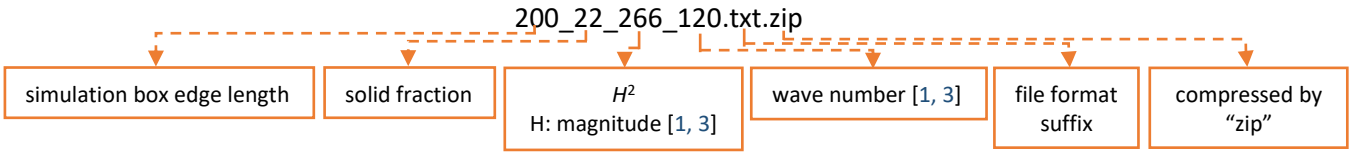
Description of Files

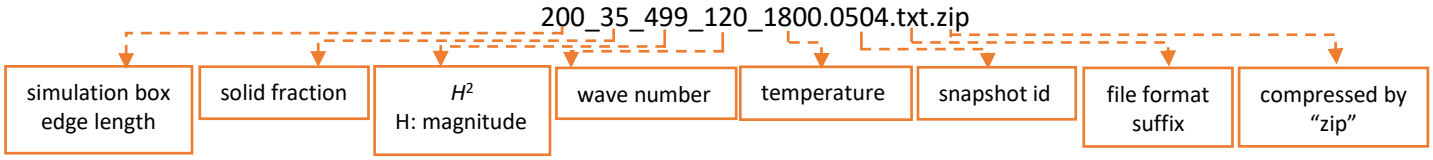
This file is the description for the datasets of "Datasets for the microstructure of nanoscale metal network structures and for its evolution during coarsening". The datasets are supplementary material of the related publication "Topology evolution during coarsening of nanoscale metal network structures" [1].

1.1 File name

1.1.1 File name for initial configurations:

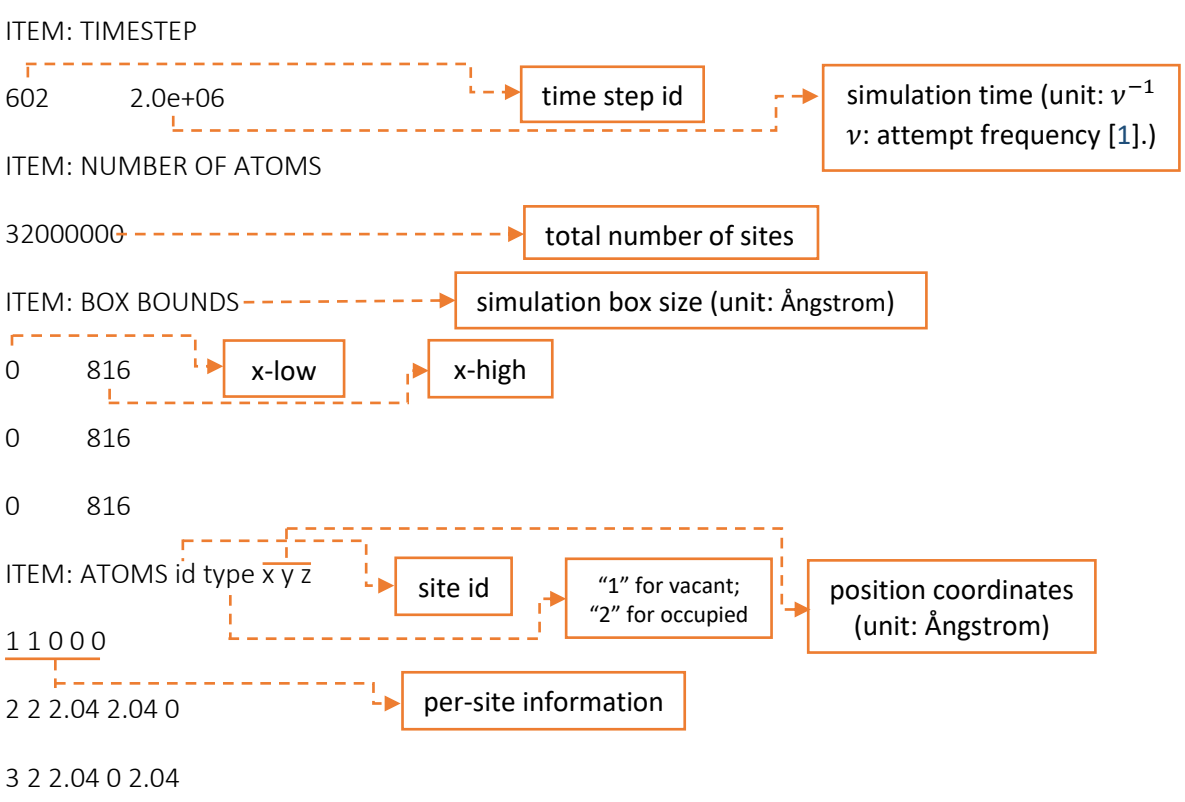


1.1.2 File name for kmc-generated structures:



1.2 Data format

The header of each snapshot:



Note:

1) Initial configurations (listed in Table 1 and 2) are stored with both vacant (type "1") and occupied (type "2") sites. The coarsened structures (listed in Table 4 and 5) are stored with occupied sites only.

2) The configurations that are produced by coarsening may contain regions of solid which are disconnected from the percolating part of the solid. This is explained in detail in Ref. [1], see specifically figure 5b there. Some conceivable applications of the structures documented here may require that these disconnected regions be removed. As just one out of several options, the open source software OVITO [6] provides a simple and convenient way of achieving this.[1]

1.3 Properties of each structure

Initial configurations (listed in Table 1 and 2) were generated by a leveled-wave algorithm [1, 2, 3] with periodic boundary conditions adapted. Table 3 listed all of Miller indices for the corresponding magnitude, H in Table 1 and 2. Coarsening KMC simulations were run on open source kinetic Monte Carlo simulation package SPPARKS [4, 5]. The structures in Table 1 were run at temperature of 900 K and output snapshots are listed in Table 4. Temperature for simulations of initial configurations in Table 2 is 1800 K and output snapshots are listed in Table 5 accordingly. Open source code Ovito [6] provided the surface area per solid volume, S_V. The apparent ligament diameter, L_{ap}, and mean ligament spacing, $\tilde{L}$, were calculated by Eqs. (3) and (4) from Ref. [1]. The topological genus, G, with $G = B_1$ (B_1 is the Betti number), was computed via open-source code CHomP [7]. Scaled genus, g, was computed from Eq. (5) in Ref. [1].

Table 1 Initial configurations for the 900 K simulations: geometric and topological characteristics, as well as parameters used for construction. Solid fraction, φ; filename of the RVE, magnitude, H, of Miller-index square; wavelength, λ, underlying the Gaussian field; specific (per solid volume) area, S_V, of surface; apparent ligament size, L_{ap}; characteristic spacing, $\tilde{L}$, between ligaments; net topological genus, G, of the RVE; scaled genus, g.

φ no units	filename	H	λ [nm]	S_V [1/nm]	L_{ap} [nm]	$\tilde{L}$ [nm]	G no units	g *no units*
0.22	200_22_266_120.txt.zip	$\sqrt{266}$	5.00	1.69	2.36	5.66	1593	0.53
0.25	200_25_306_120.txt.zip	$\sqrt{306}$	4.66	1.72	2.33	5.23	2975	0.78
0.27	200_27_350_120.txt.zip	$\sqrt{350}$	4.36	1.79	2.24	4.86	4269	0.90
0.30	200_30_386_120.txt.zip	$\sqrt{386}$	4.15	1.79	2.23	4.60	5933	1.06
0.35	200_35_449_120.txt.zip	$\sqrt{449}$	3.85	1.77	2.25	4.24	9260	1.30
0.40	200_40_525_120.txt.zip	$\sqrt{525}$	3.56	1.77	2.26	3.89	13134	1.42
0.45	200_45_649_120.txt.zip	$\sqrt{649}$	3.20	1.82	2.20	3.44	19809	1.48
0.50	200_50_754_120.txt.zip	$\sqrt{754}$	2.97	1.80	2.22	3.16	25183	1.46

[1] OVITO [6] provides the following sequence of commands: File → Load File → Add modification → Cluster analysis (Cutoff distance: 3; sort clusters by size) → Expression selection (operate on: particles; Boolean expression: Cluster >= 2) → Delete selected → File → Export File (File name: e.g. 200_22_266_120_0900.0716.txt.gz; Save as type: LAMMPS Dump File).

Table 2 Initial configurations for the 1800 K simulations. Analogous to Table 1.

φ no units	File name	H	λ [nm]	S_V [1/nm]	L_{ap} [nm]	$\tilde{L}$ [nm]	G no units	g *no units*
0.25	200_25_449_120.txt.zip	$\sqrt{449}$	3.85	2.13	1.87	4.24	5158	0.72
0.30	200_30_449_120.txt.zip	$\sqrt{449}$	3.85	1.95	2.05	4.24	7433	1.04
0.35	200_35_449_120.txt.zip	$\sqrt{449}$	3.85	1.77	2.25	4.24	9260	1.30
0.50	200_50_449_120.txt.zip	$\sqrt{449}$	3.85	1.34	2.98	4.23	11688	1.63

Table 3 : Miller indices (h, k, l) for the individual values of H as listed in Tables 1 and 2.

H	h	k	l
266	11	9	8
	12	11	1
	13	9	4
	15	5	4
	16	3	1
306	11	11	8
	12	9	9
	13	11	4
	15	9	0
	16	5	5
	16	7	1
	17	4	1
350	13	10	9
	15	10	5
	15	11	2
	17	6	5
	18	5	1
386	12	11	11
	16	9	7
	16	11	3
	17	9	4
	19	4	3
	19	5	0
449	16	12	7
	17	12	4
	18	10	5
	18	11	2
	20	7	0
	21	2	2
525	16	13	10
	19	10	8
	20	10	5
	20	11	2
	22	5	4
649	18	15	10
	18	17	6
	18	18	1
	19	12	12
	21	12	8
	24	8	3
754	21	13	12
	23	12	9
	23	15	0
	24	13	3
	27	4	3
	27	5	0

Table 4 : Contents of the individual configuration files for the 900 K simulations. Solid fraction, φ, filename of the snapshot, simulation time, t, surface area per solid volume, S_V, apparent ligament size, L_{ap}, characteristic spacing size, $\tilde{L}$, topological genus, G, and scaled genus, g of the snapshots microstructures.

φ no units	File name	t [ν^{-1}]	S_V [1/nm]	L_{ap} [nm]	$\tilde{L}$ [nm]	G no units	g *no units*
0.22	200_22_266_120_0900.0504.txt.zip	2.0E+05	0.16	2.43	5.83	924	0.34
	200_22_266_120_0900.0602.txt.zip	2.0E+06	1.45	2.76	6.60	378	0.20
	200_22_266_120_0900.0606.txt.zip	4.0E+06	1.25	3.20	7.67	159	0.13
	200_22_266_120_0900.0618.txt.zip	1.0E+07	0.92	4.35	10.42	10	0.02
	200_22_266_120_0900.0704.txt.zip	2.2E+07	0.79	5.05	12.09	1	0.003
	200_22_266_120_0900.0716.txt.zip	6.8E+07	0.67	5.98	14.33	0	0
0.25	200_25_306_120_0900.0504.txt.zip	2.0E+05	0.17	2.40	5.39	2081	0.60
	200_25_306_120_0900.0602.txt.zip	2.0E+06	1.41	2.83	6.36	1127	0.53
	200_25_306_120_0900.0606.txt.zip	4.0E+06	1.14	3.51	7.87	503	0.45
	200_25_306_120_0900.0618.txt.zip	1.0E+07	0.84	4.74	10.64	82	0.18
	200_25_306_120_0900.0704.txt.zip	2.0E+07	0.73	5.46	12.25	30	0.10
	200_25_306_120_0900.0716.txt.zip	6.8E+07	0.62	6.46	14.50	10	0.06
0.27	200_27_350_120_0900.0504.txt.zip	2.0E+05	0.17	2.31	5.03	3054	0.71
	200_27_350_120_0900.0602.txt.zip	2.0E+06	1.39	2.89	6.27	1602	0.73
	200_27_350_120_0900.0606.txt.zip	4.0E+06	1.09	3.68	7.98	655	0.61
	200_27_350_120_0900.0618.txt.zip	1.0E+07	0.82	4.87	10.57	191	0.42
	200_27_350_120_0900.0704.txt.zip	2.0E+07	0.71	5.61	12.18	113	0.38
	200_27_350_120_0900.0716.txt.zip	6.8E+07	0.60	6.72	14.59	51	0.29
0.30	200_30_386_120_0900.0504.txt.zip	2.0E+05	0.17	2.31	4.76	4720	0.94
	200_30_386_120_0900.0602.txt.zip	2.0E+06	1.30	3.08	6.33	2330	1.09
	200_30_386_120_0900.0606.txt.zip	4.0E+06	0.99	4.06	8.36	955	1.03
	200_30_386_120_0900.0618.txt.zip	1.0E+07	0.75	5.31	10.92	354	0.85
	200_30_386_120_0900.0704.txt.zip	2.0E+07	0.68	5.92	12.18	230	0.77
	200_30_386_120_0900.0716.txt.zip	6.8E+07	0.59	6.79	13.98	158	0.79
0.35	200_35_449_120_0900.0504.txt.zip	2.0E+05	0.17	2.33	4.38	7936	1.23
	200_35_449_120_0900.0602.txt.zip	2.0E+06	1.17	3.41	6.41	3398	1.65
	200_35_449_120_0900.0606.txt.zip	4.0E+06	0.89	4.48	8.42	1417	1.56
	200_35_449_120_0900.0618.txt.zip	1.0E+07	0.72	5.57	10.48	741	1.57
	200_35_449_120_0900.0704.txt.zip	2.0E+07	0.64	6.28	11.82	509	1.55
	200_35_449_120_0900.0716.txt.zip	6.8E+07	0.54	7.45	14.01	319	1.62
0.40	200_40_525_120_0900.0504.txt.zip	2.0E+05	0.17	2.35	4.04	11707	1.42
	200_40_525_120_0900.0602.txt.zip	2.0E+06	1.06	3.78	6.49	4010	2.02

	200_40_525_120_0900.0606.txt.zip	4.0E+06	0.83	4.80	8.24	1919	1.98
	200_40_525_120_0900.0618.txt.zip	1.0E+07	0.67	6.01	10.32	992	2.01
	200_40_525_120_0900.0704.txt.zip	2.0E+07	0.58	6.85	11.76	667	2.00
	200_40_525_120_0900.0716.txt.zip	6.8E+07	0.50	7.98	13.70	450	2.13
0.45	200_45_649_120_0900.0504.txt.zip	2.0E+05	0.17	2.32	3.62	17728	1.55
	200_45_649_120_0900.0602.txt.zip	2.0E+06	0.94	4.24	6.63	3937	2.12
	200_45_649_120_0900.0606.txt.zip	4.0E+06	0.77	5.17	8.08	2224	2.16
	200_45_649_120_0900.0618.txt.zip	1.0E+07	0.61	6.53	10.21	1151	2.26
	200_45_649_120_0900.0704.txt.zip	2.0E+07	0.54	7.38	11.55	790	2.24
	200_45_649_120_0900.0716.txt.zip	6.8E+07	0.48	8.33	13.04	580	2.37
0.50	200_50_754_120_0900.0504.txt.zip	2.0E+05	0.17	2.40	3.40	22394	1.62
	200_50_754_120_0900.0602.txt.zip	2.0E+06	0.84	4.77	6.77	3682	2.11
	200_50_754_120_0900.0606.txt.zip	4.0E+06	0.72	5.57	7.91	2445	2.22
	200_50_754_120_0900.0618.txt.zip	1.0E+07	0.56	7.09	10.07	1228	2.30
	200_50_754_120_0900.0704.txt.zip	2.0E+07	0.49	8.10	11.50	821	2.30
	200_50_754_120_0900.0716.txt.zip	6.8E+07	0.43	9.28	13.18	603	2.54

Table 5 : Contents of the individual configuration files for the 1800 K simulations. Analogous to Table 4.

φ no units	File name	t [ν^{-1}]	S_V [1/nm]	L_{ap} [nm]	$\tilde{L}$ [nm]	G no units	g *no units*
0.25	200_25_449_120_1800.0320.txt.zip	1.0E+04	1.83	2.19	4.95	2091	0.47
	200_25_449_120_1800.0406.txt.zip	2.5E+04	1.44	2.78	6.29	773	0.35
	200_25_449_120_1800.0420.txt.zip	6.0E+04	1.10	3.64	8.24	175	0.18
	200_25_449_120_1800.0502.txt.zip	1.5E+05	0.89	4.51	10.20	52	0.10
	200_25_449_120_1800.0508.txt.zip	3.0E+05	0.76	5.25	11.88	19	0.06
	200_25_449_120_1800.0532.txt.zip	9.0E+05	0.63	6.38	14.43	2	0.01
0.30	200_30_449_120_1800.0320.txt.zip	1.0E+04	1.71	2.34	4.83	4515	0.94
	200_30_449_120_1800.0406.txt.zip	2.5E+04	1.33	3.01	6.21	2186	0.96
	200_30_449_120_1800.0420.txt.zip	6.0E+04	1.01	3.97	8.18	820	0.83
	200_30_449_120_1800.0502.txt.zip	1.5E+05	0.81	4.95	10.21	403	0.79
	200_30_449_120_1800.0508.txt.zip	3.0E+05	0.70	5.74	11.84	232	0.71
	200_30_449_120_1800.0532.txt.zip	9.0E+05	0.57	7.02	14.48	109	0.61
0.35	200_35_449_120_1800.0320.txt.zip	1.0E+04	1.59	2.52	4.74	6890	1.35
	200_35_449_120_1800.0406.txt.zip	2.5E+04	1.24	3.23	6.08	3670	1.52
	200_35_449_120_1800.0420.txt.zip	6.0E+04	0.93	4.31	8.11	1504	1.48
	200_35_449_120_1800.0502.txt.zip	1.5E+05	0.73	5.45	10.24	776	1.54

	200_35_449_120_1800.0508.txt.zip	3.0E+05	0.63	6.33	11.91	470	1.46
	200_35_449_120_1800.0532.txt.zip	9.0E+05	0.53	7.49	14.09	305	1.57
0.50	200_50_449_120_1800.0320.txt.zip	1.0E+04	1.23	3.25	4.62	10210	1.86
	200_50_449_120_1800.0406.txt.zip	2.5E+04	0.98	4.08	5.79	6059	2.17
	200_50_449_120_1800.0420.txt.zip	6.0E+04	0.72	5.56	7.90	2406	2.18
	200_50_449_120_1800.0502.txt.zip	1.5E+05	0.55	7.23	10.27	1134	2.26
	200_50_449_120_1800.0508.txt.zip	3.0E+05	0.48	8.25	11.71	773	2.29
	200_50_449_120_1800.0532.txt.zip	9.0E+05	0.43	9.30	13.21	573	2.43

References

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