Mechanical properties of zircon for varying degree of amorphization predicted by finite element simulations

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Abstract

The level-cut Gaussian random field approach based on standing waves is used to generate bi-phase microstructures of arbitrary phase fraction. Finite Element voxel models based on such microstructures are employed to predict the mechanical properties of zircon (ZrSiO4) for varying degree of amporphization from 0 to 100% with percolation transitions at 15.9 and 84.1%. Between the percolation transitions, the microstructure is bi-continuous. The numerical simulations provide values for the volumetric swelling, density, Young´s modulus, Poisson´s ratio, yield stress, and hardness as function of the amorphous phase fraction. For achieving a fit with nanoindentation hardness data in the literature, the micromechanical model additionally considers an interface between the amorphous and the crystalline phase that can be adjusted in thickness. Yield stress and hardness data are predicted for different values of interface thickness. The repository contains the simulation results as well as the literature data used for comparison.

1. Description of Data

1.1. Experimental data from literature

The experimental data provided in the data set “ExperimentalData-Zircon.dat” are collected from references [1-3]. The sample numbers in the first column correspond to the numbers given in Table 2 in [1], Table 1 in [2], and Table I in [3]. In the following rows, the density ρ and the measured mechanical properties are given together with the measurement error. The Young’s modulus, hardness and Poisson’s ratio are denoted with E, H, and ν.

1.2. Simulation data

The simulation data are provided in the data set “SimulationData-RVE64-HS146.dat”. These data are computed with the help of a micromechanical FE-voxel model and periodic boundary conditions, which is built with the level-cut Gaussian random field approach [4] for $H = \sqrt{146}$. The resolution of the Representative Volume Element (RVE) is $64 \times 64 \times 64$ voxels and, beyond the model published in [4], includes swelling of the amorphous phase as well as a hard interface between the amorphous (a) and the crystalline (c) phase. Furthermore, each phase can undergo isotropic elastic-plastic deformation with a small amount of linear work hardening. The material parameters for each phase are given in Table 2, where the variables E, ν, σ_y, E_T, H denote the Young’s modulus, Poisson’s ratio, yield stress, work hardening rate, and Hardness, respectively. The results provided in the dataset “SimulationData-RVE64-HS146.dat” are macroscopic values obtained by homogenization over the volume of the RVE. The variables in the heading of the data set “SimulationData-RVE64-HS146.dat” are defined according to Table 3.

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Table 1: Properties of zircon. Density values ρ are taken from [1], mechanical properties are taken from [2] (yellow) and [3] (green).

Sample	ρ [1]	E	E_{err}	H	H_{err}	ν	ν_{err}
#	[g/cm³]	[GPa]	[GPa]	[GPa]	[GPa]	[-]	[-]
4407	4.69	344.09	9.06	19.98	0.81	0.175	0.002
4606	4.65	294.86	11.05	19.05	0.73	0.180	0.002
4603	4.59	279.69	6.20	18.93	0.58	0.200	0.002
4303	4.58	266.21	12.06	18.75	1.03	0.195	0.002
4605	4.58	250.55	5.61	18.35	0.53	0.195	0.002
4607	4.59	273.64	6.90	18.68	0.53	0.200	0.002
4604	4.54	251.04	6.03	16.79	0.49	0.225	0.002
4302	4.40	217.53	5.06	14.26	0.49	0.265	0.002
4204	4.40	177.49	2.88	12.62	0.27	0.265	0.002
4501	4.35	177.02	5.66	12.13	0.58	0.270	0.002
4105	4.25	158.30	4.58	10.58	0.50	0.270	0.002
4104	4.24	157.38	5.37	10.48	0.53	0.270	0.002
4102	4.27	155.43	3.39	10.69	0.35	0.270	0.002

Table 2: Material parameters for the phase constituents used in the micromechanical model.

Phase	E (GPa)	ν	σ_y (MPa)	E_T (MPa)	H (GPa)
crystalline (c)	344.0	0.173	9131	1000	19.8
amorphous (a)	129.9	0.281	4870	1000	10.4

Table 3: Description of the headings in the data set "SimulationData-RVE64-HS146.dat". All results are macroscopic values obtained from homogenization of the RVE.

Heading	Variable	Description
Job	-	PHIXYZ: Microstructure with XYZ% of amorphous volume fraction
dV/V0	dV/V_0	Relative volume change due to swelling of the amorphous fraction
phi_0	$\phi_{a,0}$	Volume fraction of the amorphous phase before swelling
phi_1	$\phi_{a,1}$	Volume fraction of the amorphous phase after swelling
rho_0	ρ_0	Density of the bi-phase microstructure before swelling
rho_1	ρ_1	Density of the bi-phase microstructure after swelling
E	E	Young's modulus (undeformed volume, nominal value)
nu	ν	Poisson's ratio (undeformed volume, nominal value)
E_tr	E_{tr}	Young's modulus (deformed volume, true value)
nu_tr	ν_{tr}	Poisson's ratio (deformed volume, true value)
sy00, sy02, sy04	σ_y	Yield stress for interface thickness of $t = 0.0, 0.2, 0.4$
H00, H02, H04	H	Hardness for interface thickness of $t = 0.0, 0.2, 0.4$

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References

[1] T. Murakami, B. C. Chakoumakos, R. C. Ewing, G. R. Lumpkin, and W. J. Weber, Am. Mineral. **76**, 1510 (1991).

[2] T. Beirau, W. D. Nix, U. Bismayer, L. A. Boatner, S. G. Isaacson, and R. C. Ewing, Phys. Chem. Minerals **43**, 627 (2016).

[3] T. Beirau, W. D. Nix, R. C. Ewing, H. Pöllmann, and E. K. H. Salje, Appl. Phys. Lett. **112**, 201901 (2018).

[4] C. Soyarslan, S. Bargmann, M. Pradas, and J. Weissmüller, Acta Mat. **149**, 326 (2018).

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