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Representative Volume Element Size of a Polycrystalline Aggregate with Embedded Short Crack

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ABSTRACT

A random polycrystalline aggregate model is proposed for evaluation of a representative volume element size (RVE) of a 316L stainless steel with embedded surface crack. RVE size is important since it defines the size of specimen where the influence of local microstructural features averages out, resulting in the same macroscopic response for geometrically similar specimen. On the other hand macroscopic responses of specimen with size smaller than RVE will, due to the microstructural features, differ significantly. Different sizes and orientations of grains, inclusions, voids,... etc are examples of such microstructural features. If a specimen size is above RVE size, classical continuum mechanics can be applied. On the other hand, advanced material models should be used for specimen with size below RVE. This paper proposes one such model, where random size, shape and orientation of grains are explicitly modeled. Crystal plasticity constitutive model is used to account for slip in the grains. RVE size is estimated by calculating the crack tip opening displacements of aggregates with different grain numbers. Progressively larger number of grains are included in the aggregates until the crack tip displacements for two consecutive aggregates of increasing size differ less than 1 %. At this point the model has reached RVE size.

1 INTRODUCTION

Classical continuum mechanics idealizes nonhomogenous microstructure of material. Microstructural features such as crystallographic orientation of grains, their sizes and shapes, phases and voids are basically not taken into account. Material properties are obtained in tests from macro specimen where the effects of the above influences are averaged out and therefore the obtained material properties are actually average values. In 1960s a concept of representative volume element element (RVE) was introduced as microstructural sub/region that is representative of the entire microstructure in an average sense. A specimen larger than RVE is then treated as having material properties equal to average material properties of RVE. However, if a specimen is smaller than RVE, its material properties must be taken as those of its constituents (grains, phases,...) which are variable from point to point.

Microstructurally short cracks have a length of up to several grain sizes. These cracks are significantly influenced by the surrounding microstructural features. Crystallographic orientation of grains and grain boundaries are of particular importance for short cracks as they can, depending upon their orientation, increase, decrease or even arrest the crack growth. Other microstructural features also play a role. From the perspective of a short crack the material surrounding the crack therefore is not homogeneous. The question that this work is dealing with is how large a polycrystalline aggregate has to be so that adding additional grains to the structure does not change the short crack parameters. Once these additional grains do not change the parameters of the crack tip we will say that the RVE has been obtained. The surrounding structure can then be modelled using homogeneous material properties.

2 MODEL DESCRIPTION

To estimate the influence of the size of the polycrystalline aggregate on the crack tip parameters we built several finite element models of aggregates. Number of grains in these aggregates ranged from 5027 down to 145.

The initial structural model includes a planar rectangular aggregate with 5027 grains and a surface crack at an angle of 45 °, Fig. 1. Finite elements are omitted from the figure so that they do not clutter it. Grains are randomly sized and shaped. The grain structure is a planar Voronoi tessellation generated using code VorTESS [1]. Each grain is subdivided into 8-noded, reduced-integration, plane strain finite elements. A study of the effect of mesh density on the crack tip opening (CTOD), Fig. 2, was performed to obtain appropriate mesh. The finite element meshing of the grains away from the crack tip is automatic and follows procedures outlined in [2]. Advanced constitutive model that includes crystal plasticity is used to describe the deformation mechanism at this scale.

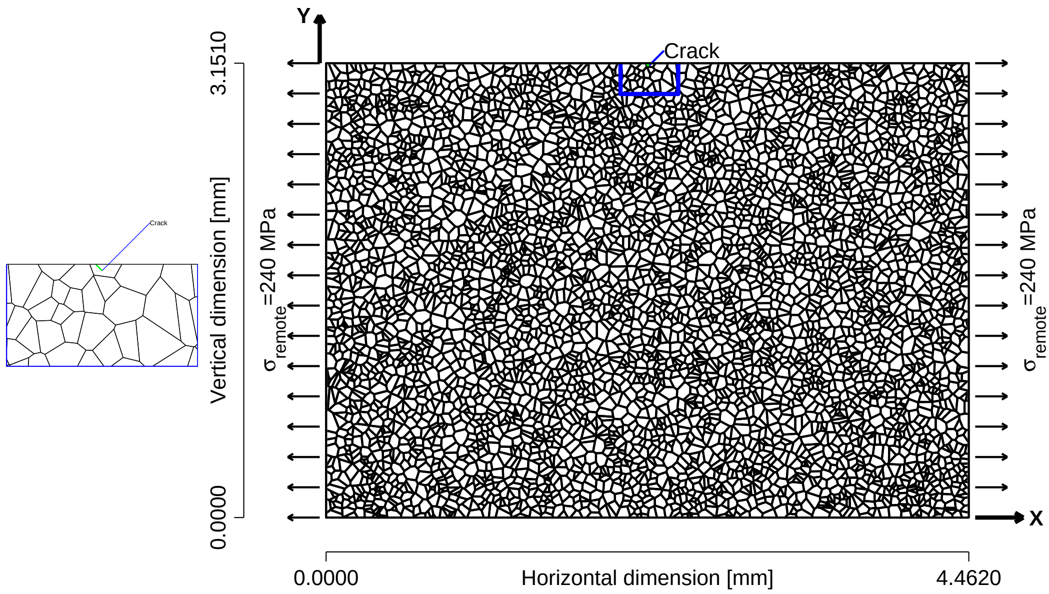

Figure 1: The outline of the finite element model. Grain with the crack is shown in the insert.

To obtain structural models with smaller number of grains rectangular sections have been cut out of the geometry of the initial structural model. The positions of the cut out sections are

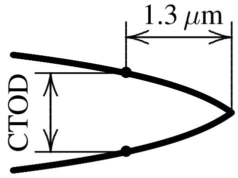

Figure 2: Definition of the CTOD.

presented in the first part of Fig. 3. The following figures represent the obtained structures with smaller number of grains. Table 1 presents their sizes.

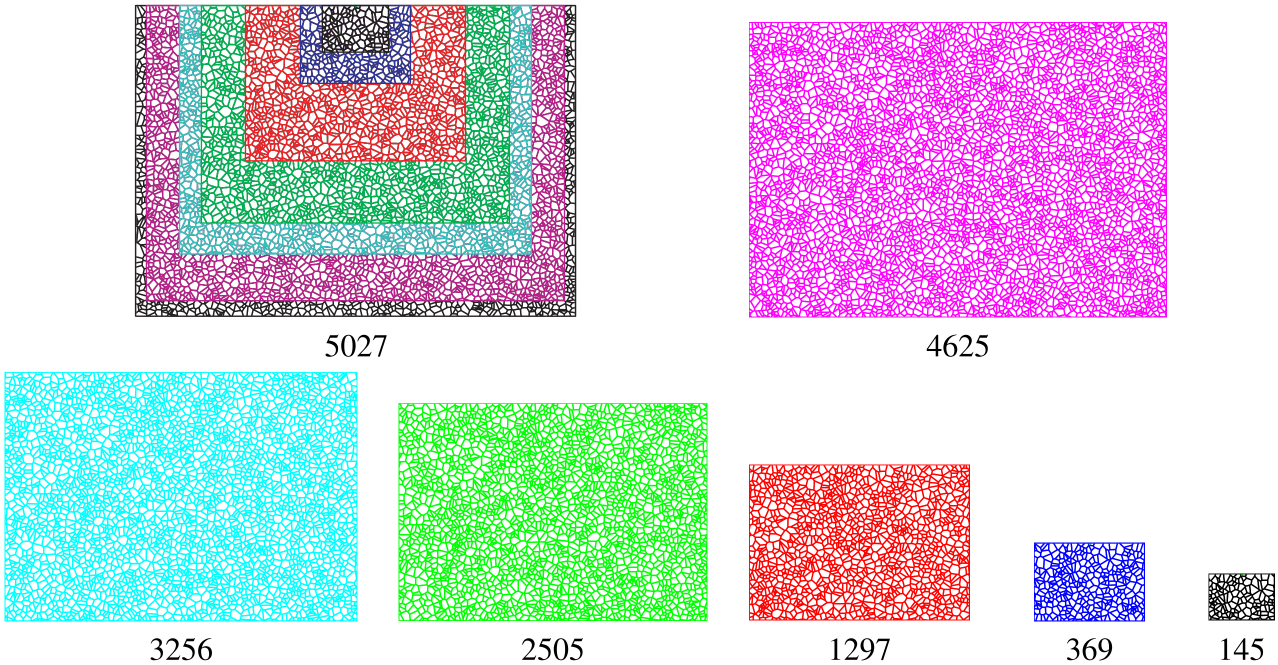

Figure 3: Polycrystalline aggregates accounting for 5027, 4625, 3256, 2505, 1297, 369 and 145 grains. Areas corresponding to smaller models are indicated on the largest aggregate.

2.1 Crystallographic orientations

Appropriate crystallographic orientations are defined by: a) setting the angle between the crystallographic [100] direction and the macroscopic X axis of all crystals in the model to 135° as shown in Fig. 4 and b) random rotation of the initial position about the global Z-axis. This results in a planar slip system model compatible with the planar macroscopic model. Within the grain the initial crystallographic orientations are identical. The resulting projections of the primary and conjugate slip planes are illustrated in Fig. 5.

For each of the aggregate sizes 100 models with different random sets of crystallographic orientations were created. One set of crystallographic orientation defines grain orientations for all the grains in the model. Although grain orientation varies from grain to grain for a given crystallographic orientation set, a specific grain has the same orientation for all the aggregate sizes. This is done to asses the size effect only. The only exception is the crystallographic orientation of the crack-containing grains which is always set to α=9.735° so that the crack falls into the slip plane as described in section 2.3.

Table 1: Size of different polycrystalline aggregates.

Number of grains	Size [mm×mm]	Scale of the largest aggregate
145	0.6692×0.4726	1/6.66
369	1.1146×0.7878	1/4.00
1297	2.2310×1.5755	1/2.00
2505	3.1234×2.2057	1/1.43
3256	3.5696×2.5208	1/1.25
4625	4.2388×2.9934	1/1.05
5027	4.4620×3.1510	1/1.00

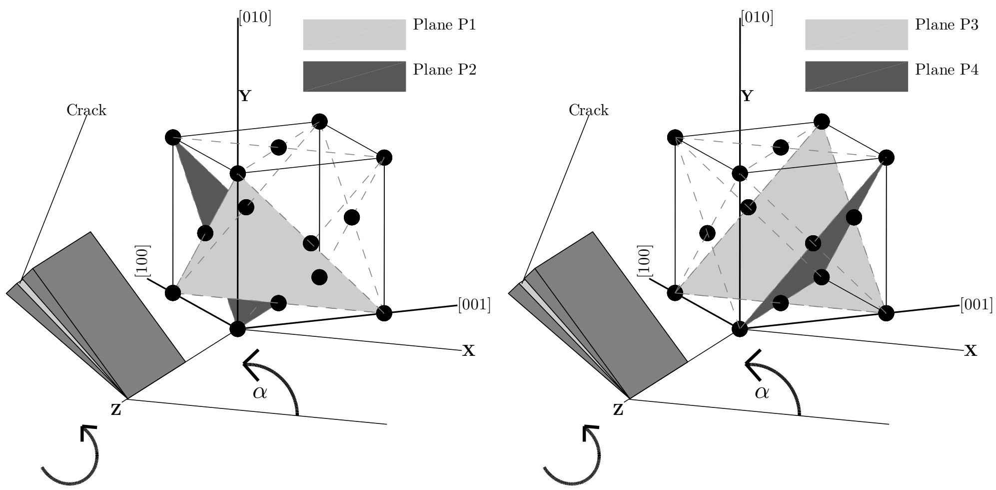

Figure 4: Relation between the slip systems of a face centered cubic material and the crack for $\alpha = 0°$.

2.2 Loading and boundary conditions

The applied macroscopic loading and boundary conditions are illustrated in Fig. 1 and are the same for all aggregate sizes depicted in Fig. 3. The left and right edges are loaded in macroscopic monotonic uniaxial tension up to a maximum load of $0.96R_{p0.2}$ (240 MPa) with zero shear traction. This load is sufficient to trigger slip systems activity in all cases analyzed. The macroscopic yielding is achieved in all the analyzed cases.

No other loads and boundary conditions are specified apart from preventing rigid body movement and the plain strain constraint. All four sides of the rectangular block are therefore modeled as free surfaces. This boundary condition results in a lower bound limit for effective material properties and reduces the constraint influences of the surrounding structure when the model is embedded into it.

2.3 The crack

A short inclined surface crack is introduced in the model with macroscopic crack orientation fixed to 45 ° relative to the global X axis. The CTOD values are calculated at a distance of 2.5 % of the average grain size behind the crack tip (i.e. 0.025·52.9=1.3 μm), see Fig. 2. This is consistent with examples found in the literature.

The crystallographic orientation of the crack-containing grain is set by rotating the initial position about the global Z-axis by α=9.735 ° which places the crack into the P2 slip plane, cf.

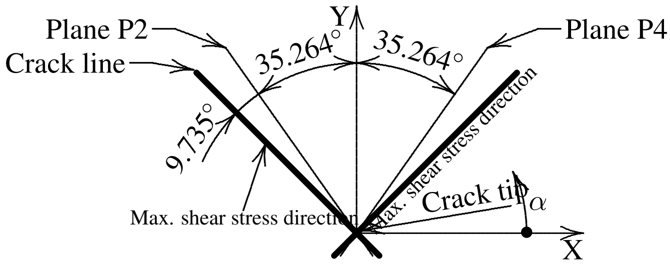

Figure 5: Orientations of slip planes, shear directions and the crack plane for crystallographic orientation of $\alpha = 0°$.

Fig. 4 and 5. This is due to our intention to model Stage I fatigue cracks that propagate through the slip planes. A model of growing crack is, however, avoided at this point in time and may be included in the model in the future. The length of a stationary crack is set to $0.5D_{4854}$, where $D_{38} = 37.446\,\mu$m is the size of the cracked grain, estimated as a square root of the grain's area. All results in this paper are therefore obtained assuming stationary crack and monotonic loading regime.

2.4 Constitutive model

Each grain is assumed to behave as a randomly oriented monocrystal governed by the anisotropic elasticity and crystal plasticity models. The elastic deformation at the monocrystal level is generally anisotropic and is governed by the generalized Hooke's law, $\sigma^e_{ij} = C_{ijkl}\epsilon^e_{kl}$, where σ^e_{ij} represents the second-rank stress tensor, C_{ijkl} the fourth-rank stiffness tensor and ϵ^e_{kl} the second-rank elastic strain tensor. The plastic deformation in monocrystals is assumed to take place via a simple shear on a specific set of slip planes. Deformation by other mechanisms such as for example diffusion, twinning and grain boundary sliding is currently not taken into the account. Details on the applied crystal plasticity constitutive model are given in [3]. This model was implemented as a user-subroutine into the finite element code ABAQUS. Further details on its theory and implementation can be found in [4, 5].

Application of the macroscopic tension in the X-direction results in macroscopic maximum shear stress planes at ±45 ° to the X-axis. Coincidence of macroscopic shear planes and microscopic primary and conjugate slip planes is achieved when the crystals are rotated around the Z axis for: α =9.735 °, 80.265 °, 99.735 ° or 170.265 °.

2.4.1 Material parameters

In this work we deal with 316L stainless steel that is for example used in certain nuclear power plants piping systems. The following elastic constants for AISI 316L single crystal are used: C_{iiii}= 163680 MPa, C_{iijj}= 110160 MPa, C_{ijij}= 100960 MPa [6]. Crystal plasticity parameters have been optimized from the macroscopic plastic response of AISI 316L polycrystal [6]: h_0= 330 MPa, τ_s= 270 MPa, τ_0= 90 MPa, n= 55, q=1.0 and $\dot{a}^{(\alpha)}$=0.001. With these parameters the proposed plain strain model is deemed sufficient to provide a correct qualitative representation of the macroscopic response, [6].

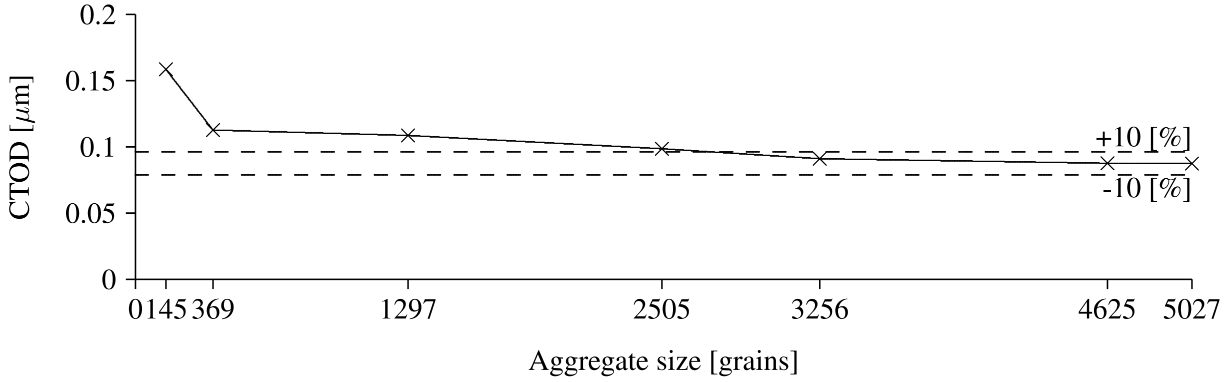

Figure 6: The dependance of CTOD on the size of the aggregate for crystallographic set number 35.

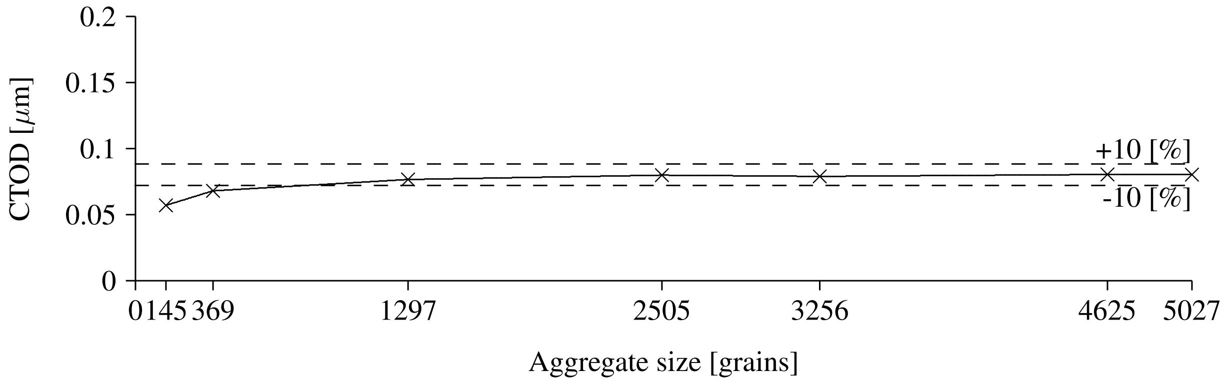

Figure 7: The dependance of CTOD on the size of the aggregate for crystallographic set number 15.

3 RESULTS

For a given set of crystallographic orientation adding additional grains to the aggregate with 145 grains inevitably changes the crack tip opening displacements. Figure 6 presents one such case for the crystallographic set number 35. We can see that the CTOD steadily decreases with the increased number of grains. This suggests that for this orientation set the increased number of grains stabilizes the crack which agrees with the theory.

However, there are cases where by adding the grains to a small aggregate actually increases the CTOD, Fig. 7. In these cases and for the smaller number of grains a strong shear band can form away from the crack tip, cf. Fig 8. In this shear band most of the deformation energy is concentrated, resulting in smaller deformation around the crack tip. As we add up additional grains, deformation structure stabilizes and deformation energy shifts away from this large shear band, decreasing its importance and increasing the deformation around the crack tip.

For determining RVE, we calculated relative difference in CTOD as we increased the number of grains in the aggregated for a given crystallographic set. We then averaged these relative differences for each number of grains. The results are depicted in Fig. 9. We can see that: a) the CTODs are decreasing with increased number of grains and b) relative differences also decrease. Between 3256 and 4625 grains the relative difference in CTODs falls below 1 %. By applying 2nd order polynomial approximation we estimated that difference of 1 % is obtained at 3739 grains. RVE size is therefore estimated to be 3739 grains. We also calculated the CTOD

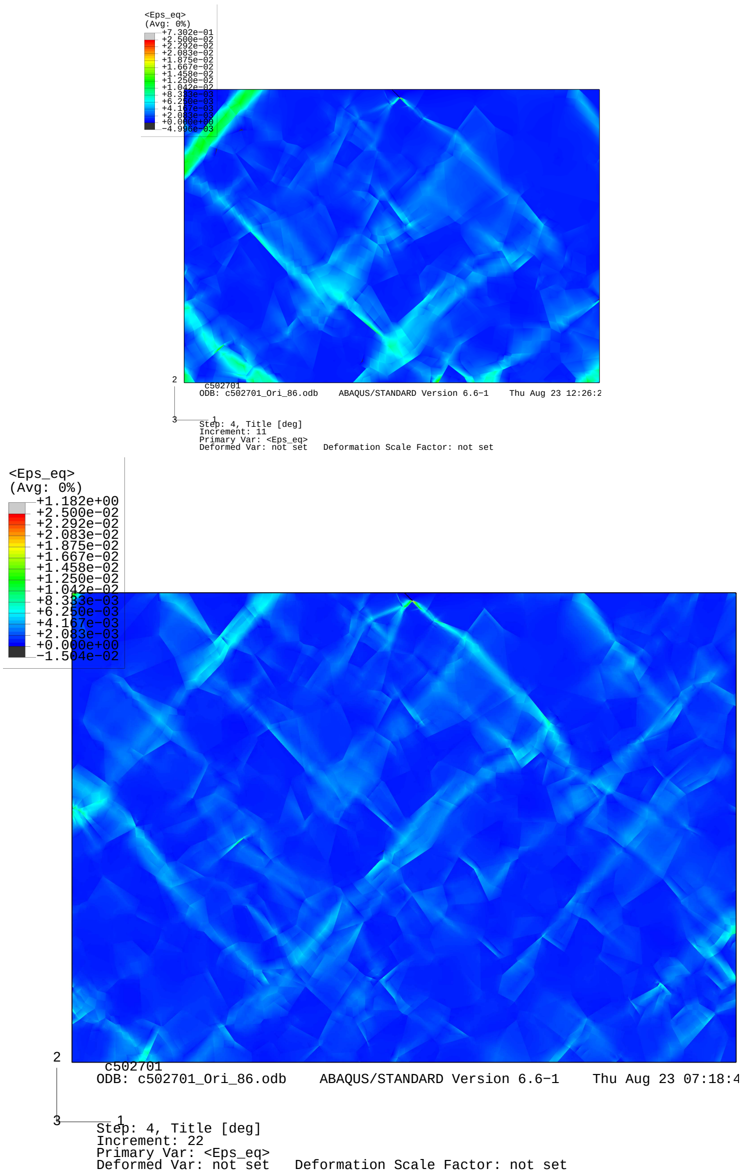

Figure 8: Equivalent strain for polycrystalline aggregates with 145 (above) and 369 (below) grains.

values for isotropic elastic material model, using the same model sizes as in depicted in Fig. 9. The difference in CTOD values are below 1 %.

It has been observed in the previous work [7] that two basic properties could dominate the CTOD response: a) orientation of grains immediately around the crack-containing grain and b) a global cluster of soft grains that results in crack tip becoming a part of the localized strain bands resulting in a large CTOD value. The individual contributions of these two mechanisms might result in two different RVEs. This is to be further investigated in the future work.

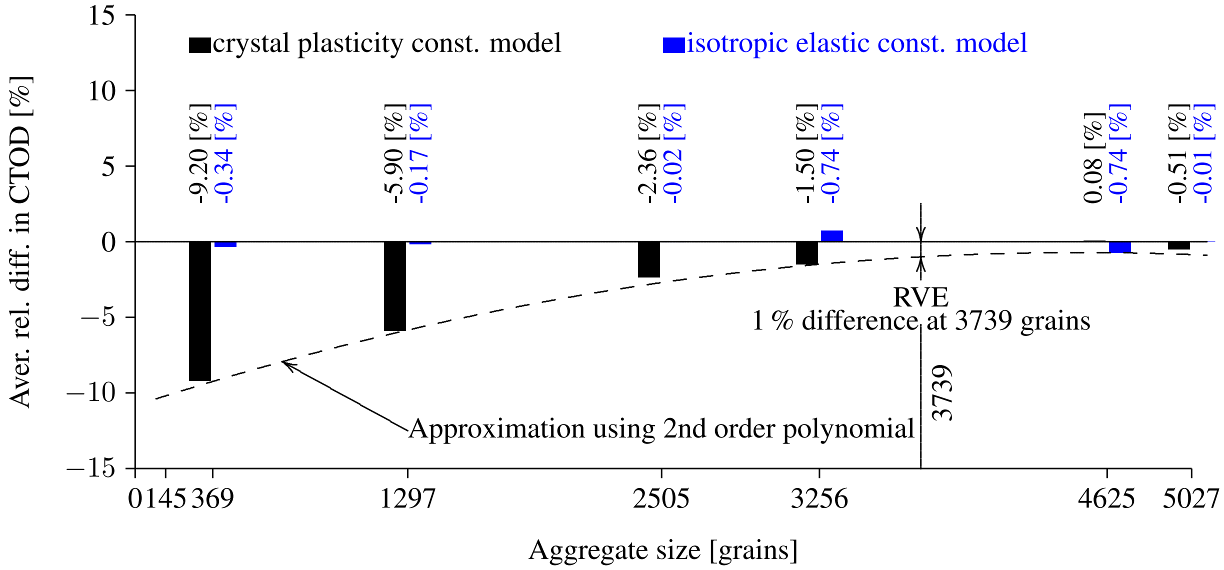

Figure 9: Average dependance of CTOD on the size of the aggregate.

4 CONCLUSIONS

This paper proposes a crystal plasticity model for determining the RVE of a polycrystalline aggregate with embedded short crack. Using a number of aggregates with different number of grains we have determined that on average the crack tip opening displacements (CTODs) decrease with increased number of grains. This decrease becomes smaller and smaller as the number of grains is increased. With aggregate consisting of 3739 grains, the CTODs change by only 1 % compared to the smaller number of grains and RVE size has been reached. In practical terms and for steel 316L this means that homogenous material properties can only be assumed for models (specimen) larger than 4x3 mm. For smaller models, advance material models that account for material's microstructure have to be employed. Future work will concentrate on clarifying the possible effect of two basic properties on the RVE: a) orientation of grains immediately around the crack-containing grain and b) global orientation of grains that can result in crack tip becoming a part of the localized strain bands.

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