Response to Anonymous Referee #2

We thank reviewer #2 for the constructive criticism, which should lead to a number of improvements in the current manuscript. Below are point-by-point responses, with the reviewer comments in *italicised red* font and our responses in normal black font.

Item I. Summary: The submitted article "Three-dimensional phase-field study of crack-seal microstructures – insights from innovative post-processing techniques" presents a 3D model for vein growth, with the possibility to model in principle crack sealing microstructures together with a modified tracking tool to track the growth of a crystal both numerically and in principle in thinsection.

We would like to add that the presented 3D model represents a general framework that can be used for simulating the growth of any arbitrary-shaped crystal under various kinds of boundary conditions. Like the referee points out, we use this model to study the tracking efficiency during the crack-sealing process.

Item II. The model itself has already been presented in a recent publication in Contr. Mineral. Petrology. There is little difference between the already published work and the presented work here.

The aim of the present study is different from the one presented by Ankit et al., Contrib. Mineral. Petrol., 2013. We enumerate the point of differences by classifying them as *major* and *minor* points below:

Major points of difference

1. The present study aims to theoretically establish the importance of accounting for the temporal evolution of grain boundaries, in determining the tracking efficiency. To achieve the aim, two new types of general tracking efficiencies (namely GTE_1 and GTE_2) are defined. A good agreement of GTE_1 with GTE_2 for both the simulation test cases 'A' and 'B' (refer to table 2) suggests that the aim of the present work is adequately achieved. On the contrary, the GTE_1^ts do not compare well with GTE_2^ts (calculated from the final vein morphology), which further strengthens our argument concerning the accountability of temporal evolution in calculation of GTE.

Ankit et al, 2013 do not account for the role of temporal evolution which could influence the accuracy of tracking efficiency. Instead, they use grain boundary contours from the last simulation frame to measure tracking efficiency.

2. The *two* general tracking efficiencies, defined as GTE_1 with GTE_2 use computationally superior post-processing techniques in comparison to GTE defined by Ankit et al., 2013 (grain boundary contours for the last simulation frame for a 2-D case).

GTE_1 : The peaks of crack surface are superimposed on the advancing crystal growth front (after numerically discarding off the crack surface) and those lying along the grain boundary/triple/ quadruple points are counted. Urai et al. 1991 use a similar technique i.e. they count the number of tracking peaks in 2-D. However, in 3-D, this becomes a challenging task from an algorithmic point of view (as shown in fig. 5), which we achieve in our present work.

GTE_2 : The barycenter of every grain present inside the shifting simulation-box represents the overall evolution pathway. The 3-D evolution pathways are more complex as compared to a 2-D case, since the former, also accounts the out-of-plane evolution of veins. The extent of deviations in the 3-D evolution pathways (obtained by joining the barycenter of every grain obtained after every simulation time-step) of veins w.r.t. the crack opening trajectory determines the tracking efficiency.

It is apparent from the above description as well as the present results, that the GTE defined by Ankit et al, 2013 cannot be directly extended for a 3-D case. Ankit et al, 2013 do not study the tracking efficiencies, in 3-D, during the crack-sealing process, unlike, the present study.

The take-home message is: *As long as the temporal evolution and the three-dimensional characteristics of the growing veins is accounted for, the derived tracking efficiency can, in principle, be calculated correctly, irrespective of the technique used.*

3. Ankit et al., 2013 do not show any grain statistics like grain size distribution, orientation-distribution and number of grains which is dependent on the crack opening rate. In fact, we were aware of the importance of grain statistics, when we drafted that article. As the grain statistics obtained after the crack-sealing process merits a separate discussion, we chose not to touch that aspect in the previous paper.

We would like to iterate the statement from Introduction - *"In the context of vein growth, we emphasize that the grain formation process is generically of 3-D nature and can be interpreted in a physically sufficient manner by methods capable of capturing the growth* characteristics *and dynamics in full 3-D space."*

The crack-sealing studies presented by Ankit et al., 2013 is predominantly 2-D, unlike, the present study which focusses exclusively on 3-D aspects and accounts for larger number of grains, which yields representative statistics.

4. One of the main results of the present simulations is: The pinning at triple junction or quadruple junction is stronger as compared to grain boundaries. We request the referee to cite a reference, if this has already been shown numerically before. To our knowledge, it has never been numerically demonstrated before.

Minor points of difference

5. Ankit et al. 2013 use an alum crystal (which is not a vein-forming material) for all the phase-field simulations. In the present work, we use an idealised quartz crystal (which is one of the common vein-forming mineral).

6. Ankit et al., 2013 use an oblique opening trajectory. In the present work, the crack opens along a quarter arc.

7. Ankit et al., 2013 used a short-range periodic (for 2-D) and an irregular (for 3-D) crack surface for the numerical simulations. In the present work, we use an algorithmically generated (diamond-square) fractal surface.

Item III. No direct comparison with real rocks are given.

We agree with the reviewer, partially. However, in principle, we do *not* think that a direct comparison of present 3-D simulations to thin sections is a good idea. This is explained in the introduction section. A 3-D re-construction from 2-D slices may be a more pragmatic approach. However, this demands a different (microscopy) expertise, which is not the focus of present work.

We explain the assumptions made in the phase-field simulations, in our previous article (Ankit et al. Contrib. Mineral. Petrol. 2013) as well as in the present write-up. The idea of using the phase-field method is to decompose the effect of every boundary condition, which influences the vein evolution process. Although, a comprehensive understanding of the crack-sealing process is long sought in the geoscientific community, we still need significant improvements in the modelling techniques to bridge the existing gap i.e. between computationally simulated and natural microstructures. With an aim to abridge the gap, we advance the model to 3-D studies, as indicated in the title of the manuscript.

With due regards to the opinion of the reviewer, we state that a more comprehensive modelling approach is required for a direct comparison of computationally simulated microstructures with naturally occurring ones. A comprehensive study, although desirable, is not the focus of current work. In the present work, we limit the discussion to the influence of crack-opening rate on tracking characteristics and grain statistics/morphologies. Within the scope of present study, a good agreement of the general tracking efficiencies (GTE_1 with GTE_2) **validates** our findings and **confirms** that the aim of conducting the numerical simulations has been adequately achieved.

The 3-D phase-field simulation of polycrystalline quartz , in absence of a barrier (shown in new fig. 2), reproduces the growth competition arising due to the mis-orientation w.r.t most-preferred orientation (vertically upwards) without any exceptions. So, it is argued that, in presence of a barrier whose opening rate is slow and surface roughness is very high,, the kinetics of the isotropic vein growth is recovered.

Item IV. Furthermore, there is a general misconception of the use of the term "Crack-seal". The presented model does not show crack-seal behaviour – but only seal behaviour. There is no true repetitive cracking and sealing going on. There is 1 crack event and then a continuous sealing event (growth of crystals). This needs to be rectified.

We clarify that the simulation results presented in the manuscript concern repetitive crack-sealing (and *not* just sealing). The overall opening trajectory is a quarter arc with crack opening horizontally and vertically in form of small steps. The magnitude of vertical and horizontal displacement change in every opening step, which constitute a quarter arc trajectory. The upper crack surface (the crystal seed bed) remains static while the lower crack surface is the one which is displaced. The size of the vertical steps (constant) are given in table 1. The horizontal displacement is therefore determined automatically, according to the equation of the circle.

If the presented study concerned only one crack-opening event, why would the numerically calculated tracking efficiency be related to the opening trajectory? If it was just one sealing event, opening trajectory would have *no* meaning. Obviously, there is a misunderstanding on the part of referee. Additionally, we are not able to find the source that causes such a confusion, in the manuscript. The arched crack opening trajectory is shown clearly in Fig. 6(a). Figs. 6(b) - (h) (in the old manuscript version) show the opening trajectories as well. We humbly request the referee to point out the lines/words/figures in the manuscript which led to such a confusion, so that this can be clarified in the final version of the manuscript.

Reply to General Comments

A) Title: This is Uniaxial Vein Growth not Crack Sealing – needs rectification

The word "unitaxial" can be added to the title. We agree, as the present simulations concerns one-sided growth.

However, not calling it crack sealing will be unreasonable. Kindly consider our reply to referee comments in Item IV.

B) Organisation of paper: The paper is generally correctly organized, however, it is not made clear what really the difference between this contribution and the latest publication of Ankit (Contr. Mineral. Petrology) is. The General tracking method has already been presented int that very paper (Ankit et al. 2013). The dependence of grain number with rate of crack opening has also already been shown.

We request the referee to consider the detailed reply in Item II. which highlights the points of major and minor differences of the present work with Ankit et al., Contrib. Mineral. Petrol., 2013.

To warrant publication especially as a Modell Assessment paper – direct comparison with experiments or nature need to be given.

Kindly refer to our reply to the referee comments in Item III.

C) Abstract: The paper promises to look at realistic boundary conditions, but how realistic is the fractal surface used – this is not being tested/discussed or questioned in the contribution and not even based on any natural examples of cracks in nature. Thus the abstract promises research that is not presented.

The phrase "realistic boundary condition" needs to be comprehended in its entirety. When we talk of a realistic boundary condition, it means the following:

(a) The crack surface profile used in numerical simulations resembles a naturally occurring rock surface.

(b) The crack-opening trajectory is more complex as compared to an oblique line.

(c) The magnitude and direction of crack-opening increments are *not* uniform/consistent.

In the present work, we account for (a) and (b) but do not change them for the two simulation test cases 'A' and 'B'. Only the influence of changing (c) is considered.

It is a widely accepted fact that a "real roughness is often fractal and can be measured." (refer to the book: The Fractal Geometry of Nature, B. Mandelbrot). In the present work, we implement the above idea to generate a rough surface, by the aid of a numerical pre-processing algorithm (diamond-square). However, the surface roughness has not been varied (although this can be done by the algorithm we use) for the two simulation test cases 'A' and 'B', as we do not intend to do a parameter-study, which is similar to Ankit et al., 2013.

D) Introduction: Generally fine. However, should go more into the literature of how veins crack, what governs crack opening rates, and the known surface roughness in different rocks. Needs more *review of data from the geological community as input for the numerical simulation presented here. Work by Koehn et al. in the early 2000 on fringe development should be discussed and cited as there they have shown the clear dependence of growth behaviour and crack roughness.*

We wrote a short literature review of the numerical studies presented before the phase-field method was used for modelling the vein growth process. Urai et al., 1991; Hilgers et al., 2001; Bons, 2001; Nollet et al., 2005, all these very nice papers have been cited before by Ankit et al. 2013.

In the present manuscript, we do not study the influence of crack roughness. Rather, the aim is to decompose the effect of crack-opening rate on tracking efficiency. Therefore, we do not find it reasonable to cite Koehn et al., 2000. The aim of conducting a short literature survey is already clear i.e. the front-tracking approach and the other derived models have not been used for a 3-D study. In the light of above argumentation, we still choose to cite Koehn et al., 2000 in the revised version, giving due regards to referee comment.

We also clarify that the aim of the present work is not just to appeal to a specific section of structural geologists. The multiphase-field method is capable of capturing the physics of any phase-transition and therefore, is considered to be interesting for material scientists alike. The numerical techniques adopted and the three dimensional domain-decomposition involved makes the topic interesting for computer scientists as well; vein growth, *merely,* being the simulation test case.

E) Methods: As far as I can see, the numerical method is the same model as presented in Ankit et al. 2013. In general it is o.k. like this, however since the model was already explained it would have been good to provide an extra figure showing graphically how the model works (to complement figures in Ankit et al. 2013).

We agree with the reviewer's suggestion. The picture explaining the diffused interface approach can be included in the final version of the manuscript (Fig. 2).

F) Results. The Tracking efficiency that is written in the results section, should really be in the methods section. The emphasis of this paper is this tracking efficiency as actually the boundary conditions are not varied or tested. This is a slightly refined version of the Ankit et al. 2013 version. Please put method of tracking into the Methods section. In the results you can have the tracking results, and the statistics of grains. Again none of this is really new or novel though.

We agree with the reviewer's suggestion that the description of general tracking efficiencies needs to be moved to the Methods section. This can be implemented before the final submission.

In order to appreciate the difference w.r.t Ankit et al., 2013, kindly refer to point number 2 of Item II.

The novelty of the current work can be established only if the differences are clearly understood by the reader w.r.t Ankit et al., 2013.

G) Discussion Actually, the results presented are very few and not new and not com- pared to nature. For an Model assessment paper there should be some comparison as the Model itself has been already presented. This seem very much a double-dipping technique. If you compare with experimental or natural samples, then you give this publication an extra dimension (which is necessary)

The aspect concerning comparison of present simulations with natural samples is addressed in Item III.

The novelty aspect of the present work can be appreciated only if the difference w.r.t. Ankit et al. 2013 can be established. Kindly refer to Item II.

H) Conclusion Conclusions are very similar to that given in Ankit et al. 2013. And has little to do with the abstract "realistic boundary conditions" – I do agree that 3D models are very valuable, however a lot can be learnt from 2d models and in many cases it is much easier to assess if results are just an artefact of the numerical method used or true. This needs to be discuss

On a careful comparison of the conclusion section presented by Ankit et al., 2013, following differences can be identified:

(a) Ankit et al. 2013 conclude about the influence of different boundary conditions on the grain boundary morphology. The aspect of multi-junction morphologies is not mentioned

(b) Ankit et al., 2013 presented a detailed study of 2-D crack-sealing process. However, it is important to understand that adding an extra dimensionality to the numerical simulations especially, in the case of crack-sealing, helps us to access the "complete story" as explained in the introduction. The present work concerns 3-D, and the conclusion is made on similar lines.

(c) Concerning the "realistic boundary conditions", kindly refer to the response to general comment (C). We offer to clarify the same in discussion and conclusion sections, if the editor agrees.

The question concerning numerical artefacts is adequately answered by a good agreement of GTE_1 and GTE_2. The model is tested by Ankit et. al, 2013 to reproduce the crystal growth competition during free-growth in 2-D and 3-D alike (refer to figs. 2 and 3 of Ankit et al., Contrib. Mineral. Petrol., 2013), an example of which is included in the revised version (Fig. 2). Moreover, the 2-D phase-field results are able to reproduce the 2-D results of the front-tracking method (without any artefacts like "crystal terminations" or "long-distance effect"; Nollet et al. 2005).

We believe that the reviewer does not warrant the publication of this work, mainly because of being not able to establish the difference with the previous work of Ankit et al. 2013. The comparison of numerical simulation results with natural samples, as suggested by the referee, is great to have. But again, this demands adoption of a comprehensive modelling approach, which is not the aim of the current work. We make several assumptions in the present 3-D simulations, so a comparison with natural samples is difficult to establish.