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COMPREHENDING THE MECHANISM OF VEIN FORMATION - INSIGHTS FROM THREE-DIMENSIONAL PHASE-FIELD MODELING AND INNOVATIVE POST-PROCESSING TECHNIQUES

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Vein formation in earth's crust involves a complex interplay of material transport and local precipitation during ongoing deformation. The geological experts try to correlate the different indicators which may vary across length scales, to reconstruct the past events, in order to gain an understanding of vein formation. However, it is difficult to decompose the effect of different processes that might have acted in sequence or simultaneously in such studies. The approximate reconstruction, which determines the final vein morphology could often be misleading and may result in erroneous interpretation of evolution mechanism. On the contrary, numerical methods applied to the study of vein microstructure formation improves the general understanding, as it is possible to decompose the effect of various boundary conditions. Further, computations provide an in-situ look into the temporal evolution of grains. In spite of numerous attempts in the past to simulate the dynamics of vein growth process, numerical studies are limited to two dimensions. It is to be noted 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.

In the present work, we extend the previous numerical studies [1] and primarily focus on the three-dimensional phase-field study of crystal growth in veins under crack-sealing conditions. Fig. 1 illustrates the successive steps of the simulation work-flow, starting from an initial wall crack surface/voronoi structure up to the various microstructural characterization methods. By the aid of innovative post-processing and advanced visualization techniques, the major advantages of accounting for the third dimensionality are highlighted. The grain growth statistics obtained from simulation studies provide valu-

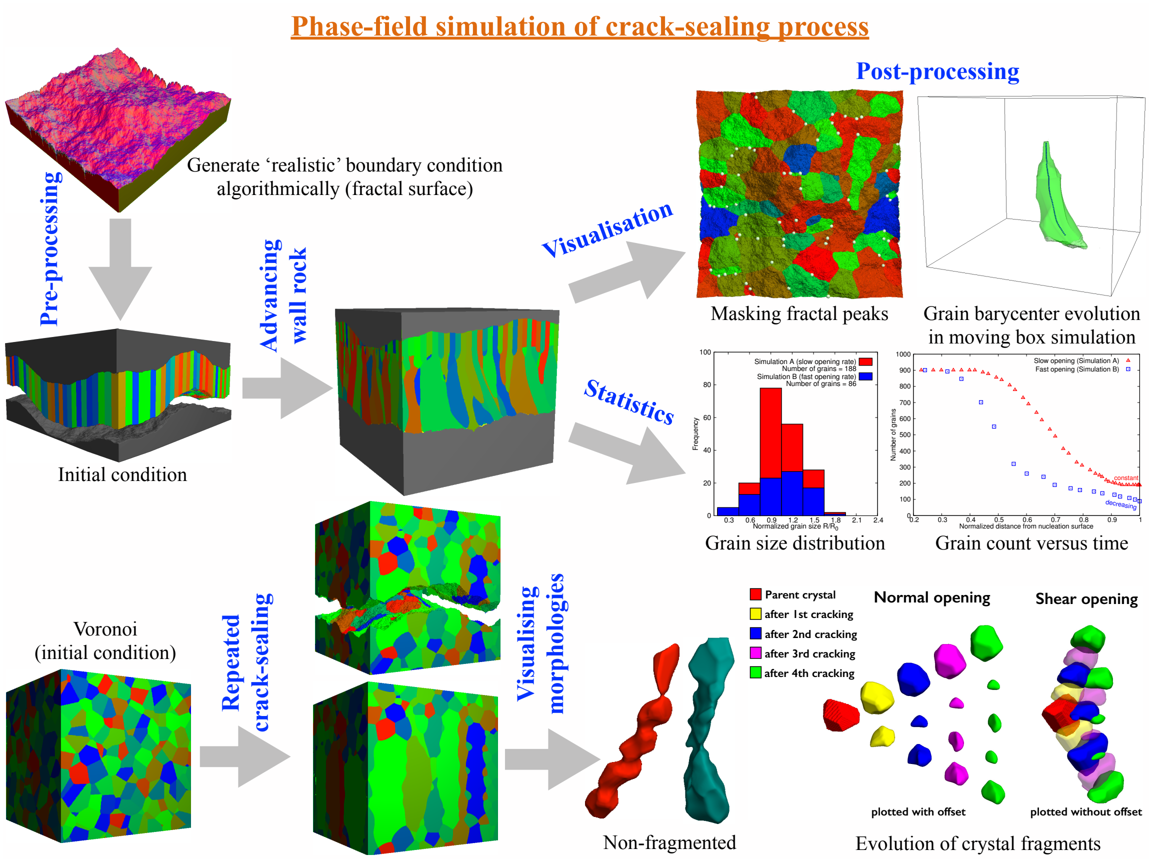

Figure 1: A general work-flow adopted for three-dimensional phase-field simulation of the crack-sealing process in geological veins under different boundary conditions.

able insights into the evolution characteristics; no such information is usually accessible in field studies and is essentially difficult to obtain from laboratory experiments as well. We also propose a general framework based on multiphase-field modeling [2], which allows an efficient use of modern high super-computing power, so that even the consideration of large grain systems (up to 500,000 grains) in 3-D computational studies becomes feasible.

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