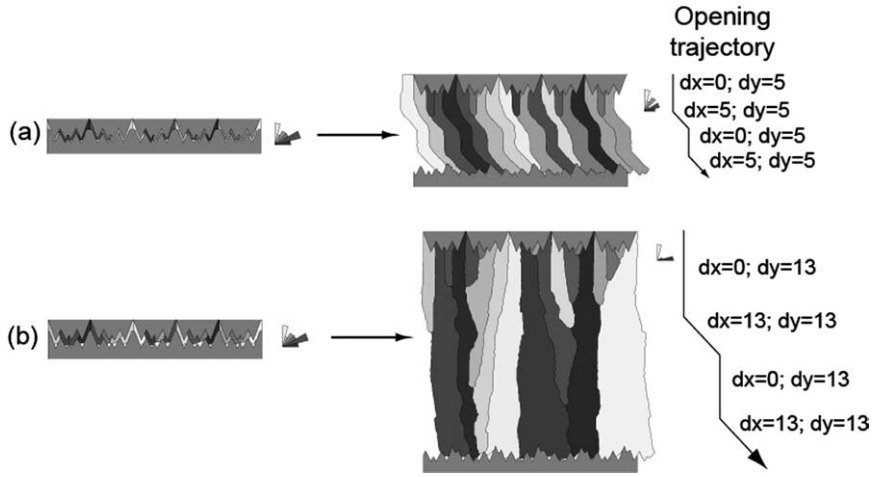


Fig. 12. Numerical simulations with oblique opening trajectories in *Vein Growth*. The same seed crystals, crystal properties (square anisotropy) and wall morphology were used as in Fig. 11. (a) Oblique opening in small increments (5 pixels lateral offset). (b) Oblique opening in larger increments (13 pixels lateral offset). Fibres only track the opening trajectory when opening increments are sufficiently small.

microstructure can be used as a kinematic indicator of progressive deformation because the grain boundaries track the opening trajectory of the vein walls under these circumstances (Fig. 12a). With larger opening increments (Fig. 12b) and the same oblique opening trajectory, the grain boundaries only partly reflect the opening trajectory. The crystals are elongate but the grain boundaries do not exactly follow the opening trajectory because there is enough space to allow growth competition. Such microstructures cannot be used to derive the opening trajectory. When the amplitude of roughness is reduced using anisotropic growth, the open space between crystals and wall rock becomes larger and allows growth competition with an elongate-blocky microstructure as the result. Using isotropic growth, Hilgers et al. (2001) showed a transition from displacement-controlled towards face-controlled growth with the fibre orientation normal to the vein wall interface regardless of the opening direction.

In the next series of tests, we varied the number of initial crystals to study the relationship between growth competition and irregularities in the wall morphology (Fig. 13). The fracture was opened in small opening increments to avoid growth competition based on orientation effects. The crystals have a random orientation.

The simulations show the absence of growth competition if the initial number of grain boundaries corresponds to the number of peaks (Fig. 13a). When there are initially more crystals than peaks, competition occurs until all the peaks have attracted one single grain boundary each (Fig. 13b). Further decreasing the number of grain boundaries (Fig. 13c) has no effect on the final microstructure.

Grain boundaries attracted by a peak during their growth are stable and survive during the further evolution of a crack-seal vein. The unstable places for the grain boundaries are the troughs or deeper places of the crack surface (Fig. 13b and c) (see also Urai et al., 1991; Koehn et al., 2000). When a grain boundary is located between two peaks, it tends to grow towards the nearest peak and will finally be consumed by a neighbouring grain boundary, which was already located at the favourite position.

The inaccuracies that were recognized in the *Vein Growth* code during simulations of growth in an open space do not have consequences for the crack-seal simulations. Moreover, once the underlying wall rock has an influence on the microstructures, i.e. when opening distances are small enough, the crystals behave isotropically and the effects described above were found to be caused by anisotropic growth rate functions. The transitional microstructures that were simulated here are not influenced by the inaccuracies in the program, except for the facet terminations in the simulations with larger opening distances where the crystals behave mainly anisotropically.

5. Discussion

Vein Growth is a useful tool to simulate the microstructural evolution of crack-seal veins, covering elongate-blocky to fibrous microstructures, because it is able to switch from anisotropic growth to isotropic growth when the crystals touch the wall rock in a crack-seal environment (Fig. 14). However, the growth algorithm is limited with respect to the simulation of crystal growth in an open space and needs an extension to produce the exact facet orientation simulations of blocky crystals in a free growth environment. This can be achieved by using the traditional facet propagation algorithm for those parts of the growing surface that have evolved into facets. The algorithm may be improved by expanding the simulation code to include the growth algorithm used in FACET. The growth algorithm from *Vein Growth* is used as long as the crystals do not develop low-index facets (Fig. 14a). The growth rate

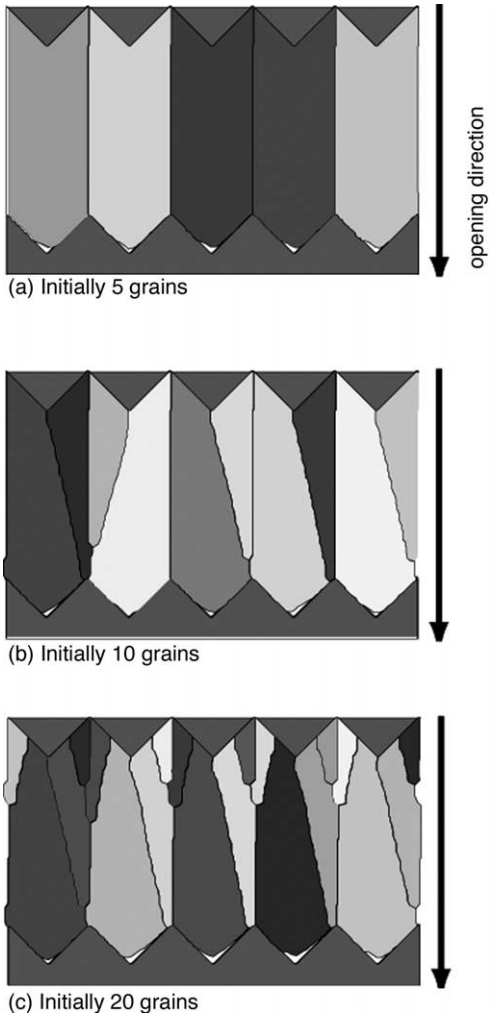


Fig. 13. Numerical simulations of square-like growing crystals with small opening distances and a wall rock with five peaks with varying numbers of seed crystals in *Vein Growth*: (a) initially 5 crystals (b) initially 10 crystals and (c) initially 20 crystals. Opening of the crack is in all the simulations strictly vertical. The simulations show that there is growth competition when not every grain boundary faces a peak in the wall rock. Growth competition occurs until the number of grain boundaries equals the number of peaks in the wall rock. In (c), three grain boundaries tend to grow towards the favourite position on the GBA. The grain boundary that was located in the most unfavourite position, i.e. the trough, outgrows grain boundaries that were located closer to the GBA and survives longer.

anisotropy will lead to semi-rational crystal facets. These segments are then classified as rational, and the algorithm switches to the growth algorithm of Schmidegg (1928) and Zhang and Adams (2002). The crystals with well-oriented facets grow, and growth competition occurs between different crystals (Fig. 14b). The movement of the triple junction is calculated by the vector sum of the two free facets next to the triple junction in free growth, without solid-state boundary motion. However, when crystals have grown close to the opposing wall, the model will again switch to the algorithms of *Vein Growth*, which allow the influence of the wall morphology on the final microstructure (Hilgers et al., 2001) (Fig. 14c). This hybrid algorithm will

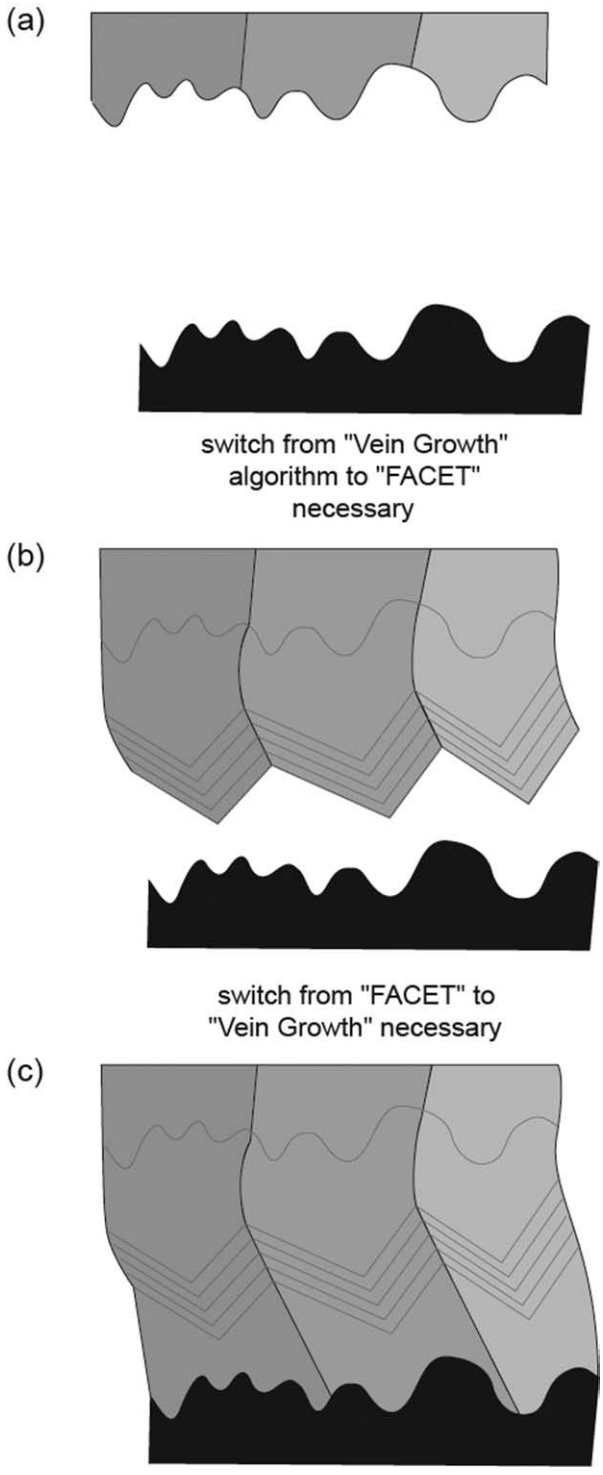


Fig. 14. Sketch showing the hybrid simulation algorithm. (a) At first, the *Vein Growth* algorithm is used to simulate the evolution from a crystal with random morphology to a faceted crystal. The model should then switch to the FACET algorithm for the calculation of the movement of the triple junction nodes. (b) Once the growing crystals are grown close to the wall rock, the algorithm should switch again to the *Vein Growth* model, because then the calculation of the triple junction nodes is dominated by the irregularities in the wall rock.

require a criterion for classifying a crystal segment as facet or irrational. Details of this criterion are difficult to define, because in the crystal growth literature the transition from irrational, rough faces to facets is not well understood and further studies are needed to determine the nature of this transition.

The change from elongate-blocky crystals to completely fibrous veins, which track the opening trajectory, will depend on the nature of this transition. One consequence of the algorithm of *Vein Growth* is that a critical free growth distance is required for the development of facets. At a shorter distance, growth is effectively isotropic and the propagation of grain boundaries is dominated by the wall rock morphology. This critical distance has been already discussed by Urai et al. (1991) as the factor controlling the onset of growth competition. Based on numerical simulations in *Vein Growth*, Hilgers et al. (2001) found an upper limit of 10 μm, below which growth competition is absent. Typical opening increment lengths in natural crack-seal veins are described as 10–100 μm, correlated with inclusion band separations (Ramsay, 1980; Cox, 1987; Fisher and Brantley, 1992). However, there is almost no experimental data available on this transition, although it seems likely that it is variable and complex. Therefore, at this point it is difficult to discuss the effect of details of the *Vein Growth* algorithm on this transition.

6. Conclusion

Microstructures formed by precipitation of a supersaturated fluid in an open cavity or in a progressively opening fracture have a specific morphology, depending on different parameters. The parameters controlling vein microstructures were studied using numerical simulations. Growth of crystals in an open space results in microstructures that are controlled by the crystallographic orientation and the growth anisotropy of the crystals. The transition between free growth and crack-seal growth occurs when peaks in the wall are regularly touched by the grain boundaries. These peaks then become grain boundary attractors. Incomplete sealing during crack-seal vein growth will produce a wide range of transitional microstructures characterized by elongated crystals and growth competition. Fibrous veins are formed when sealing is sufficient to bring grain boundaries in contact with the smallest peaks in the wall rock before the next opening event. Growth competition in a crack-seal environment will occur until the number of grain boundaries equals the number of grain boundary attractors. If a fibrous vein microstructure shows no growth competition with all grain boundaries located at peaks in the wall, it displays the opening trajectory and can be used to derive the deformation history. *Vein Growth* can be improved by incorporating a hybrid growth algorithm, which simulates free growth based on the algorithms of facet growth. In order to understand the mechanisms occurring at the vein–wall interface, experimental studies of the transition between irrational (rough) and faceted growth are required.

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