Science of Sintering, **51** (2019) 459-467

doi:https://doi.org/10.2298/SOS1904459H

UDK: 675.92.027; 539.4; 539.217

Numerical Modeling of the Porosity Influence on Strength of Structural Materials

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Abstract:

The effect of micro-scale structural low-level porosity on strength of structural materials was studied using the three-dimensional Unit Cell Numerical Model - UCNM. A comparison between proposed UCNM and available experimental data in literature was done by comparing obtained values for stress concentration factor – SCF for different sizes and shapes of pore. Results for normalized strength obtained by proposed UCNM model are in agreement with available experimental data published in literature. It was confirmed that material porosity in form of closed pores, regarding pores' size (volume fraction) and shape, has note cable influence on strength of structural material. Less porosity in the material microstructure generally leads to higher values of material strength. For fixed porosity volume fraction, shape of pores has an impact on strength of structural material.

Keywords*: Numerical modeling; Strength; Porosity; Structural materials.*

1. Introduction

The development and application of porous structural materials are motivated by the continuous demand in different fields of possible applications. For instance, in a field of structural engineering there is a demand for lightweight constructions with enhanced mechanical properties. On the other hand, in the field of medicine, porous biocomposites are used as bone replacement in implant surgery. Therefore, different porous materials such as ceramics and bioceramics, porous shape memory alloys, foam-like structures, and thermal spray deposits have been used in a wide range of applications in various engineering structures. Anyhow, presence of porosity usually degrades mechanical properties of structural material [1]. The fact that porosity reduces mechanical properties is important when material is used as structural member carryingload. In this case porosity is considered a flaw which generally causes a decrease in the mechanical properties of structural material such as strength and stiffness. As defined in metallographic studies, pores can be mainly classified as: closed round pores, long and broad pores, long and fissured pores, and small, fissured pores [2].

When the presence of porosity is evident, mechanical properties of structural materials are strongly influenced by microstructure of pores size and shape. This impact was in focus of number of the prior studies which confirmed the fact that less porosity in the material microstructure leads to higher material stiffness and strength, while an irregular shape of pores strongly influences the material fracture toughness and strength [3-7]. It should

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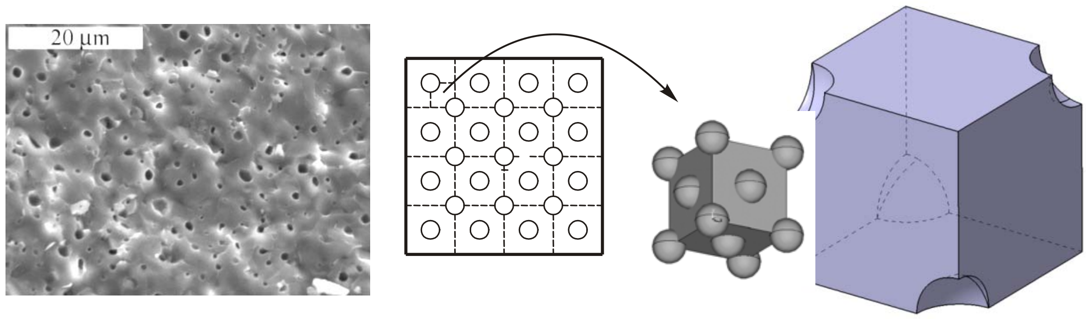
be emphasized that sometimes presence of porosity is quite necessary and desirable. In implant surgery porous materials have been shown to effectively provide stable long-term anchorage for biological fixation of the implant due to bone tissue ingrowth through the pores [8]. Nielsen [9] developed a number of empirically-based relations between stiffness (modulus of elasticity) and strength (modulus of rupture) of materials in order to control quality without damaging or destroying the material or the building component considered. Some theoretical methods have been developed to correlate porosity size and shape with material stiffness and strength. A detailed summary of these methods could be found in and Wang and Tseng [10].

Through past decades numerical modeling became a powerful tool for studying the influence of microstructure on mechanical properties for different types of materials. Three dimensional Unit Cell Approach is widely used for simulating real microstructure of different types of materials. In the Unit Cell Approach, real microstructure having random distribution of pores shape and size is idealized by periodically distributed pores of the same shape and size which are represented by a periodic repeating cell which is usually simple cube. The Unit Cell Approach requires relatively little computational efforts in comparison to simulations of real structures. For instance, in some prior studies the Unit Cell Approach was used to investigate the effect of the mutual arrangement of phases in different composite materials [11, 12] and to study effect of structural porosity on the mechanical and elastic properties of sintered materials [13, 14].

In this study, the focus is on low-level porosity in form of closed round pores and their influence on strength of structural materials by using proposed UCNM. A face-centered-cubic (FCC) finite element (FE) unit cell model which was previously designed to evaluate the compressive stiffness and strength of biocomposite material for a range of porosity volume fractions [11] is used here for simulating spherical geometry of pores. An extension of FCC model is developed to simulate non-spherical geometry of pores.



(a) (b) (c)

Fig. 1. The idealization of the random pore distribution, shape, and size by arranging the pores of same size and same shape (sphere) on a FCC packing array.

2. Materials and Experimental Procedures

A typical example of microstructure of porous material is SEM micrograph of HAP sample sintered at 1250 ºC for 2h – Fig. 1(a) [14]. Sintering usually leads to a denser microstructure, with closed pores and parts of well-sintered grains. To fully simulate such a microstructure, a three-dimensional (3D) model of a random distribution of pores shape and size is required. The present study aims at carrying out an influence of closed pore's shape and size on strength of structural materials. In this study, distribution of pores is idealized by face-centered-cubic arrange of pores where there is one spherical pore at each corner and one spherical pore centered in each face of the cube cell as shown on Fig.1(b). With assumption of isotropic material properties, for analysis in this study, one-eighth of the original unit cell is used – Fig. 1(c). The irregular shape of porosity appearing in real microstructure is idealized as ellipsoid geometry shape (Fig. 2(d)) with chosen orientation, aligned with main coordinate ax *z*. The aspect ratio of pores - AR, defined as diameter to diameter ratio – $AR=D_1/D_2$, were chosen to be 1 (sphere), 2, and 3 respectively, while volume fraction of porosity (V_p) is chosen to be 3, 5 and 7 percent, respectively. A unit cell is loaded by compression in vertical direction (NL load case) or horizontal direction (PL load case). The symmetry of geometry and load potentially allows unit cell to be reduced to the one-eighth of original unit cell as shown in Fig. 2.

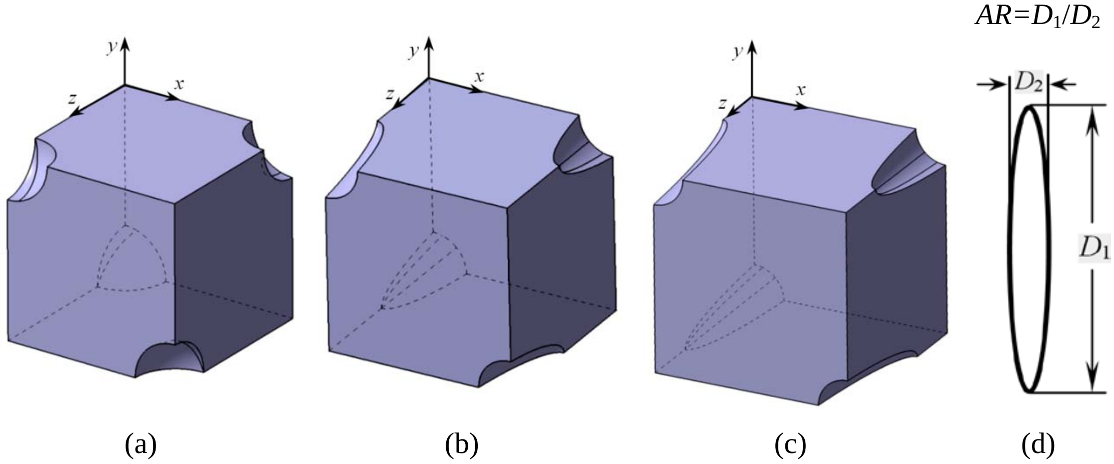


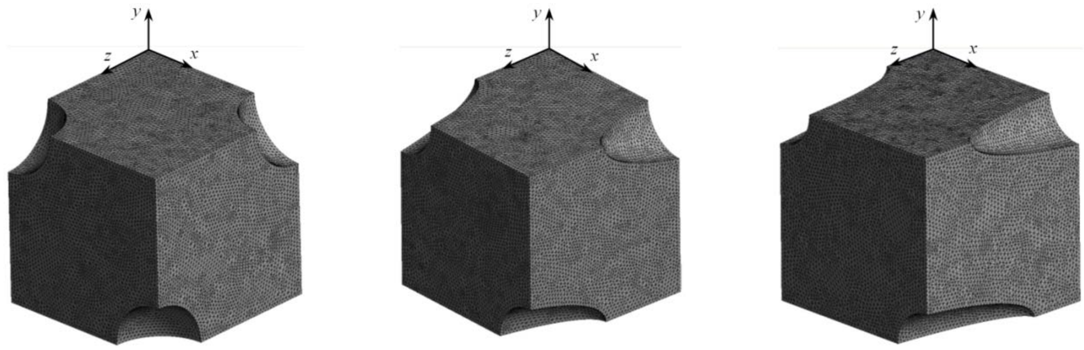
Fig. 2. UCNM with 3 % of porosity volume fraction (V_p): (a) AR=1, (b) AR=2, (c) AR=3 and (d) dimensions of ellipsoid (D_1, D_2 - principal axe diameters).

The assumptions for all models are: (a) the elastic properties of material are linear, (b) the material is isotropic, (c) in every model, all sphere and ellipsoid like pores are of the same size, (d) the material will not fail at the prescribed loads and (e) pores do not intersect each other.

Due to the symmetry of the unit cell and the applied loads, as well as adopted isotropic material properties, analysis was reduced to one-eighth of the unit cell for all models as shown in Fig. 2 (a,b,c). Dimensions of reduced unit cells presented in Fig. 2 are 10×10×10μm.

All 3D finite element (FE) models were produced using ANSYS 16.4, a general-purpose FE software package for structural analysis. The elements used in analysis are 10-node tetrahedral structural solid elements (an option of 20-node solid brick elements). Each node has three degrees of freedom corresponding to the three degrees of translation. Boundary conditions constrain the unit cell to remain in its original shape. After loading, the sides remain parallel and orthogonal, but changes in length. The load was introduced in form of displacement in vertical or in horizontal direction. In the vertical load case (NL) nodes positioned at upper surface of the cube (y=0μm) were displaced by Δ_y=-0,01 μm in vertical direction while nodes positioned at lower surface of the cube (y=-10μm) were constrained by displacement in y direction. In horizontal load case (PL) nodes positioned at side surface of the cube (z=10μm) were displaced by Δ_z=-0,01 μm in horizontal direction while nodes positioned at z=0μm were constrained by displacement in z direction. The local coordinate system aligns with the global one.

A representative FE grid for evaluation of compressive strength with porosity volume fraction V_p = 5 %, shown in Fig. 3(a), contains 116513 elements and 169724 nodes. The material data used for FE analyses, adopted based on literature data [11], with the following values: E= 16,04GPa, ν=0.124, where E is Young's modulus and ν is Poisson's ratio.



(a) (b) (c)

Fig. 3. Finite element grid of unit cell with 5 % of porosity volume fraction (V_p): (a) AR= 1, (b) AR= 2, (c) AR= 3.

After loading, maximum equivalent stress is divided by nominal stress (stress in non-porous material) to obtain stress concentration factor, SCF:

$$\mathrm{SCF} = \frac{\sigma_{max}}{\sigma_{nominal}} \quad (1)$$

Higher values of SCF can significantly lower the strength of structural material. Therefore, there is a need to investigate how porosity volume fraction and porosity shape influences SCF of structural material.

3. Results and Discussion

Results presented in this section are obtained numerically with assumptions for ideally elastic material adopted in the previous section.

Summary of obtained results (maximal and nominal stress and SCF) for different AR (1, 2, and 3) and different V_p (3, 5, and 7 %) for PL load case are presented at Table I. PL load case refers to load applied parallel to direction of pores.

Tab. I Summary of obtained results for SCF for different AR for PL load case.

AR = 1			
Porosity volume fraction V_p (%)	3	5	7
Maximal stress (MPa)	391,43	390,18	375,01
Nominal stress (MPa)	190,04	181,11	173,35
SCF	2,059	2,166	2,161
AR = 2			
Porosity volume fraction V_p(%)	3	5	7
Maximal stress (MPa)	308,17	363,59	403,39
Nominal stress (MPa)	195,16	188,35	181,48
SCF	1,579	1,93	2,223
AR = 3			
Porosity volume fraction V_p(%)	3	5	7
Maximal stress (MPa)	244,34	273,8	289,19
Nominal stress (MPa)	195,64	190,07	184,76
SCF	1,249	1,44	1,565

Comparisons of obtained values of SCF from equation (1) for different AR for load parallel to direction of pores – PL load case is presented in Fig. 4.

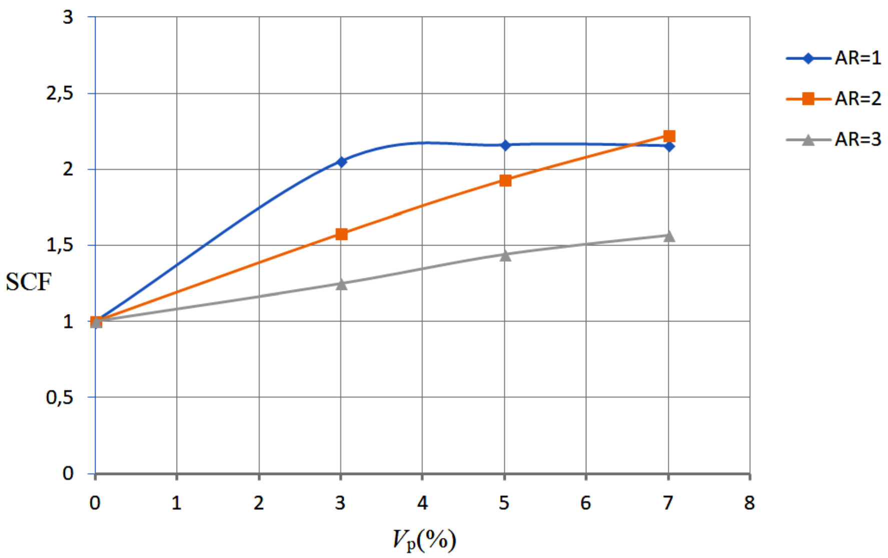


Fig. 4. Comparisons of obtained values of SCF for PL load case for different fixed aspect ratios and for different porosity volume fractions - V_p.

Summary of obtained results (maximal and nominal stress and SCF) for different AR (1, 2, and 3) and different V_p (3, 5 and 7 %) for NL load cases are presented in Table II. NL load case refers to load applied normal to direction of pores.

Tab. II Summary of obtained results for SCF for different AR for NL loads case.

AR = 1			
Porosity volume fraction V_p(%)	3	5	7
Maximal stress (MPa)	391,43	390,18	375,01
Nominal stress (MPa)	190,04	181,11	173,35
SCF	2,059	2,166	2,161
AR = 2			
Porosity volume fraction V_p(%)	3	5	7
Maximal stress (MPa)	342,17	403,65	449,68
Nominal stress (MPa)	195,16	188,35	181,48
SCF	1,753	2,143	2,478
AR = 3			
Porosity volume fraction V_p(%)	3	5	7
Maximal stress (MPa)	270,17	303,91	332,75
Nominal stress (MPa)	195,64	190,07	184,76
SCF	1,381	1,599	1,801

Comparisons of obtained values of SCF for different AR for load normal to the direction of pores – NL load case is presented in Fig. 5.

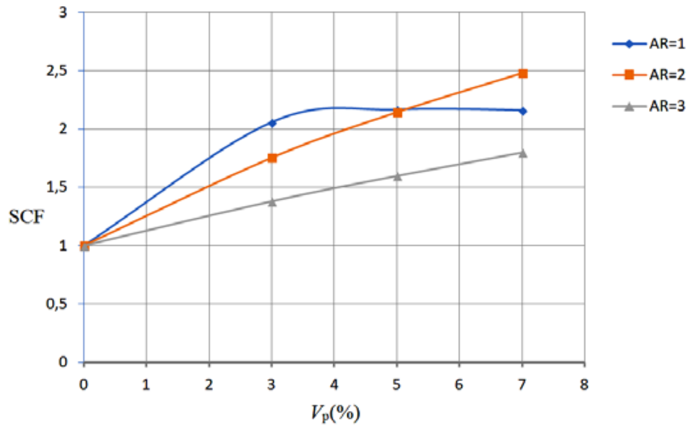


Fig. 5. Comparisons of obtained values of SCF for NL load case for different fixed aspect ratios and for different porosity volume fractions - V_p.

Additionally, obtained results for PL load case for AR= 2 and AR= 3 are compared to the experimental values available at literature [15], as presented in Fig. 6. For comparison purposes normalized experimental strength $S_{nor.}^{exp.}$ is calculated from:

$$S_{nor.}^{exp.} = \frac{S_{por.}}{S_{nom.}} \qquad (2)$$

where $S_{nom.}$ is measured strength of non-porous material sample and $S_{por.}$ is measured strength of porous material sample.

Numerically obtained results for SCF were used for calculating estimated normalized strength as:

$$S_{nor.}^{est.} = \frac{1}{\text{SCF}} \qquad (3)$$

As obvious from obtained results, for non-porous structural material SCF=1 and therefore, $S_{nor.}^{est.} = 1$. For porous structural material, porosity influences the strength by the fact that increasing V_p is increasing SCF which in turn is lowering the strength.

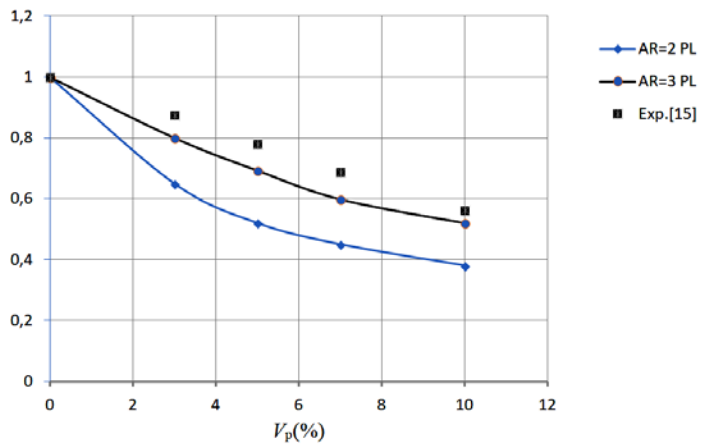


Fig. 6. Comparison of obtained results for estimated normalized strength - $S_{nor.}^{est.}$ with normalized experimental strength $S_{nor.}^{exp.}$ (data from [15]).

As obvious from Fig. 6 with the increase in porosity content strength decreases. For example, for PL load case and AR= 3, the presence of 5 % of porosity leads to estimated decrease of strength for approximately 30 %. For porosity of 7 % estimated decrease in strength is approximately 40 %. For this comparison additional numerical models having 10 % of porosity with AR= 2 and AR= 3 (for PL load case) were made. Experimentally obtained values [15] are similar to values obtained numerically for PL load case and AR= 3 within 10 % difference. For all other aspect ratios and load cases estimated decreases of strength were much lower than the values obtained experimentally. It should be emphasized that SCF is important but not the only one parameter contributing to strength decrease in structural materials. Type of load, post-yield behavior, hardening low, etc. are contributing to strength as well. Therefore these numerical models generally underestimate real values of strength in structural materials. Estimated values obtained by these models are always on the side of safety.

Fig. 7 presents the influence of pores shape (AR) to SCF for PL load case for different fixed porosity volume fractions - V_p. Figure 8 presents influence of pores shape (AR) to SCF for NL load case for different fixed porosity volume fractions - V_p. As it is evident from Figs. 7 and 8, shape of porosity has an impact on strength. With increasing aspect ratio (AR) of pore for fixed porosity of 3 and 5 % value of SCF is lowering. The same trend is observed for both load cases NL and PL. With increasing aspect ratio (AR) of pore for fixed porosity of 7 % value of SCF has a light higher value for AR= 2 while for AR= 3 value of SCF is lower than the value obtained for AR= 1. It can be concluded that this influence is moderate when comparing to influence of volume fraction which is clearly dominant.

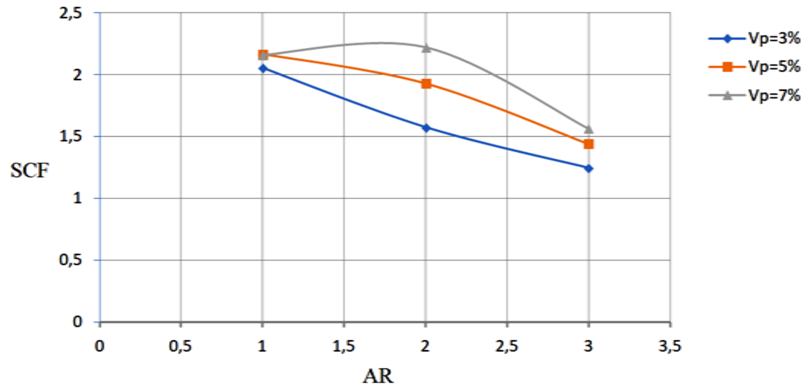


Fig. 7. Influence of pores shape (AR) to SCF for PL load case for different fixed porosity volume fractions - V_p.

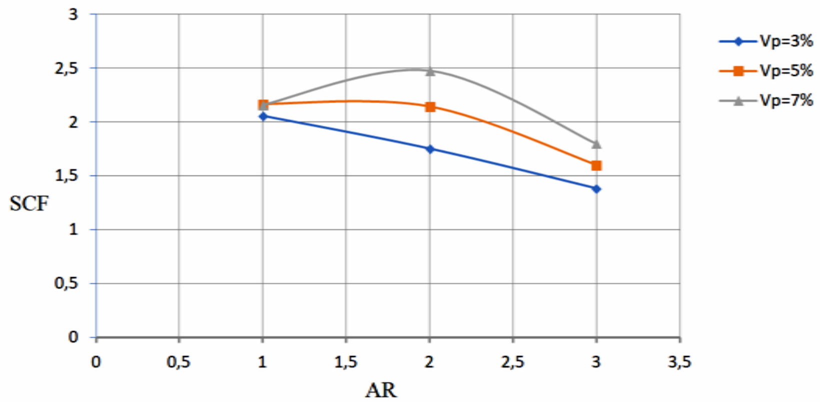


Fig. 8. Influence of pores shape (AR) to SCF for NL load case for different fixed porosity volume fractions - V_p.

4. Conclusion

A 3D unit cell FE model of low-level porosity in form of closed pores is developed and compared with available experimental results. The low-level porosity has significant influence on strength of structural material.

The shape of porosity has an impact on estimated strength of structural material. For fixed volume fraction, changing shape of pores by increasing aspect ratio (AR) in general slightly decreases values for SCF which contributes to higher strength.

The volume fraction of porosity has a significant impact on strength. Less porosity in the material microstructure generally leads to noticeable higher values of strength. It is shown that values of estimated strength predicted by UCNM model for PL load case and AR= 3 are in good agreement with previously published experimental data. For all other aspect ratios and load cases estimated decreases of strength were much lower than the values obtained experimentally.

Finally, the presented UCNM model is capable to simulate microstructure irregularity of closed pores shape and size regarding the influence of presence of such porosity to strength of structural material.

Acknowledgments

This investigation was supported by the Ministry for Education, Science and Technological Development, project III 45019 and TR 35006.

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Садржај: *Анализиран је утицај порозитета ниског нивоа на чврстоћу структуралних материјала применом тродименsионалног unit cell нумеричког модела - UCNM. Извршено је поређење резултата за фактор концентрације напона SCF добијених применом UCNM нумеричког модела за различите величине и облике порозитета са резултатима добијеним на основу података из раније публикованих радова добијених експерименталним путем. Добијени резултати за нормализовану чврстоћу за различите запреминске уделе порозитета су у сагласности са експерименталним подацима из литературе. Потврђено је да материјална порозност затвореног типа са својом величином (запреминским уделом) и обликом утиче на чврстоћу конструкцијских материјала. Мања порозност у микроструктури материјала доприноси значајном повећању вредности чврстоће. Са друге стране, сам облик порозитета такође има утицаја на чврстоћу за одређени запремински удео порозитета.*

Кључне речи: *Нумеричко моделирање, Чврстоћа, Порозитет, Конструкцијски материјали.*

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