On the basis of a careful examination of referee comments, two important inferences are drawn:

- The referee is **NOT** aware of the previous numerical results reported (Hilgers et al, J. Struc. Geol. 2001; Nollet et al, J. Struc. Geol., 2005 to name a few) which are also validated by field studies. The review is full of factual errors which arise due to the misunderstanding concerning the crack-sealing process in veins.

- The referee fails to recognise that Urai et al, 1991 assumed isotropic crystal growth rates, i.e. the growth surface propagates equally fast in all directions (refer to page number 830, 4th paragraph of Urai et al, Journal of Structural Geology, Vol 13, No 7, pp 823-836, 1991). On the contrary, we use faceted-type anisotropy function to model crystal-liquid interfacial energies (see the polar plot of interfacial energy and the simulated crystal equilibrium shape in Fig. 2 of the present manuscript). Therefore, referee arguments disputing our current work for not having drawn a meaningful connection to the numerical results of Urai et al 1991, is not reasonable (also see a detailed reply to the corresponding comment below).

Since the comments are not itemised, we split the referee's comments in numerous lines (in *italicised blue* font) and provide a detailed reply (in black font colour)

The manuscript "Three-dimensional phase-field study of crack-seal microstructures - from innovative post-processing techniques" by K. Ankit, M. Selzer, and B. Nestler does not contain new physics or new models in the applied area (within the scope of Geoscientific Model Development).

We are not aware of any three dimensional numerical study of crystal growth in veins, that is published earlier. As the referee suggests that the present work does not contain any new physics or new models in applied area, we request to supply the required references. In particular, we would like to know and congratulate the authors who have already published a **three dimensional** numerical study of crystal growth in veins, as it is a computationally challenging task.

We also request the referee to cite the articles (if any) concerning the phase-field study of crack-sealing in veins. We are aware of only one such article which we published recently (**K. Ankit,** B. Nestler, M. Selzer, M. Reichardt. Phase-field study of grain boundary tracking behavior in crack-seal microstructures. Contributions to Mineralogy and Petrology, Volume 166, Issue 6, pp 1709-1723, 2013). We request the reviewer to read the detailed literature review presented in the article mentioned above.

A thorough literature review on the numerical simulation of vein growth reveals that there is **NO** such article that was published earlier which addresses the 3-D aspect. In fact, such a *thermodynamically consistent* model has been long sought in the geoscientific community. Till date, the numerical studies on crack-sealing is limited to 2-D. The 2-D front-tracking algorithm which is a well known technique (and most widely accepted in view of dearth of any other numerical model) to simulate vein

growth (namely “FACET” and “VEINGROWTH”) suffers from model artefacts as reported by Nollet et al, Journal of Structural Geology 27 (2005) 217–230. Further, both the front-tracking methods mentioned above, do not account for any thermodynamic parameters which influence crystal growth in veins. As compared to the front-tracking approach, the thermodynamic aspects are accounted for in the present phase-field simulations, which directly answers the referee comment: “does not contain new physics”.

Model assumptions: Unlike Wendler et al Journal of Crystal Growth 327 (2011) 189–201, we do not account for the role of kinetic anisotropy in crystal growth but only the anisotropy in interfacial energy. In view of non-availability of a kinetic wulff shape, this appears to be a reasonable choice. Further, the long range diffusion is not modelled, and we use a constant driving force for evolving crystals. The equilibrium shape of the evolving crystals represents an idealised quartz.

The importance of a three dimensional numerical study of the crystal growth in veins is very important and explained in the first paragraph of page 633 of the present manuscript. The presented study is not reported elsewhere. As far as the question of new physics is concerned, the present study shows, how a rough surface pins the grain-growth as the vein evolves. The same is reflected by the grain statistics obtained from 3-D simulations. The present study also introduces the concept of **General Tracking Efficiency** and a near overlap of the two GTE^t shows the importance of accounting the temporal evolution in the calculation of tracking efficiency.

We observe that the referee does not cite any references while disputing the aspect of novelty. As we are aware that Geoscientific Model Development publishes articles concerning model assessment, it is fully within the scope of publication.

Moreover, there are no connections to the previous results presented in Ref. [Urai et al 1991].

We request the referee to comprehend the present work and compare it with Urai et al 1991, once again. A careful examination of the model used by Urai et al 1991 would reveal that the crystal growth was assumed to be **isotropic**. On the contrary, we use anisotropy in surface energy; therefore, the two models are not comparable.

As far as “connections” are concerned, the ability of phase-field method to reproduce the results of Urai et al 1991 is already reported in our recent article (compare plots in fig. 5(g) of **K. Ankit** et al. Contributions to Mineralogy and Petrology, Volume 166, Issue 6, pp 1709-1723, 2013 with fig. 7(a) of Urai et al, Journal of Structural Geology, Vol 13, No 7, pp 823-836, 1991).

In spite of both models being not comparable, the reason why the plots look alike is because when the crack-opening rate is small and the surface roughness is sufficiently high, veins evolve like-isotropic. In such cases, anisotropy in interface energy does not play any role (even if it is taken into consideration in the model). This also

happens to be classical instance where front-tracking as well as the phase-field method agree quite well for a comparable simulation setup.

We also request the reviewer to compare the diagram shown in fig. 2(g) of **K. Ankit** et al. Contributions to Mineralogy and Petrology, Volume 166, Issue 6, pp 1709-1723, 2013 with fig. 6 of Nollet et al, Journal of Structural Geology 27 (2005) 217–230. The area "Both survive" in the latter represent the artefact of front-tracking algorithm whereas no such area is visible in the former. It should be intuitive that for such a simulation setup, there always exist a most preferable orientation, which outgrows the mis-oriented neighbours. Since 'A' and 'B' represent crystals with dissimilar orientations, there is no question of both of them, surviving the growth competition simultaneously, when anisotropy in surface energy is taken into consideration. This represents the model advancement i.e. getting rid of artefacts and the same has been reported well in our previous article.

There are ample evidences which suggest that the phase-field method is able to reproduce the previous findings sans model artefacts, hence we do not agree with the view point of the referee.

That means no results about the dependency of the tracking efficiency on the angels of the crack surface are presented.

We do not understand the meaning of "angels of the crack surface". We assume that there is a typing error in the above comment, the referee actually meant "angles of the crack surface".

The choice of the terminology "angles of the crack surface" appears to be confusing. As the referee does not make it clear, what he actually meant (spelling error does not help either), there can be two possibilities:

1. We assume that what the referee meant was a short range periodicity of crack surface, the apex angle of which being the "angle of the crack surface".

We would like to update the referee that such a study was one of the focus points of our already published article: **K. Ankit** et al. Contributions to Mineralogy and Petrology, Volume 166, Issue 6, pp 1709-1723, 2013. Kindly refer to figure 5 of the published manuscript. Here 'β' represent the angle of periodic crack surface, which is a measure of surface roughness.

We would also like to clarify that definition of such a unique angle 'β' is limited to periodic surfaces. However, in the present study we do not use a short-range periodic crack surface. Therefore, invoking a similar argument which was already tested in a previous article using the same model for a 2-D case, will not be necessary and undesirable. This is the precise reason, why we develop the concept of general tracking efficiency which accounts for a more complex trajectory of evolving veins (GTE_2), an aspect the referee seems to overlook all together.

2. The angles could also be interpreted as crack opening trajectory. In the present study, we use a curved opening trajectory as against to our previous study on oblique openings (fig. 7 of the above paper). For the present case, we relate the tracking efficiency with the temporally changing opening angle using GTE_2 (also see Fig. 6 in present manuscript).

The used random crack surface does not have any characteristics from which the tracking trajectory and the tracking efficiency can be analyzed (see Ref. [Urai et. al 1991]).

We would like to add that the "used random crack surface" is a fractal surface which is constructed by the well known diamond-square algorithm (G. Miller Definition and rendering of terrain maps, in: Proceedings of the 13th annual conference on Computer graphics and interactive techniques (ACM), SIGGRAPH '86, New York, NY, USA, 39–48, 1986).

We would also like to clarify that in a crack-sealing process, it is the crack surface which opens up temporally and it is the veins whose tracking characteristics are studied. The tracking efficiency depends on a number of factors such as the surface roughness, crack-opening rate and trajectory. The focus of the present study is limited to the study of crack opening rate and the resulting general tracking efficiency of the vein, while keeping the surface roughness as well as opening trajectory to be same for both the test cases 'A' and 'B'.

We do not intend to merely repeat the numerical experiments of **K. Ankit** et al. Contributions to Mineralogy and Petrology, Volume 166, Issue 6, pp 1709-1723, 2013 for a fractal surface in 3-D. On the contrary, the focus of the present work is to define the tracking efficiency in a way, which accounts for a more complicated 3-D case, as the veins temporally evolve out of the plane in 3-D space. Further, the importance of accounting for temporal evolution in the calculation of general tracking efficiency is highlighted.

We provide a detailed discussion concerning the comparison of the two general tracking efficiencies GTE_1 (which is an extension of definition from Urai et al for a 3-D case) and GTE_2 in section 4 and table 2.

The comparison of phase-field results with Urai et al 1991 is already addressed above.

The coarsening process in the paper is only a standard microstructue evolution simulated by a standard phase field model.

There are multiple errors in the above comment. We will address these errors which seems to arise due to the misunderstanding of the referee.

First of all, unitaxial crack-sealing in veins is not same as normal grain coarsening process. To be more precise, we study the effect of barrier (crack wall) pinning the

evolving grain boundaries/triple/quadruple point in 3-D for a complex (rough and also temporally moving) boundary condition. During the evolution of veins, there are numerous external boundary factors which influences (or hinders) the growth process. In order to simulate the crack-sealing process correctly, the boundary condition needs to be modelled suitably which is a challenging task. Crack surface roughness, opening rate and trajectory are a few, to mention. K. Ankit et al, Contrib Mineral. Petrol., 2013 have already presented a detailed phase-field study on each of these aspects. On the contrary, in a normal grain coarsening process, periodic boundary conditions are sufficient to reproduce the grain coarsening law.

From the above comments, it is clear that the referee misunderstands the current work to be grain coarsening. In fact, grain coarsening (solid-solid interaction) is one of the aspects we suppress in the present simulations by appropriate choice of kinetic coefficient τ (for solid-solid and solid-liquid interaction). We allow only the solid-liquid interaction. There is also an additional optimisation technique we have used in the present phase-field simulations to suppress grain coarsening known as the shifting-box algorithm. We shift the domain in the vertically downward direction, every time the clearance between crack surface and veins falls below 10%. Thus, we are able to cut off the evolved veins from the numerical domain, which could have otherwise started to coarsen. Further, for quartz sealing in veins, it is reasonable to assume that there is huge magnitude of difference in the time scale of sealing (which occurs w.r.t liquid) and grain coarsening (which is a solid-solid interaction). We offer to append these clarifications in addition to the explanation given in lines 8-18 on page 638 in the present manuscript, if required.

A constant driving force is assumed for evolving crystals. The hindrances to the vein sealing process together with the modelling aspects results in a significant deviation from the normal coarsening laws. The present article is about decomposing the effect of one such hindrance, i.e. crack-opening rate in 3-D. The present work focusses on an accurate determination of tracking characteristics when the rate of crack opening increment is varied but the surface profile and trajectory (circular arc) is kept consistent. Further, the facing wall rock pinning along the grain boundaries and grain triple/quadruple point is studied in detail with supporting statistics. We request the referee to supply the reference where the barrier pinning on grain triple/quadruple point during vein evolution has been numerically studied before.

The expression “standard microstructure evolution” is again, quite vague. Kindly cite the concerned references (if any to clarify), which explain the difference between standard and non-standard microstructure evolution. In our opinion, there is no such thing which can be described as a standard microstructure evolution. If the referee wanted to mention “normal grain growth”, an explanation citing the points of differences is already provided in previous paragraph.

As far as we are aware of, the multiphase-field model from Nestler et al, Phys. Rev. E. 2005 which is also used in the present work, has been used only once by us (in the context of vein growth) for simulating 2-D evolution of veins during crack-sealing

process. A 3-D study is still missing and we aim to bridge this gap using the current study. The intention of the present work is also to show the model capabilities applied to simulation of vein growth in 3-D and the importance of post-processing techniques.

The kinetics of coarsening should depend on the thermodynamic parameters, but in the paper there are no real thermodynamic parameters.

As already stated in 3rd paragraph of the reply to previous comment, the study of grain coarsening kinetics is not the focus of current work. In fact, every effort has been made to suppress the grain coarsening i.e. by choosing an appropriate kinetic coefficient and using shift-box algorithm.

Kindly refer to the model description Nestler et al. Phys. Rev. E 71, 041609, 2005 to appreciate the thermodynamic consistency of the present phase-field model.

Section 2.1, in the present manuscript lists the model equations briefly. A detailed description of the involved model parameters (both thermodynamic or kinetic) are given in K. Ankit et al, Contrib. Mineral. Petrol. (2013) 166:1709–1723 and need not be repeated in the present write-up. The same is mentioned in section 2 of the present manuscript.

Furthermore, the coarsening should depend on the kinetics of the crack propagation, but there are no representative results in the paper. Moreover, the coarsening in the paper does not depend on the crack propagation kinetics after any time for both cases A and B.

Kindly, consider our replies to the previous two comments.

In view of above comments, the aspect of crack-sealing process that is numerically simulated needs to be clearly understood. In the present numerical study (just like the previous studies of Urai et all, 1991; Hilgers et al 2001; Nollet et al 2005), the focus is to comprehend the kinematics of sealing by assuming a pre-determined crack opening incremental rate and trajectory.

Modelling the kinetics of crack propagation may be an interesting direction, but in all certainties, not the focus of current work.

The results in the manuscript show that the tracking efficiency does not depend on the crystal orientations, too. It can be caused by the wrong parameters.

This happens because the crystals grow isotropically when the surface roughness is high and crack-opening rate is small. It is to noted that in such a case, crystals grow isotropically even if anisotropy in the interfacial energy is considered. This result was published in a proceeding (in Deutsch) where no change in the grain boundary morphology was reported by switching off the anisotropy in interfacial energy. We attach a copy of this proceeding as a supplement. In support of our argument, we

request the referee to refer to figures 6 and 7 of the attached proceeding. English translation of the corresponding figure caption:

Figure 6: Simulation of a polycrystalline crack sealing in a geological setup with isotropic grain boundary energies with a random initial configuration in a) and b). Three time-steps are presented during a repeated stepwise crack event.

Figure 7: Simulation of a polycrystalline crack sealing in a geological setup with facetted grain boundary energies with a random initial configuration in a) and b). Three time-steps are presented during a repeated stepwise crack event.

If required, it will also be possible for us to translate a portion of the attached supplementary file into English.

On the contrary, in the free growth regime i.e. absence of any barrier, the effect of anisotropy in interfacial energy is clearly seen as the evolving crystals develop well defined facets and sharp corners. Additionally, the growth competition based on mis-orientation w.r.t most-preferred-orientation also takes place for the case of freely evolving polycrystals (see Fig. 2 in Ankit et al, Contrib. Mineral. Petrol, 2013).

The main reason attributed to such a growth regime is the hindrance of the facing wall rock (barrier) which inhibits the free growth of veins and forces them to track the opening trajectory. The peaks on the crack surface arrest the grain boundaries and there are ample 2-D numerical results available in literature, which accentuate these findings. In the present study, for the first time ever, the pinning mechanism of the facing barrier (in 3-D) on the grain triple/quadruple points (shown in fig. 8 of the manuscript).

These findings date back to the time of Urai et al 1991 who used an isotropic crystal growth rate and Hilgers et al, 2001; Nollet et al, 2005, both of whom used the anisotropic crystal growth rate using the front-tracking method and demonstrated the above behaviour. This was also reproduced by Ankit et al, 2013 who used the phase-field method to simulate crack-sealing in veins.

In absence of any crack surface which could inhibit the free growth of crystals, a growth competition based on mis-orientation sets in. In such a scenario, the most preferred orientations outgrows the mis-oriented neighbours as shown by K. Ankit, Contrib. Mineral. Petrol., 2013 in 2-D as well as 3-D studies.

It is worth clarifying that the present work does not aim to represent the vein growth process, in totality. As it is clear from the above reply as well the manuscript in question, we make several assumptions and within the limit of these assumptions, we investigate the physics of crack-sealing process in veins. A close resemblance of the present numerical work with the field studies reported earlier (read the Discussion of results in Ankit et al, Contrib. Mineral. Petrol., 2013) suggest that the model assumptions are reasonable and the chosen parameter set is correct.

There are not enough data for the validation of the anisotropic model.

The faceted type anisotropic function using in the model, that was used to simulated quartz crystals is well explained in Nestler et al, Phys. Rev. E **71**, 041609 (2005). As mentioned in the lines 4-16, page 636 of the submitted manuscript, the equilibrium shape that is simulated represents an idealised quartz where only three important facets are considered, while the other fast growing facets are ignored (assumption). A similar approach was also used for the case of alum crystals simulated in Fig. 1 of Ankit et al, Contrib. Mineral. Petrol. (2013) 166:1709–1723.

Wendler et al. Journal of Crystal Growth 327 (2011) 189–201 compared the role of anisotropy in interfacial energy as well as the kinetic anisotropy in polycrystalline growth. However, in the present study, we do not account for the kinetic anisotropy (but only the anisotropy in interfacial energy).

The faceted anisotropic model used in the present work is able to reproduce the growth competition based on mis-orientation (with respect to the most preferred orientation) observed in polycrystalline growth, This also serves as a sufficient model test case. Kindly refer to Figs. 2 and 3 of Ankit et al, Contrib. Mineral. Petrol. (2013) 166:1709–1723.