SAND2011-1581C

Quantifying the Microstructure-Induced Uncertainty in Strain Concentrations at Engineered Defects

Corbett Battaile[1], Brad Boyce[1], Luke Brewer[2]
John Emery[1], Charlie Robino[1]
[1] Sandia National Laboratories
[2] Naval Postgraduate School

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Introduction: What is Uncertainty Quantification?

• Uncertainty Quantification usually describes the connection between "the answer" and the underlying mathematical models, geometries, boundary conditions, algorithms, etc:

"Uncertainty: How accurately does a mathematical model describe the true physics and what is the impact of model uncertainty (structural or parametric) on outputs from the model?"[1]

"Uncertainty quantification (UQ) is the quantitative characterization and reduction of uncertainty in applications. Three types of uncertainties can be identified. The first type is uncertainty due to variability of input and/or model parameters and the characterization of the variability is given (for example, with probably density functions). The second type is similar to the first type except that the corresponding variability characterization is not available, in which case work can be directed to gain better knowledge. The third type, which is the most challenging, is uncertainty due to an unknown process or mechanism..."[2]

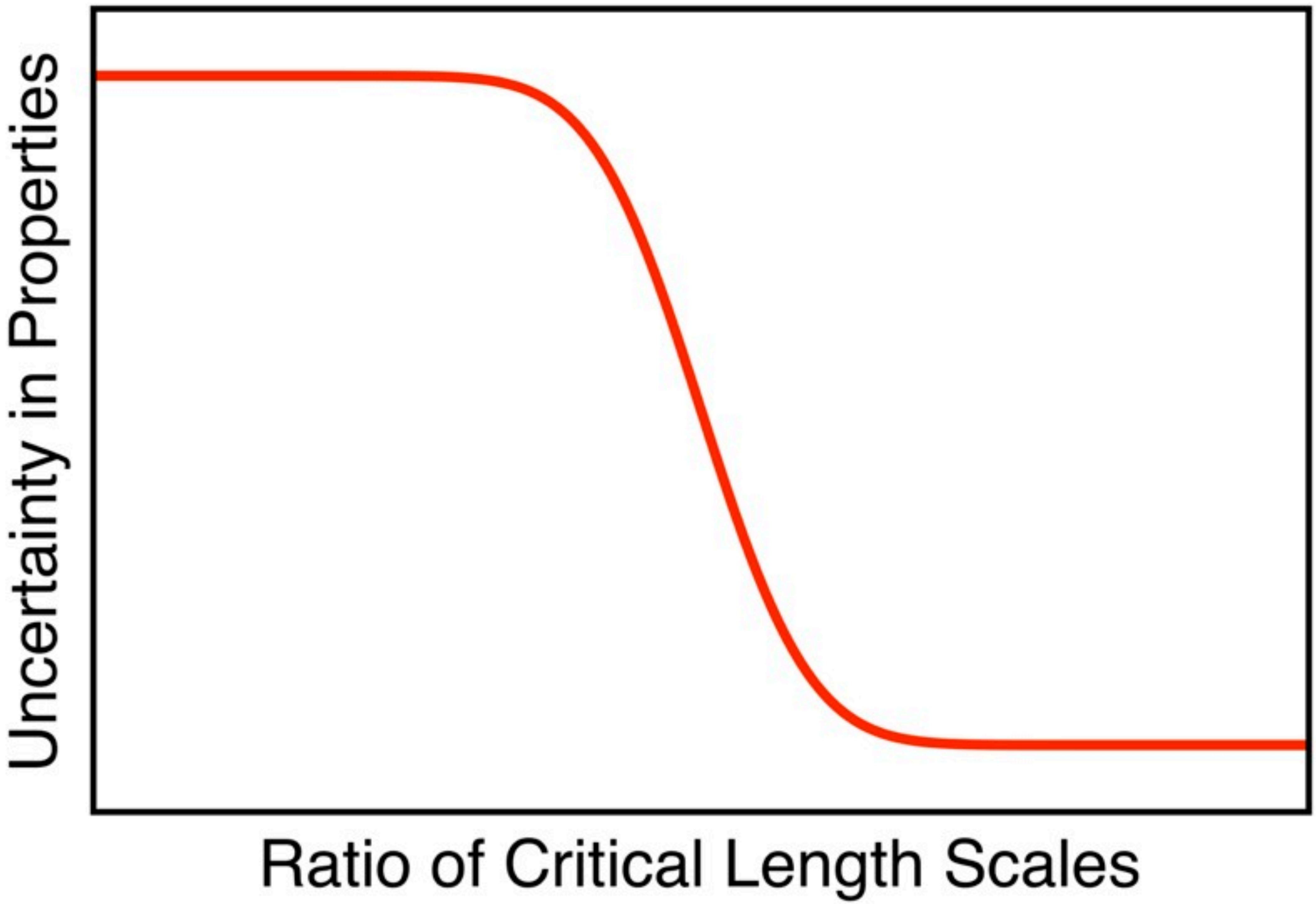
1) T.J. Barth, "A Brief Overview of Uncertainty Quantification and Error Estimation in Numerical Simulation," www.stanford.edu/group/cits/pdf/lectures/barth.pdf
2) From https://computation.llnl.gov/casc/uncertainty_quantification/

Introduction: What is Uncertainty Quantification?

- But there are other potential sources of uncertainty:
- Most engineering materials are inherently inhomogeneous.
- Variability in a material's microstructure can have a direct and profound impact on it properties.
- Variability can occur locally from point to point; globally from region to region; from part to part and lot to lot; and in time as a material ages.

Introduction: When is Variability Important?

When the length scale of the critical phenomena are comparable to, or less than, that of the microstructure.



Outline

- **Introduction**
- **Strength and Ductility of 304L Welds**
  - Experiments: tension tests
  - Simulations
- **Deformation near Holes in Brass**
  - Experiments: electron backscatter diffraction
  - Simulations
- **Summary**

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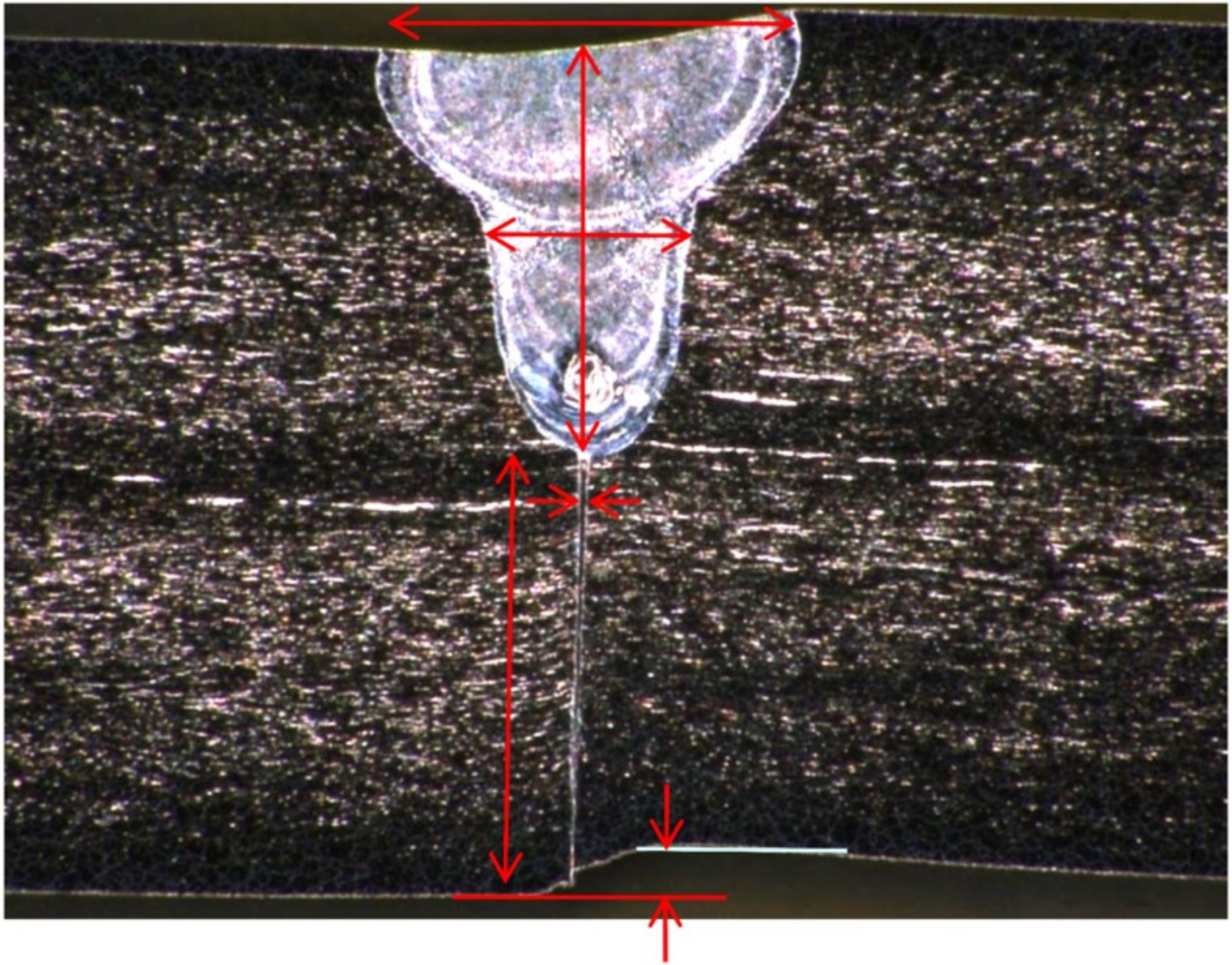
Welds in 304L: Micrograph w/ Geometry Variables

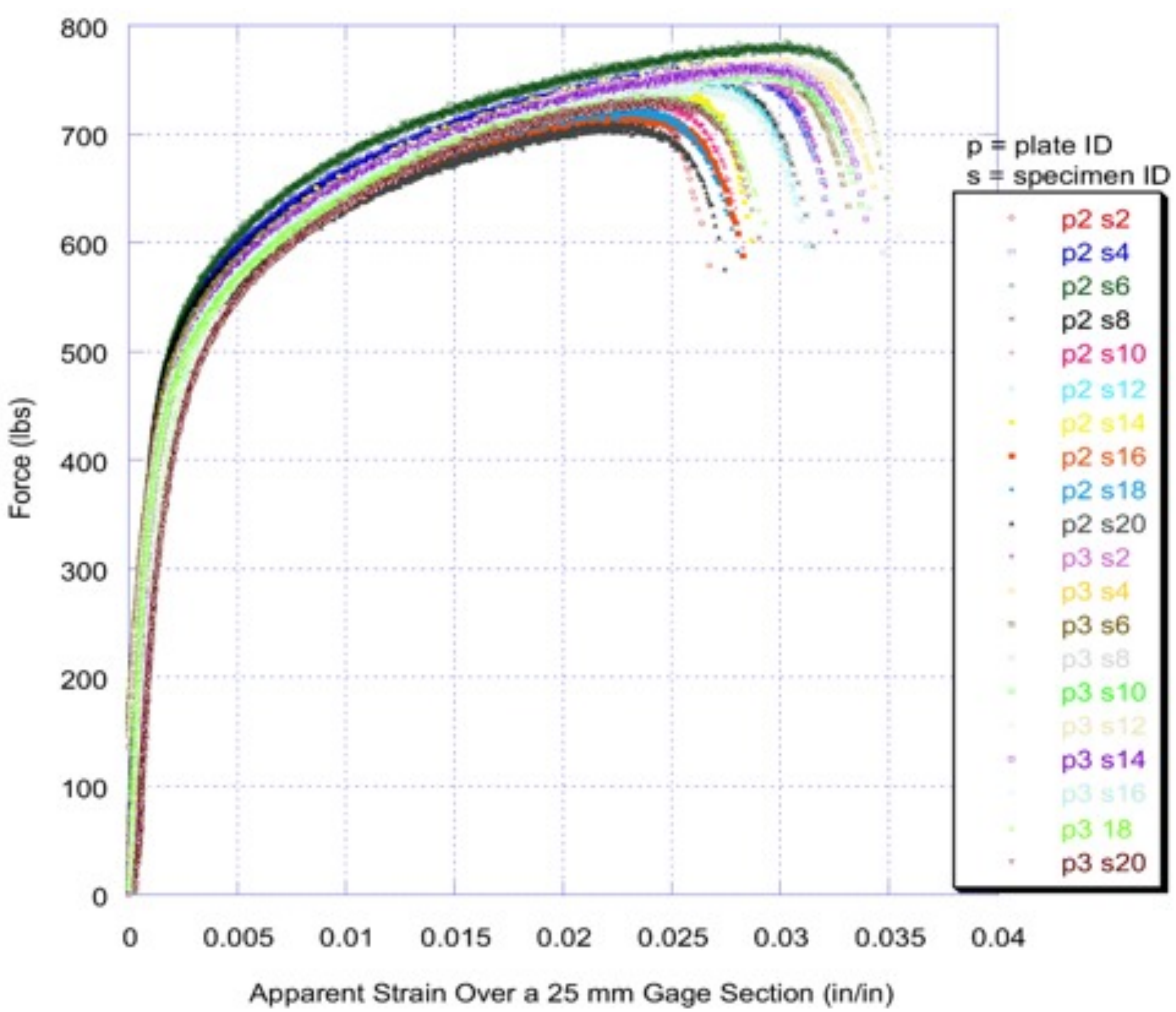
Optical Micrograph of a Partial Penetration Weld



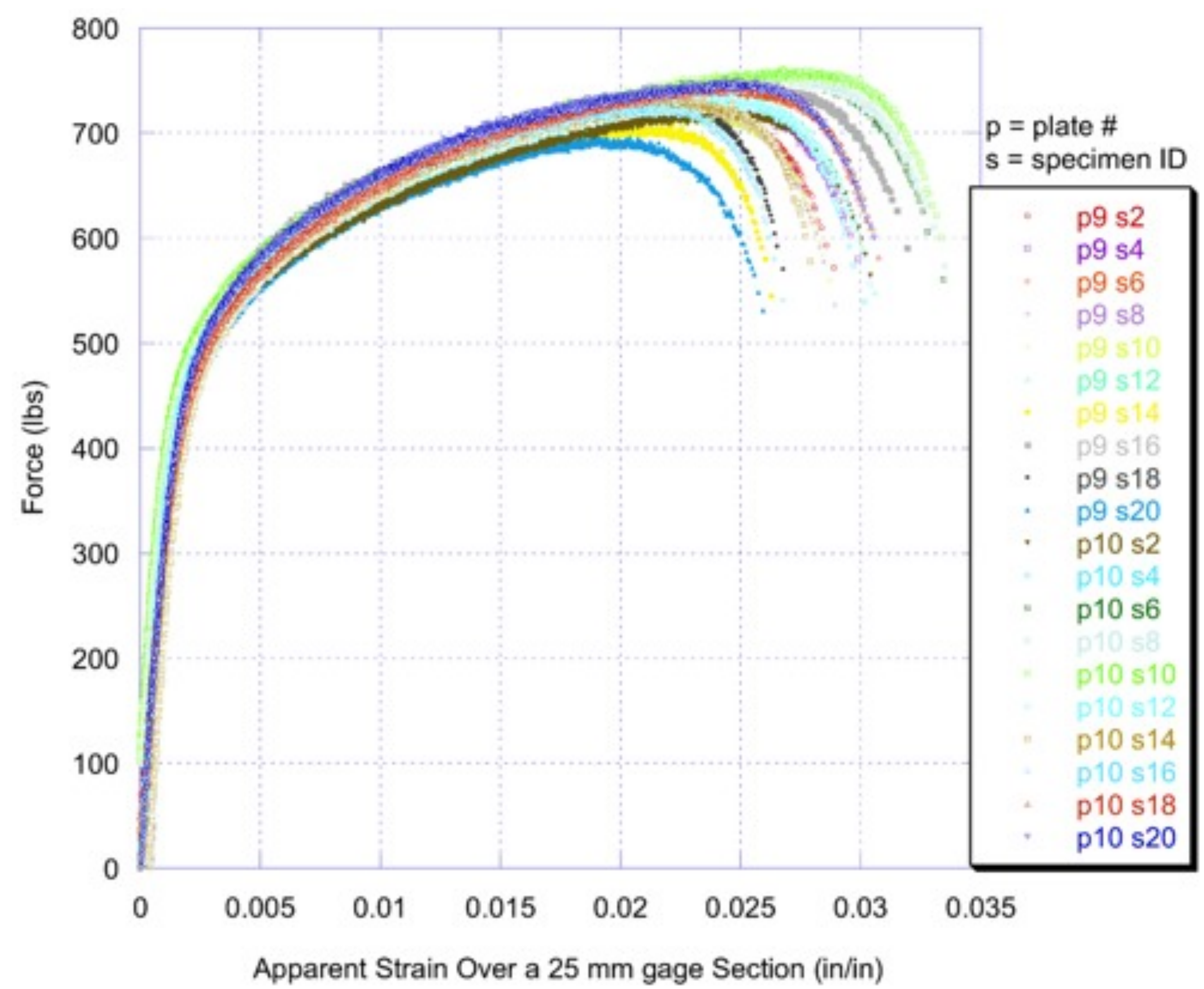
Welds in 304L: Force-Displacement Data

Tensile samples cut from nominally homogeneous welded plates show significant variability.

Continuous Welds

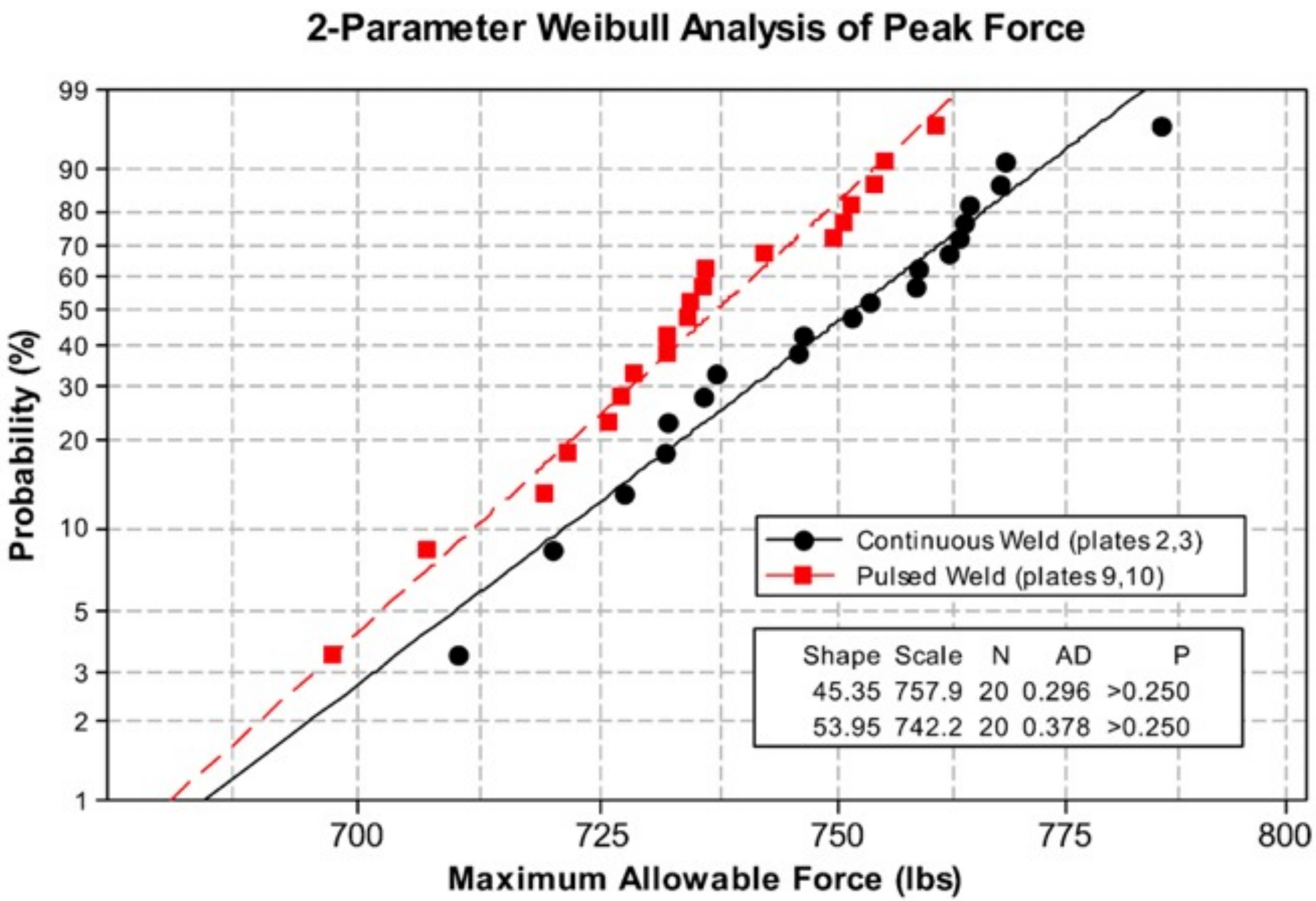


Pulsed Welds



Welds in 304L: Cumulative Probability Distributions

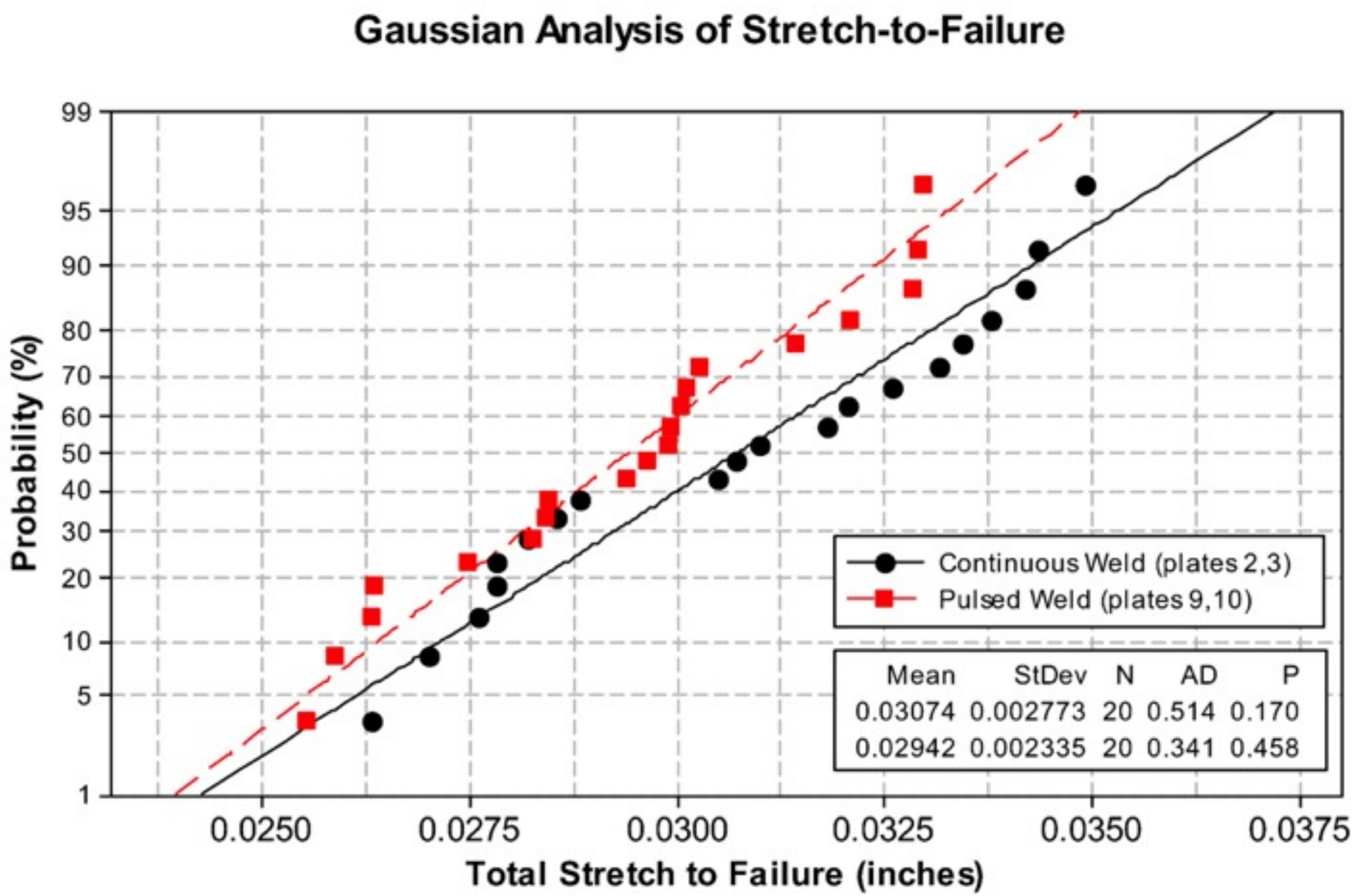
Among 15 common distributions, the 2-parameter Weibull distribution provided the best fit to the maximum force data based on the Anderson-Darling goodness-of-fit metric.



Extrapolating 'pulsed weld' distribution to a low allowable probability of failure:
1-in-1,000 Allowable Force: 650 lbs
1-in-1,000,000 Allowable Force: 550 lbs
$\Rightarrow$ ***Weld must be de-rated 25% below its average strength for 1-in-1,000,000 Failure***

Welds in 304L: Cumulative Probability Distributions

Among 15 common distributions, the Gaussian distribution provided the best fit to the stretch data based on the Anderson-Darling goodness-of-fit metric.



Extrapolating 'continuous weld' distribution to a low allowable stretch:
1-in-1,000 Allowable Stretch in Weld: 22.2 mils
1-in-1,000,000 Allowable Stretch in Weld: 17.6 mils
⇒ ***Weld must be de-rated 43% below its average stretch for 1-in-1,000,000 Failure***

Welds in 304L: What Variables Control Properties?

plate	sample	max force	stretch to failure (inch)	number of pores	total area of pores	area of biggest pore	average pore area	reinforcement width at surface (mm)	Penetration depth (mm)	Width at 1/2 penetration (mm)	notch depth (mm)	notch gap (mm)	plate offset (mm)	approx weld volume (mm^2)
2	2	731.7287	0.02633	30	344885.2	48461.04	11496.17	0.8155	0.7145	0.3665	0.771	0.005	0.0565	0.42227
2	4	764.3476	0.031814	28	504380.8	67351.97	18013.6	0.8025	0.7185	0.388	0.7675	0.008	0.029	0.427687
2	6	785.6429	0.03436	26	266235.2	44637.72	10239.82	0.7985	0.7035	0.3915	0.7775	0.013	0.0385	0.418583
2	8	753.4464	0.030999	25	537060.2	66261.64	21482.41	0.806	0.7175	0.382	0.781	0.0145	0.0395	0.426195
2	10	731.9822	0.027829	31	435196.5	62946.16	14038.6	0.7995	0.76	0.3595	0.7895	0.0195	0.0185	0.44042
2	12	751.5873	0.030714	26	308716	55588.3	11873.69	0.7835	0.758	0.3445	0.776	0.0235	0.0175	0.427512
2	14	745.672	0.02821	32	212601.9	22193.46	6643.81	0.779	0.722	0.35	0.755	0.0245	0.05	0.407569
2	16	719.898	0.027835	29	438360.8	53003.06	15115.89	0.782	0.686	0.3745	0.7795	0.03	0.0745	0.39668
2	18	727.2499	0.027609	35	354673.2	37476.05	10133.52	0.782	0.664	0.3855	0.7905	0.032	0.0825	0.38761
2	20	710.0954	0.02702	36	372310.9	44018.25	10341.97	0.792	0.7065	0.3925	0.7085	0.029	0.047	0.418425
3	2	758.6013	0.032052	29	481844.9	52864.41	16615.34	0.804	0.7005	0.378	0.7855	0.013	0.0475	0.413996
3	4	768.2348	0.033789	26	337065.6	49955.08	12964.06	0.7955	0.7175	0.383	0.7705	0.0085	0.0535	0.422787
3	6	763.1645	0.032605	30	346742.9	36935.88	11558.1	0.7805	0.7285	0.378	0.7545	0.0115	0.0565	0.421984
3	8	758.7703	0.034193	34	386876	41873.32	11378.71	0.7865	0.723	0.384	0.755	0.014	0.067	0.423136
3	10	762.0659	0.033158	27	460016.9	47660.59	17037.66	0.7875	0.7325	0.3715	0.732	0.0145	0.0945	0.424484
3	12	767.6433	0.034913	21	368383.8	62139.42	17542.09	0.7935	0.709	0.378	0.726	0.014	0.1245	0.415297
3	14	763.756	0.033426	35	300459.3	47282.13	8584.552	0.8125	0.68	0.383	0.7195	0.0115	0.151	0.40647
3	16	746.2635	0.0305	30	331717	39365.89	11057.23	0.8135	0.661	0.367	0.72	0.0125	0.1725	0.390155
3	18	737.0525	0.028834	27	317016.6	45480.49	11741.36	0.8095	0.648	0.372	0.7295	0.009	0.1735	0.382806
3	20	735.7004	0.028555	29	298972.9	35753.25	10309.41	0.826	0.6555	0.478	0.6125	0.0105	0.158	0.427386
9	2	728.3485	0.02843	44	363719	39415.14	8266.341	0.899	0.623	0.41	0.7565	0.0045	0.2065	0.407754
9	4	734.0948	0.029399	38	401812.9	48320.67	10574.02	0.8835	0.6705	0.41	0.799	0.0035	0.1115	0.433646
9	6	742.2918	0.030054	32	402231.7	76218.67	12569.74	0.8725	0.6985	0.4205	0.8355	0.002	0.032	0.45158
9	8	725.7288	0.028466	33	476366.9	67738.92	14435.36	0.933	0.69	0.42	0.838	0.002	0.03	0.466785
9	10	719.0529	0.028257	34	717368.5	56351.47	21099.07	0.9235	0.69	0.412	0.797	0.0045	0.0695	0.460748
9	12	735.7849	0.030113	41	636322.9	82478.43	15520.07	0.9375	0.6855	0.443	0.758	0.0135	0.0925	0.473166
9	14	706.9687	0.025872	36	750598.6	81757.19	20849.96	0.9455	0.6895	0.441	0.726	0.0195	0.1165	0.477996
9	16	751.4183	0.031445	43	531461.7	55421.27	12359.58	0.8725	0.714	0.423	0.682	0.024	0.144	0.462494
9	18	731.9822	0.026336	35	527197.1	51616.68	15062.77	0.858	0.6935	0.4075	0.6615	0.034	0.1635	0.438812
9	20	697.5042	0.025533	41	626131.7	71328.11	15271.5	0.915	0.6875	0.415	0.6065	0.046	0.166	0.457188
10	2	721.4191	0.029941	34	505079.6	46905.18	14855.28	0.9575	0.688	0.426	0.8605	0.0045	0.02	0.475924
10	4	734.4329	0.029661	39	496797	65343.21	12738.38	0.8955	0.6925	0.4025	0.8505	0.008	0.02	0.449433
10	6	755.1365	0.032914	29	353073	45028.03	12174.93	0.87	0.7105	0.4245	0.82	0.0115	0.033	0.459871
10	8	754.1225	0.032974	27	408711.1	70921.59	15137.45	0.8925	0.7425	0.4385	0.77	0.015	0.0185	0.494134
10	10	760.7984	0.032837	32	381440.4	59819.77	11920.01	0.904	0.7395	0.4385	0.7735	0.016	0.007	0.496389
10	12	736.0384	0.029911	35	620600.6	88394	17731.45	0.87	0.714	0.4215	0.8025	0.021	0.0345	0.461066
10	14	731.9822	0.027478	31	512465.1	61636.75	16531.13	0.8425	0.7185	0.4075	0.778	0.0275	0.0695	0.449063
10	16	727.1654	0.026342	38	505874.6	78496.16	13312.49	0.8715	0.74	0.4285	0.7205	0.031	0.094	0.481
10	18	749.5593	0.03028	22	341599.2	50304.31	15527.24	0.84	0.7465	0.4305	0.7015	0.029	0.0925	0.474214
10	20	750.7423	0.032082	44	439447.8	47962.89	9987.45	0.8855	0.8475	0.452	0.562	0.0345	0.058	0.566766

According to multivariate linear regression, the notch gap accounts for 63% of the variability in peak force, and 48% in strain-to-failure.

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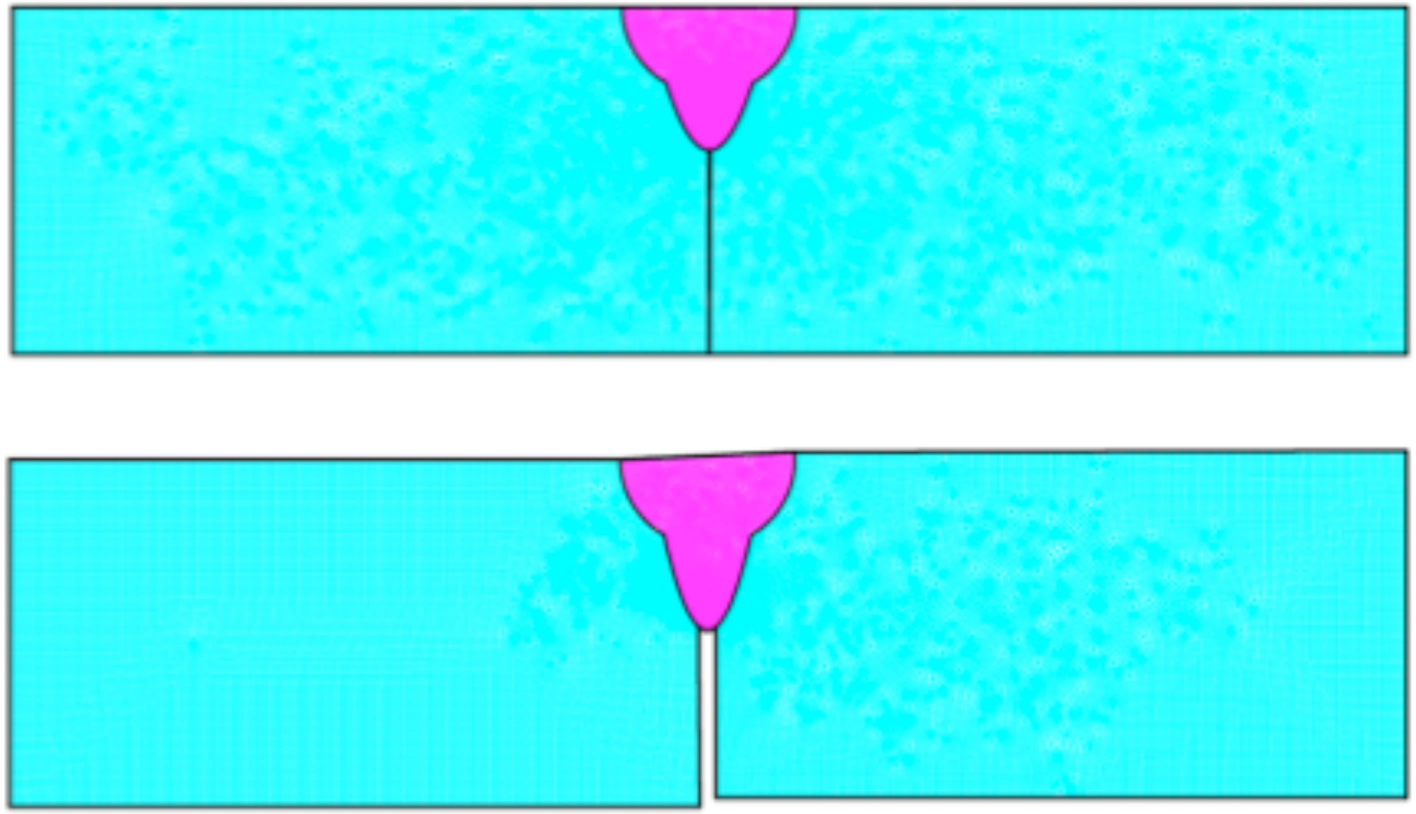
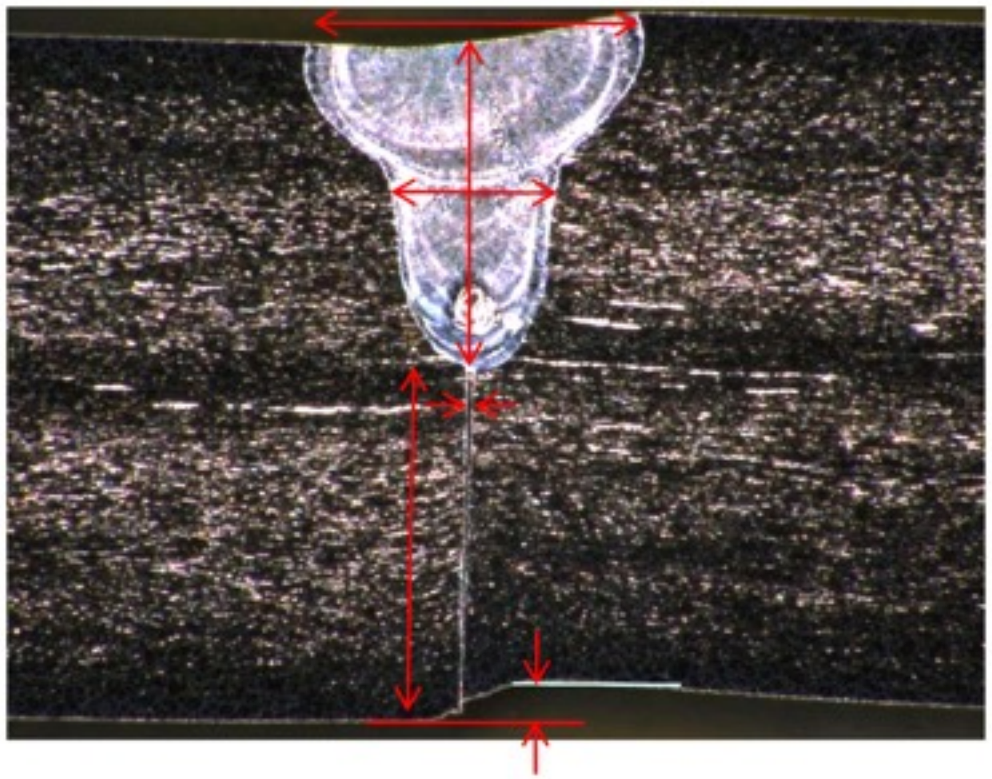
Welds in 304L: FE Meshes with Geometrical Variability

Simulated weld geometries attempt to capture realistic weld shape, in addition to variability in weld depth, plate gap, and plate offset.



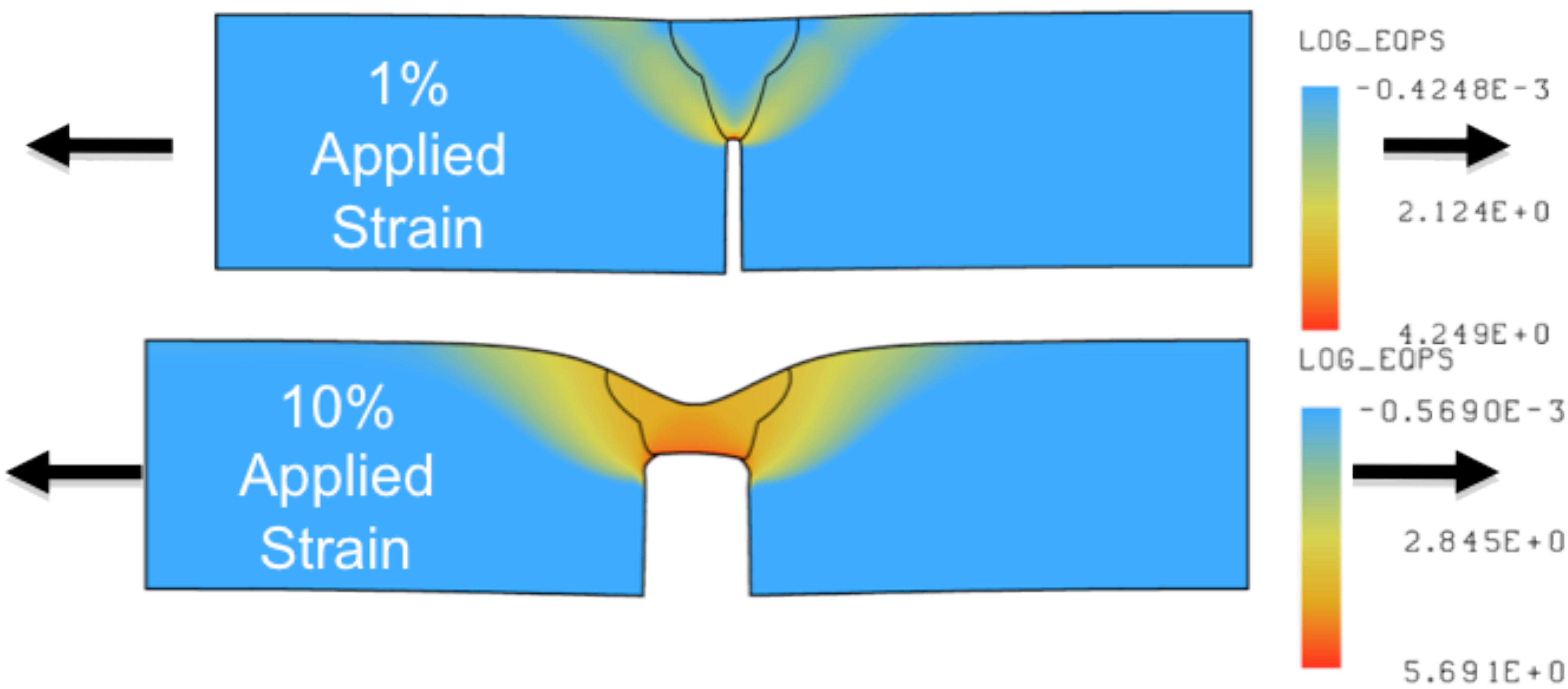


Welds in 304L: Model and Simulation Details

- Simple elastic + power-law plastic constitutive law
- Parameters fit to data from both plate and weld
- "2+1 D" geometries
  - Plane strain boundary conditions in Z
  - Prescribed displacements in X
  - Unconstrained in Y

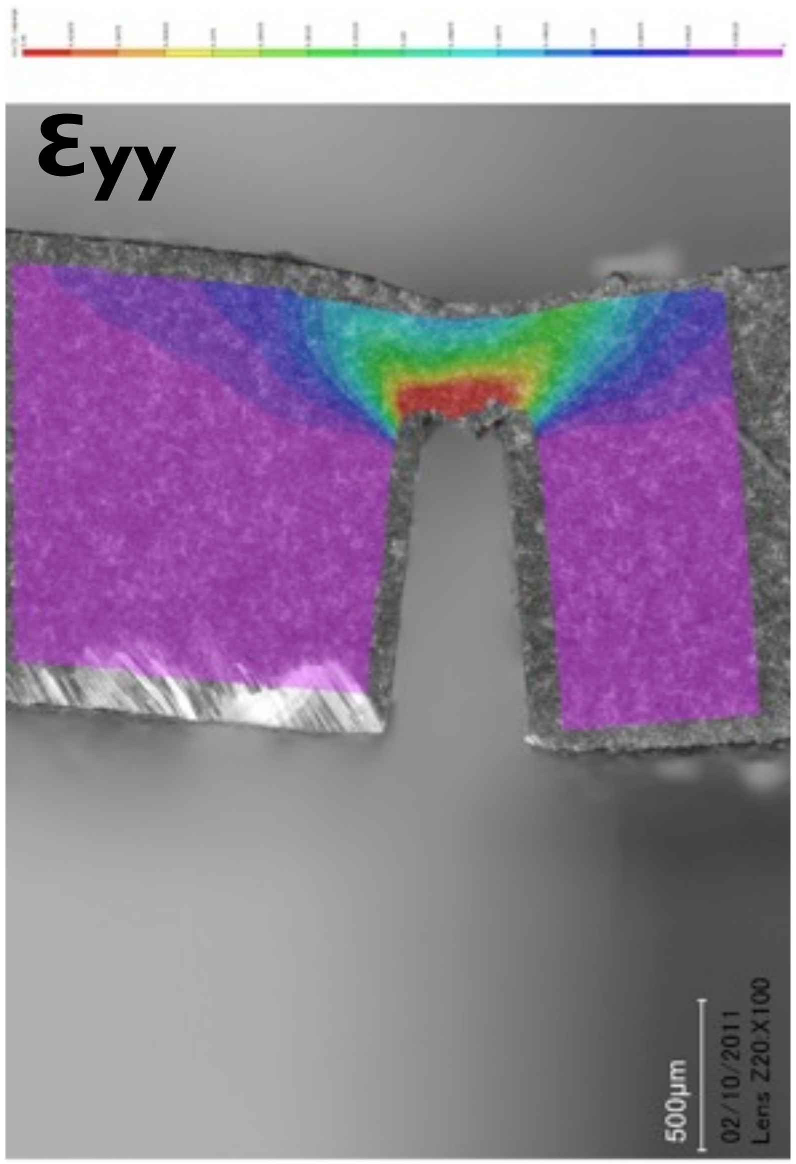
Welds in 304L: Simulations of Tensile Deformation

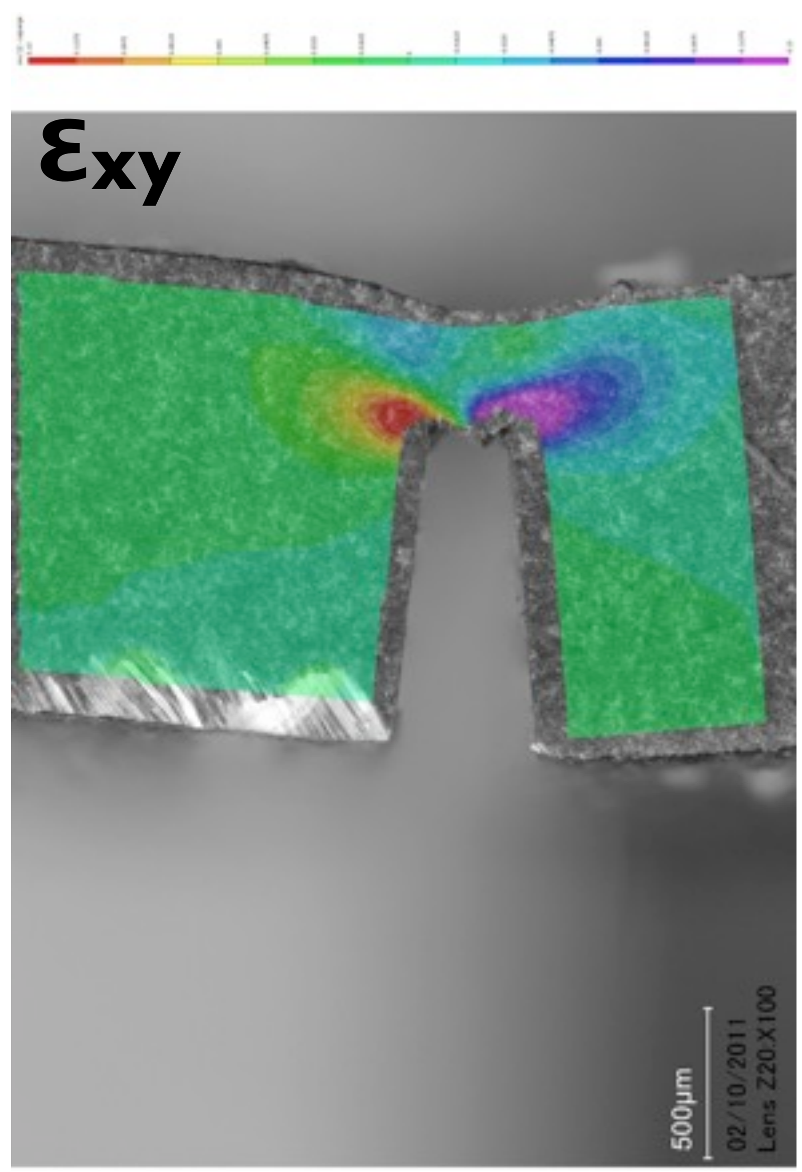
Weld deformation simulations suggest strain concentration localized at the notch root.

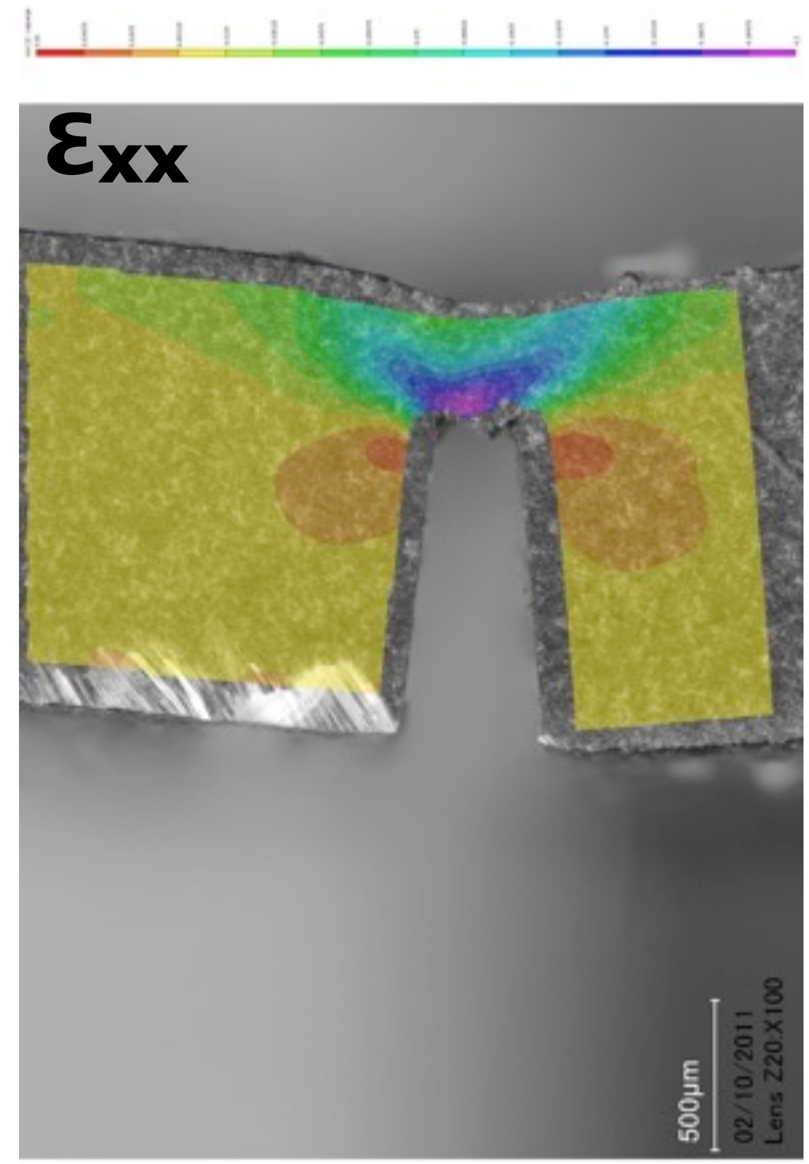


Welds in 304L: DIC Experiments of Tensile Deformation

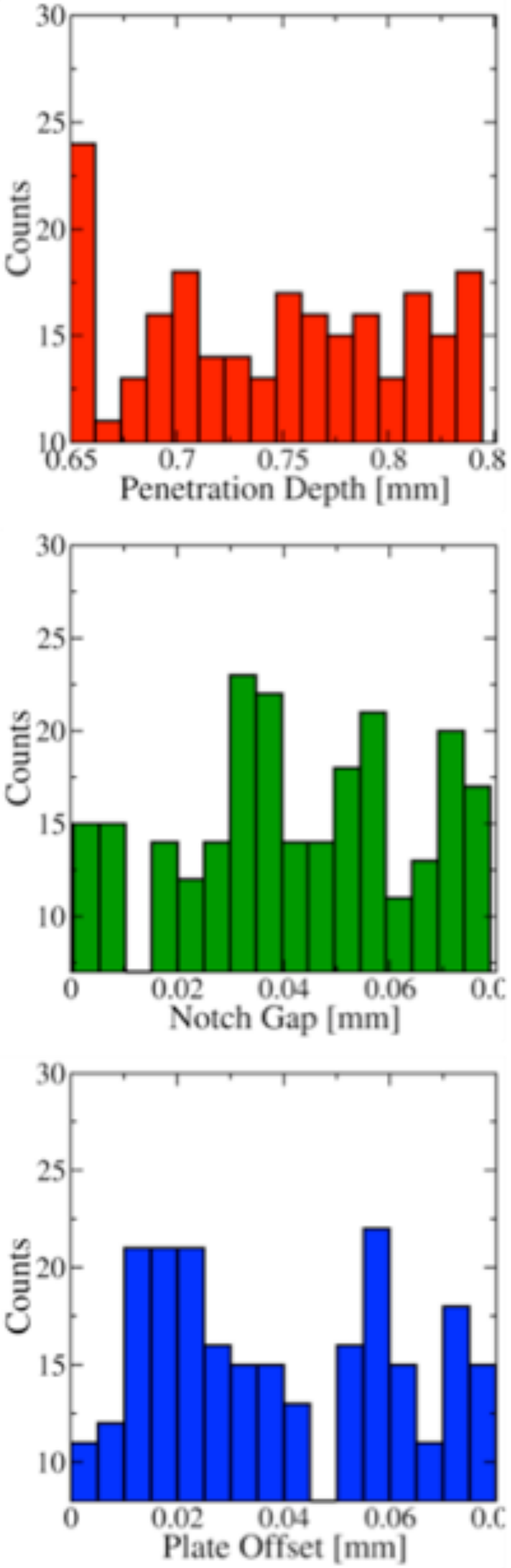
Digital image correlation experiments show similar behavior...





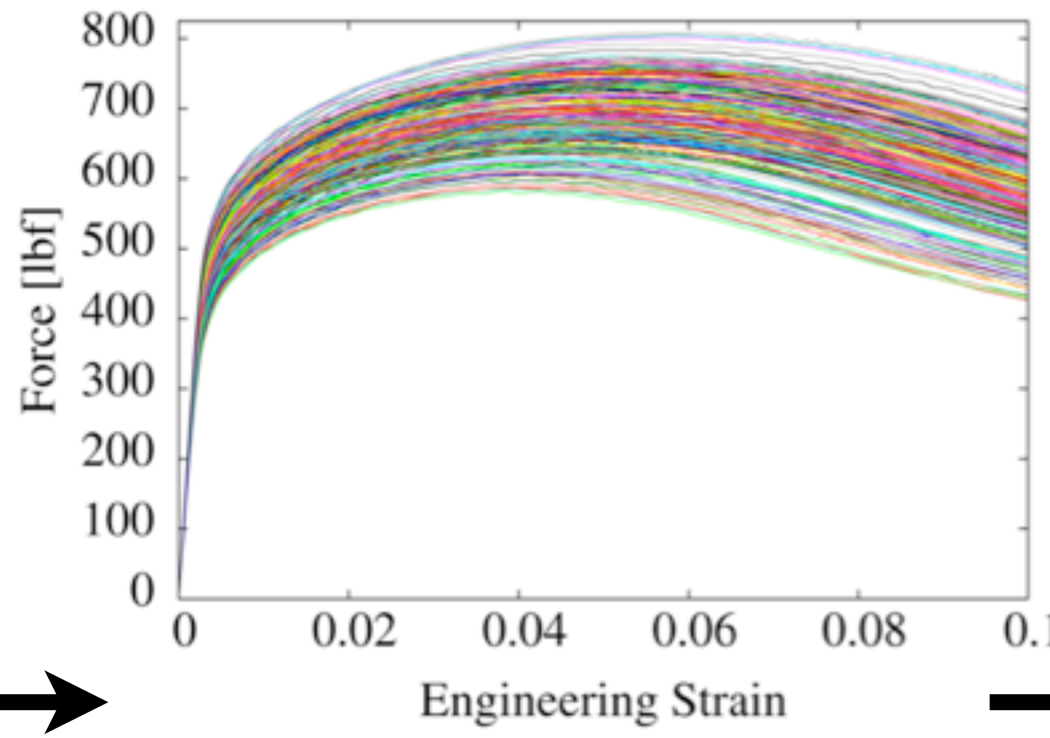


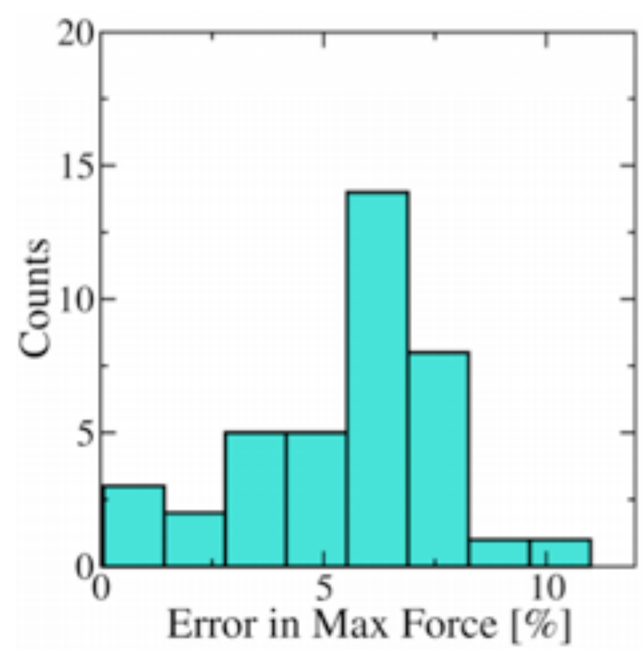
Welds in 304L: Geometry-Induced Property Statistics



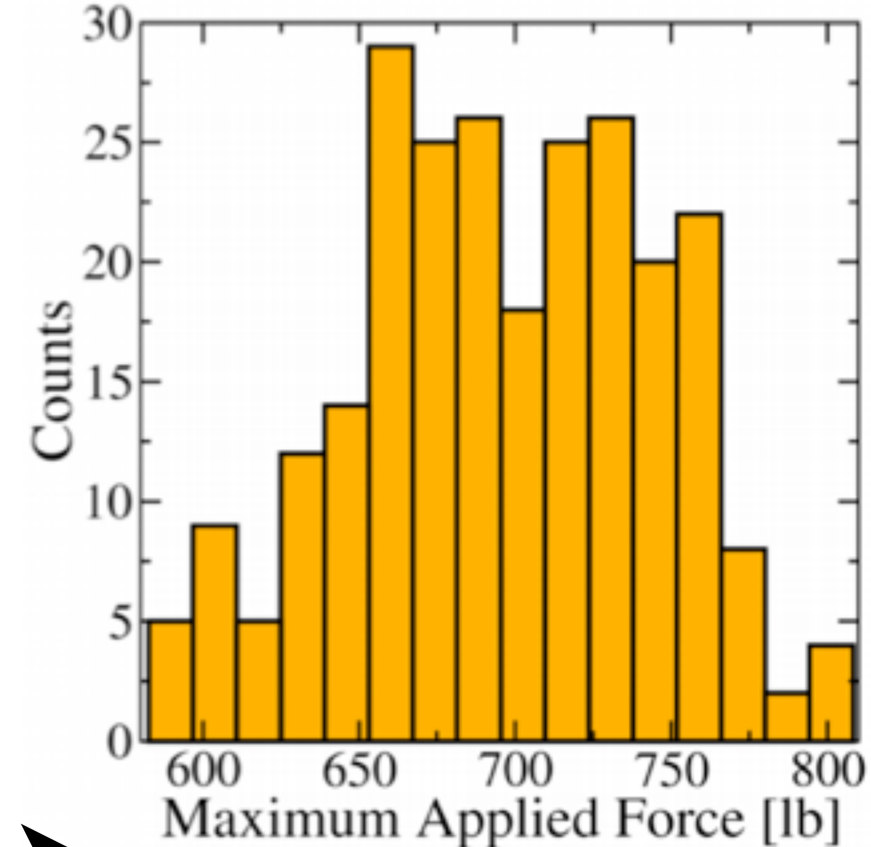
Inputs

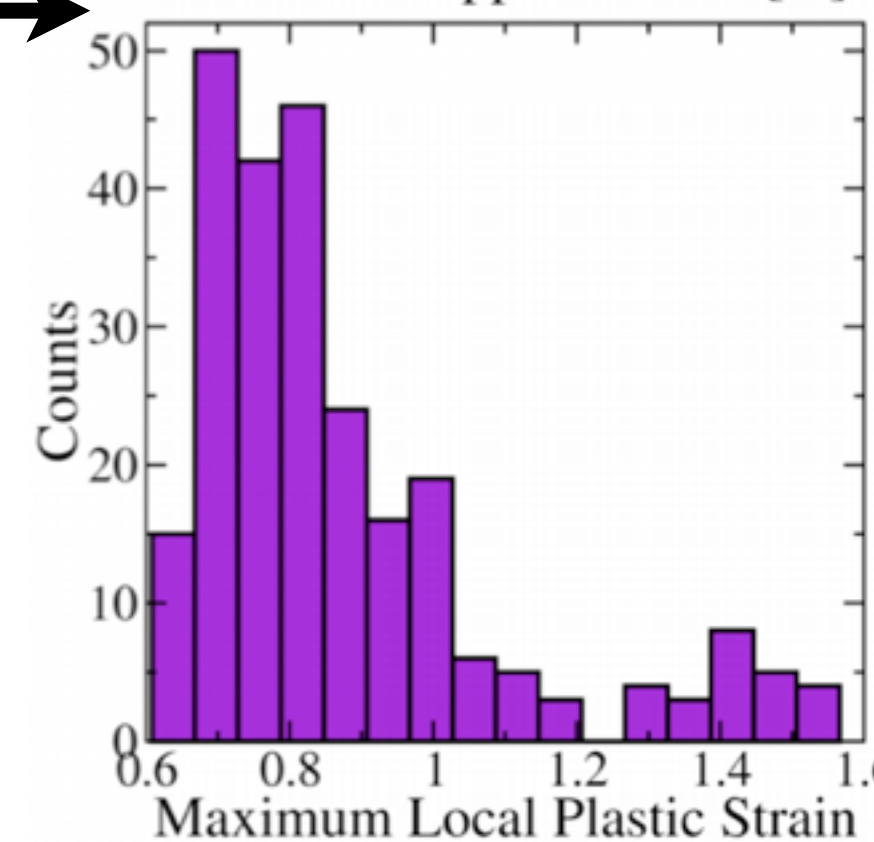
Tensile Behavior





Validation

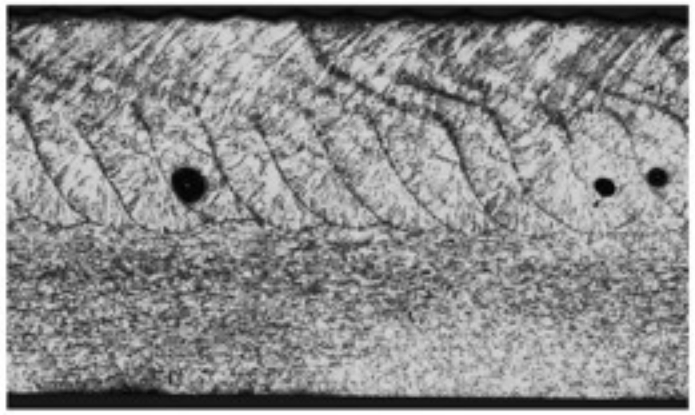




Property Statistics

Welds in 304L: Microstructure Characterization

Microstructure variability can play an important role in governing variability in properties (though not so prominently in 304L-to-304L welds).



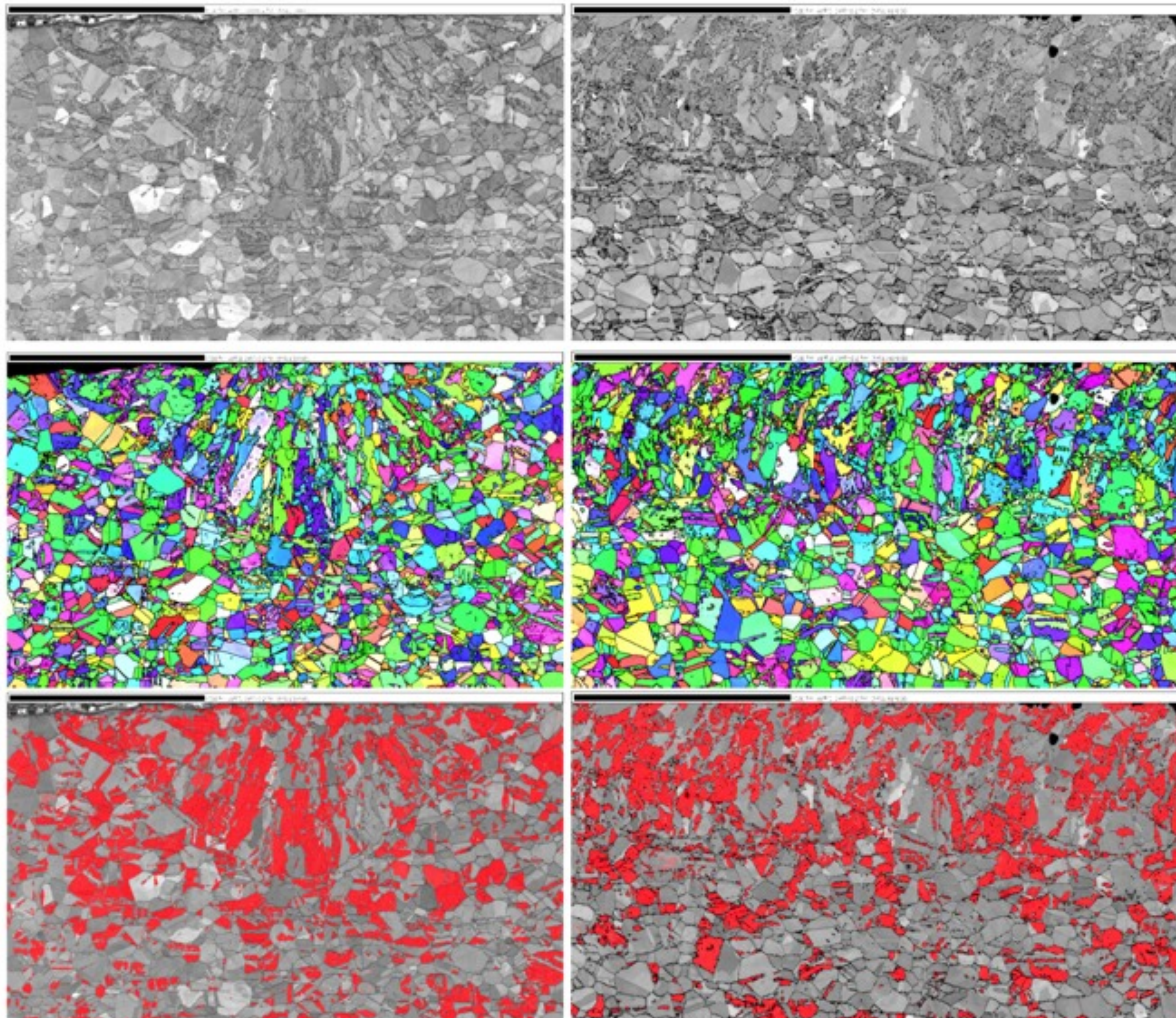
Weld microstructures are extremely complex

In pulsed welding solid liquid interface motion is not monotonic

This results in non-homogeneous interfaces, grain shapes, and and phase distributions

These distributions have not previously been quantified

Our long term goal is to quantify this variation and incorporate it into properties simulations



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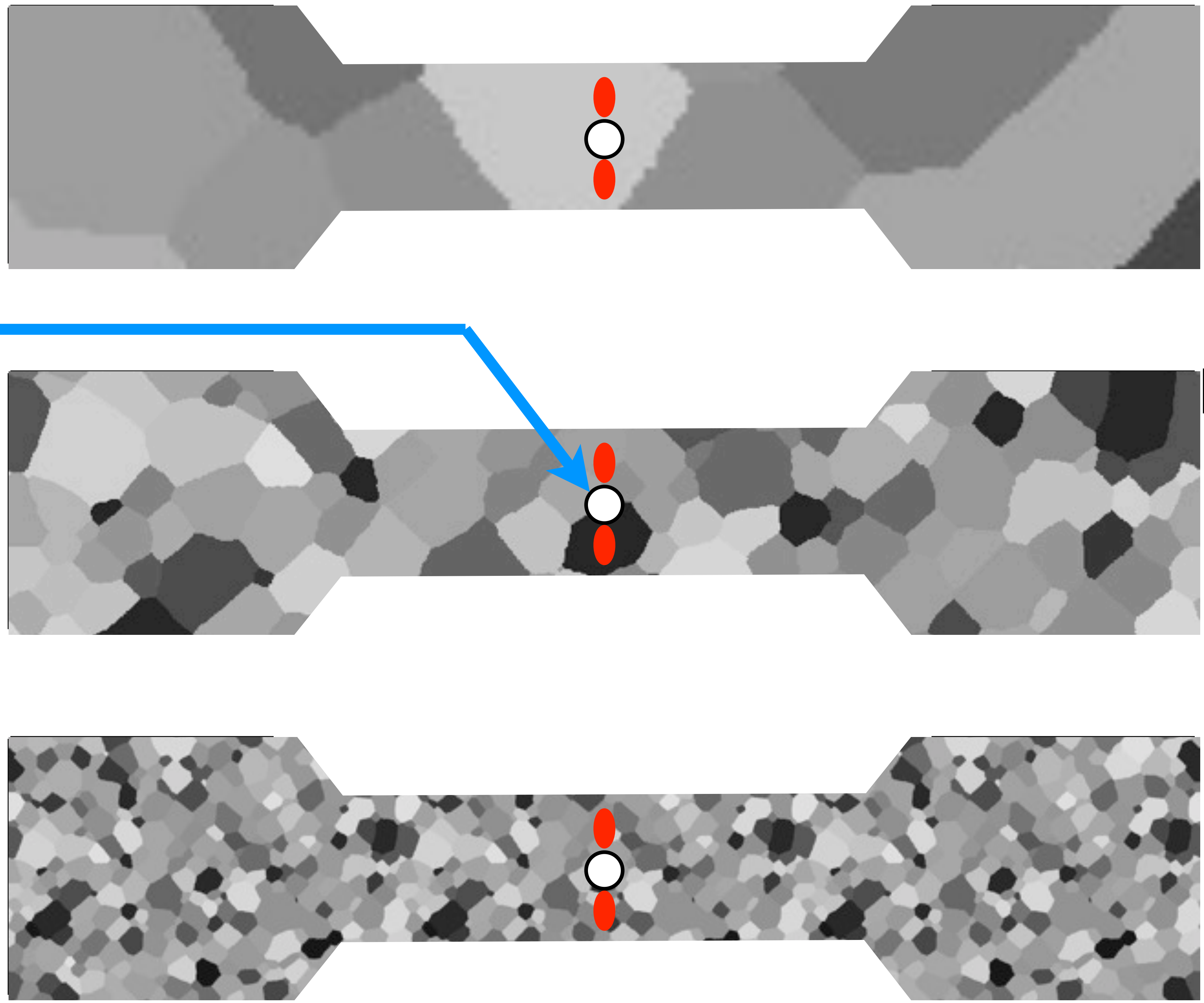
Punched Brass: Schematic of Tensile Samples

Localization of deformation near a small hole should interact directly with microstructure if the relevant scales are appropriate.

Hole ~100µm diameter, via femtosecond laser.



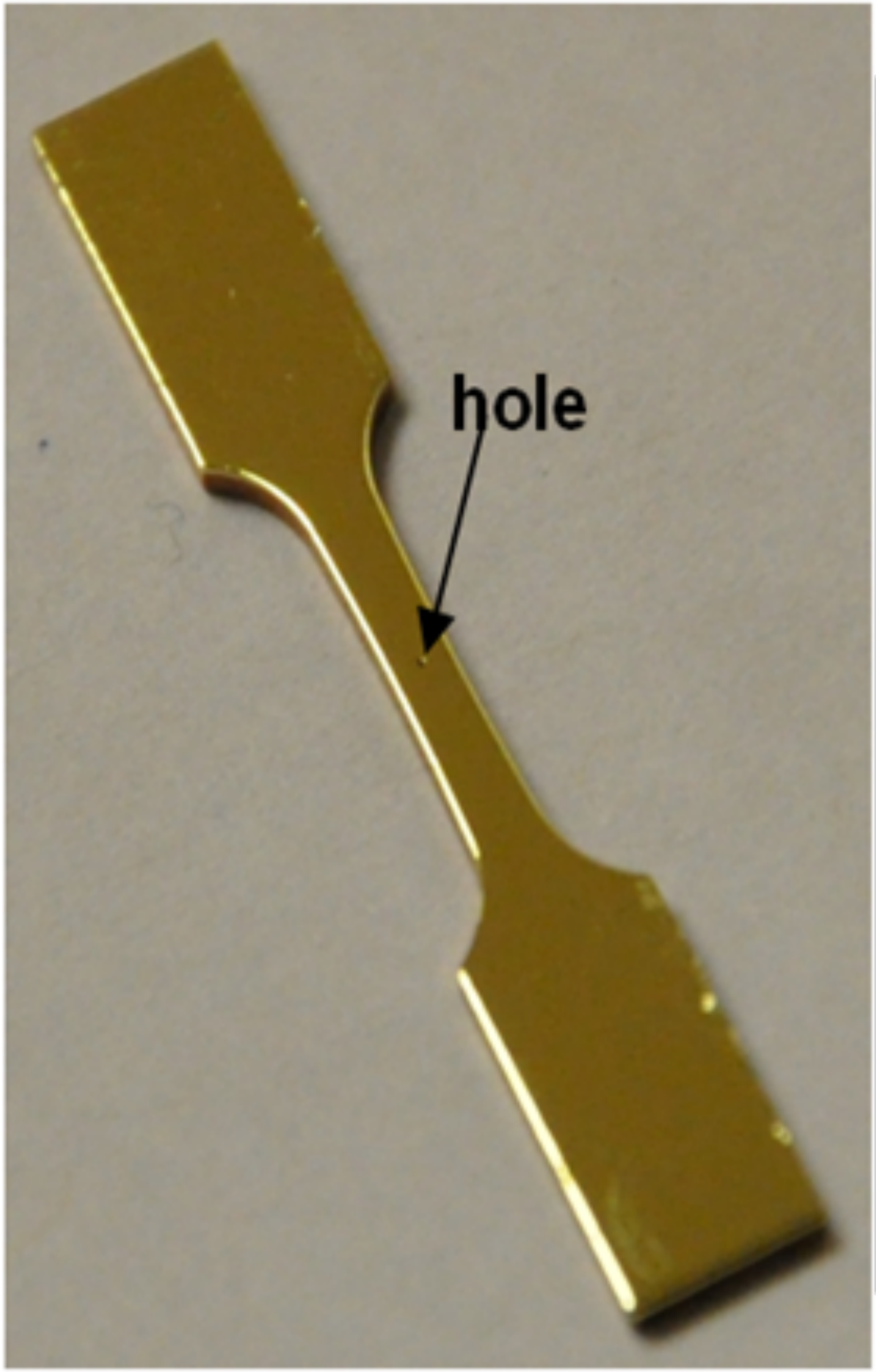
Coarse (R<1)
8 hr, 800 °C
725.2 µm
62.7 MPa

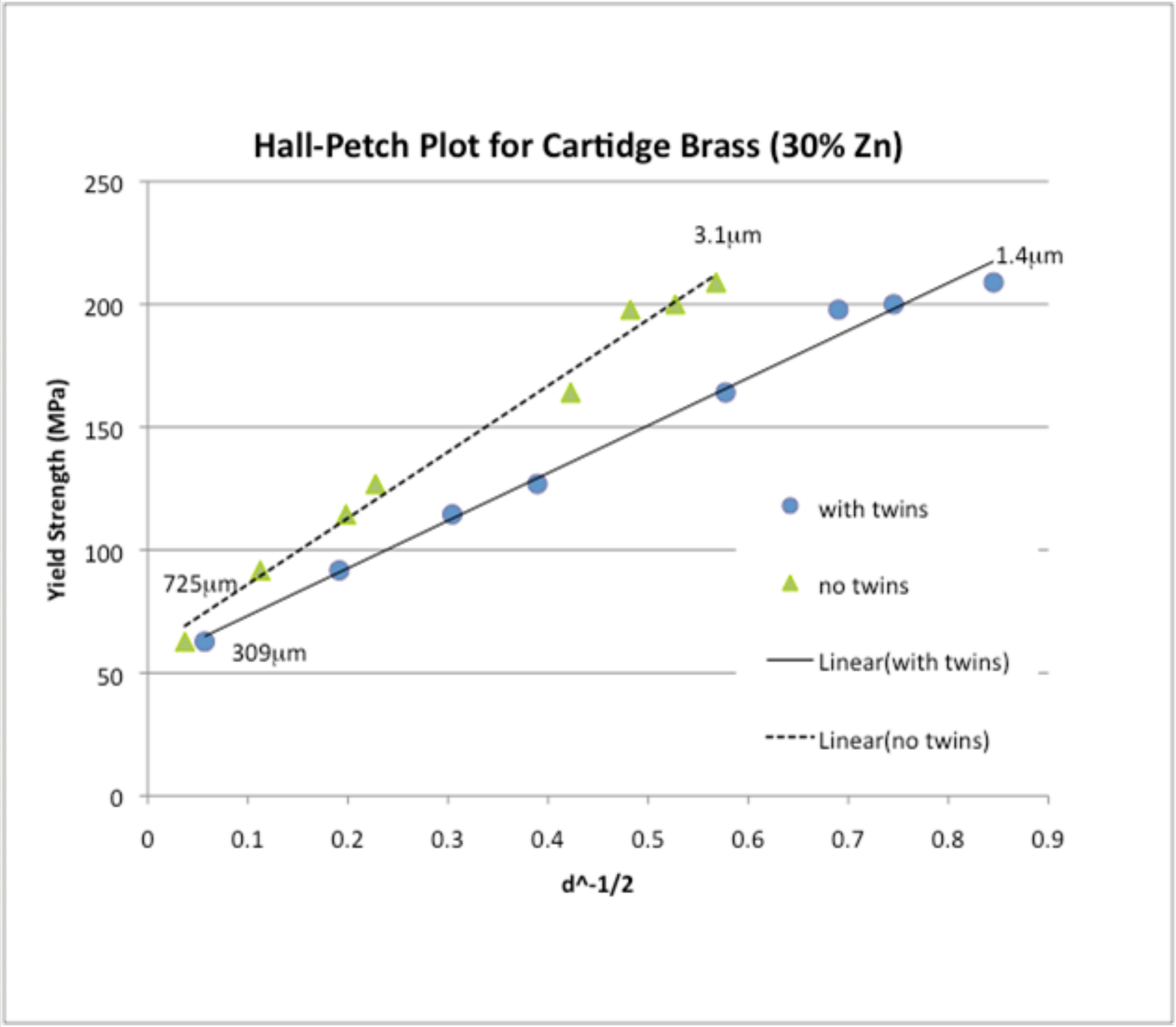
Medium (R=1)
8 hr, 600 °C
79.1 µm
91.7 MPa

Fine (R>1)
8hr 450°C
725.2µm
62.7MPa

R is the ratio of HOLE SIZE to GRAIN SIZE!

Punched Brass: Hall-Petch Behavior

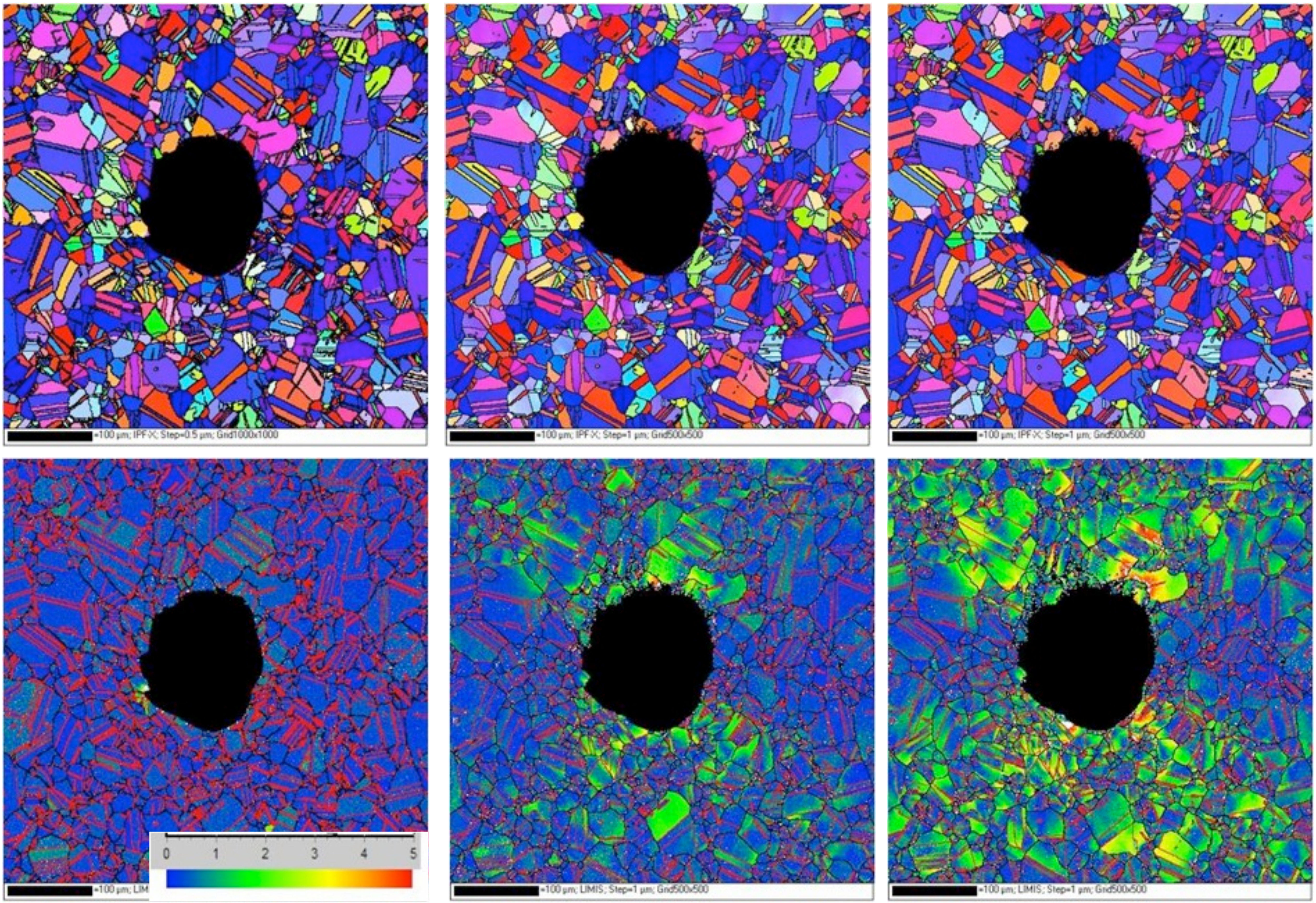




Punched Brass: EBSD, R=7

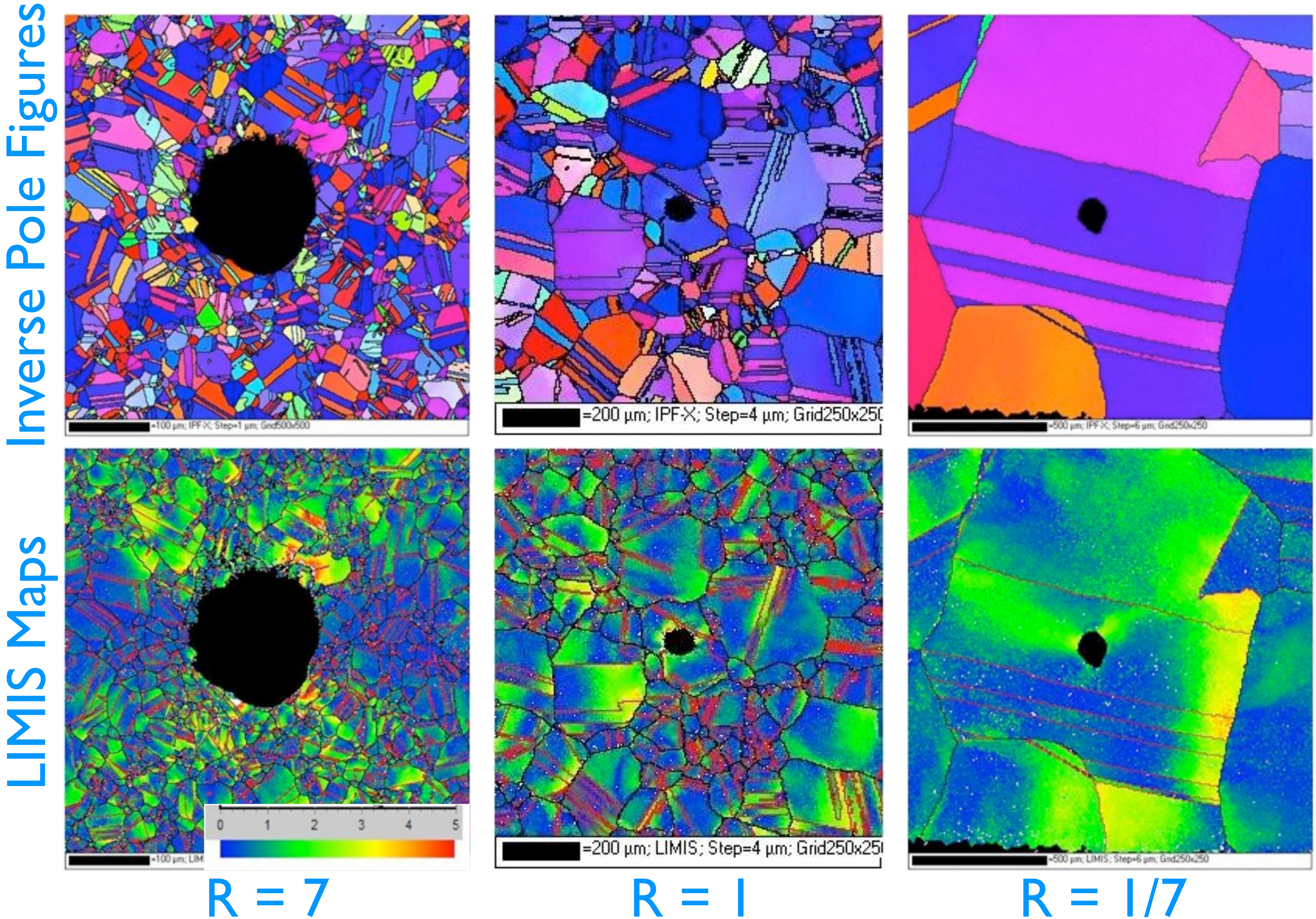
Inverse Pole Figures

LIMIS Maps



0% Strain | 1% Strain | 2% Strain

Punched Brass: EBSD, 2% Strain



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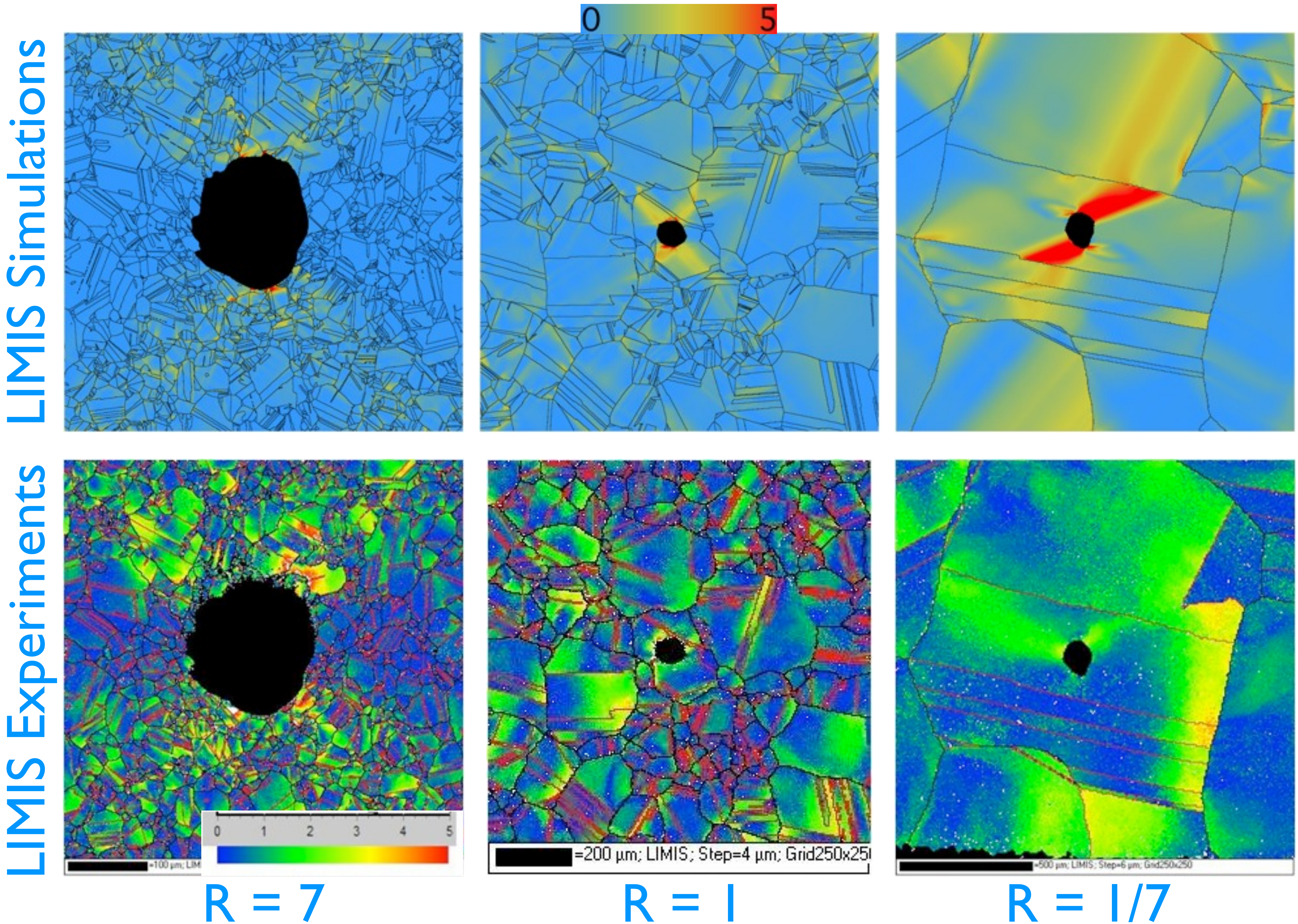
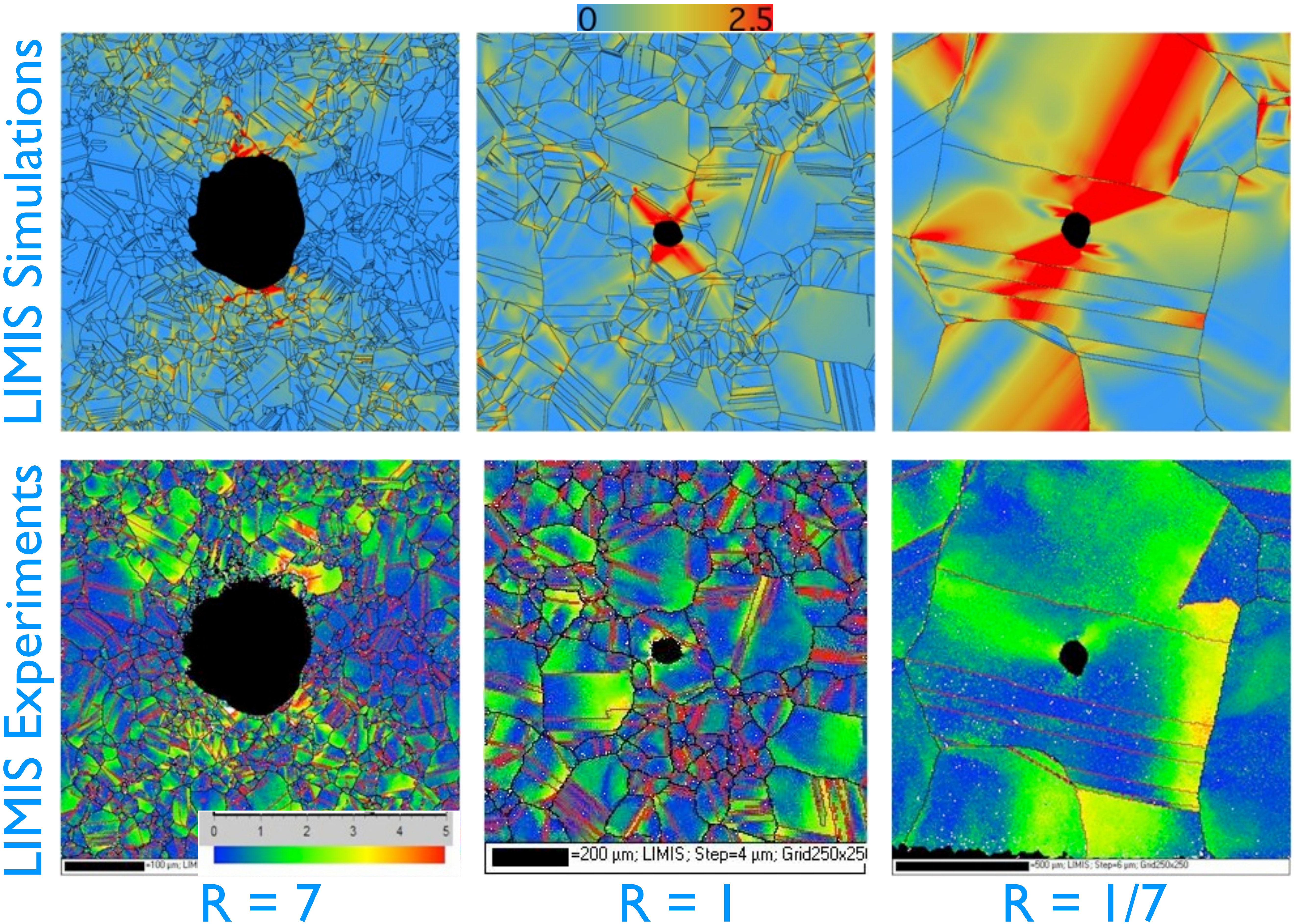
Punched Brass: Polycrystal Plasticity Simulations

- "Simple" polycrystal plasticity:
  - Anisotropic linear elasticity
  - Anisotropic power-law slip
  - Isotropic power-law hardening
- Parameters fit to tensile data from cartridge brass
- "2+1 D" geometries:
  - Plane strain boundary conditions in Z
  - Prescribed displacements in X
  - Free surfaces in Y (!)
- Approximately 100,000+ elements

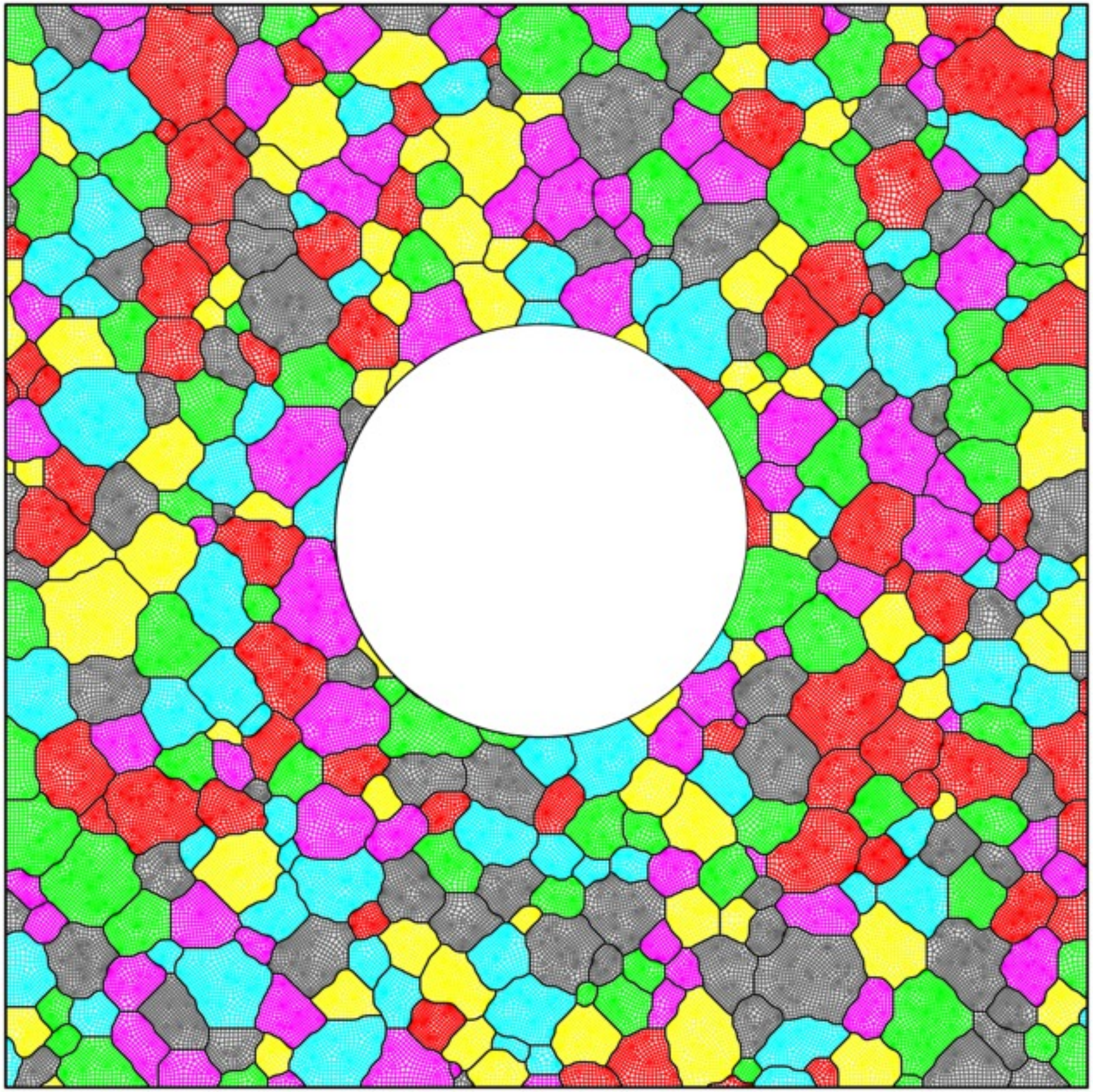
Punched Brass: Validation with Experiments



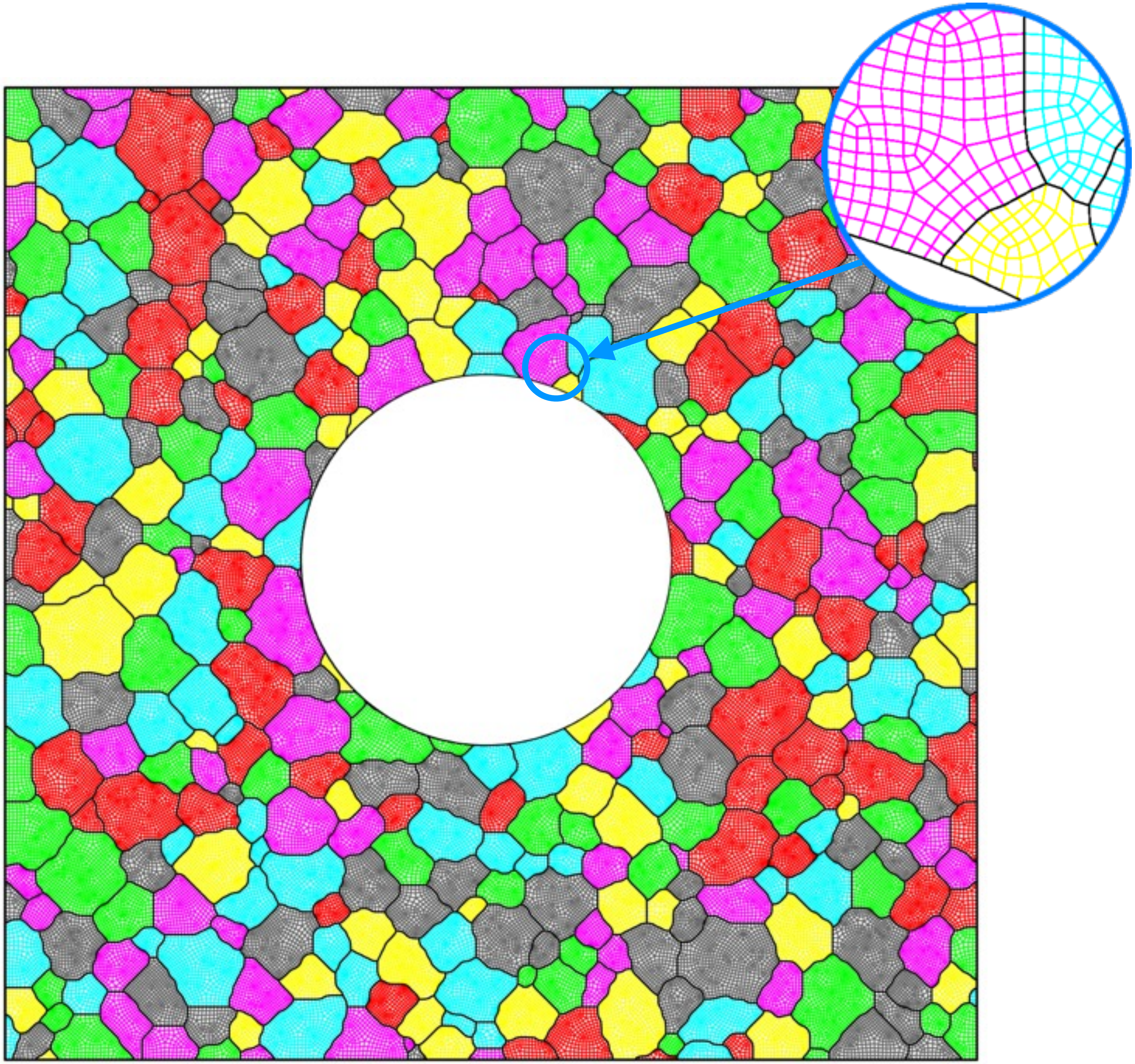
Punched Brass: Validation with Experiments



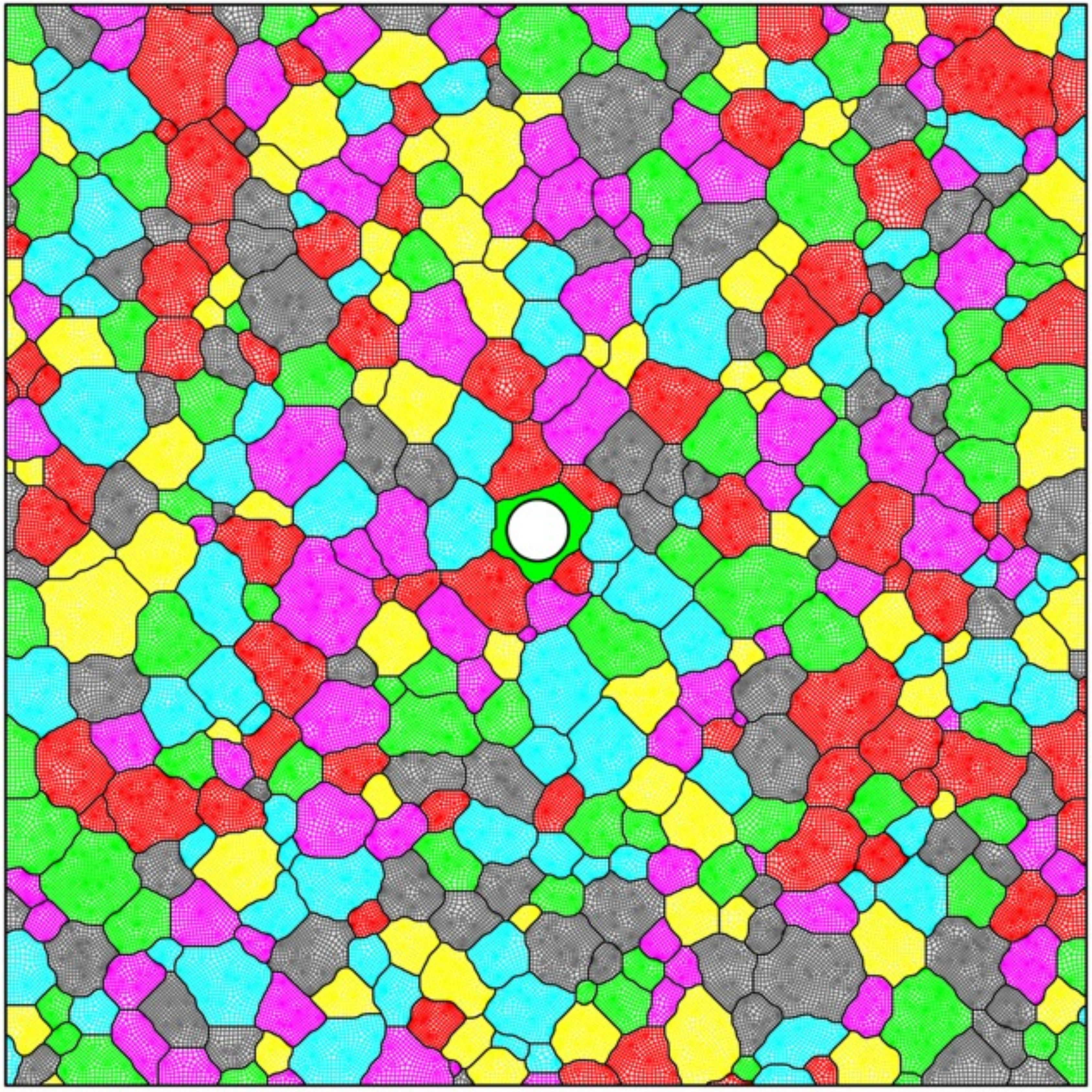
Punched Brass: Finite Element Mesh, R=7



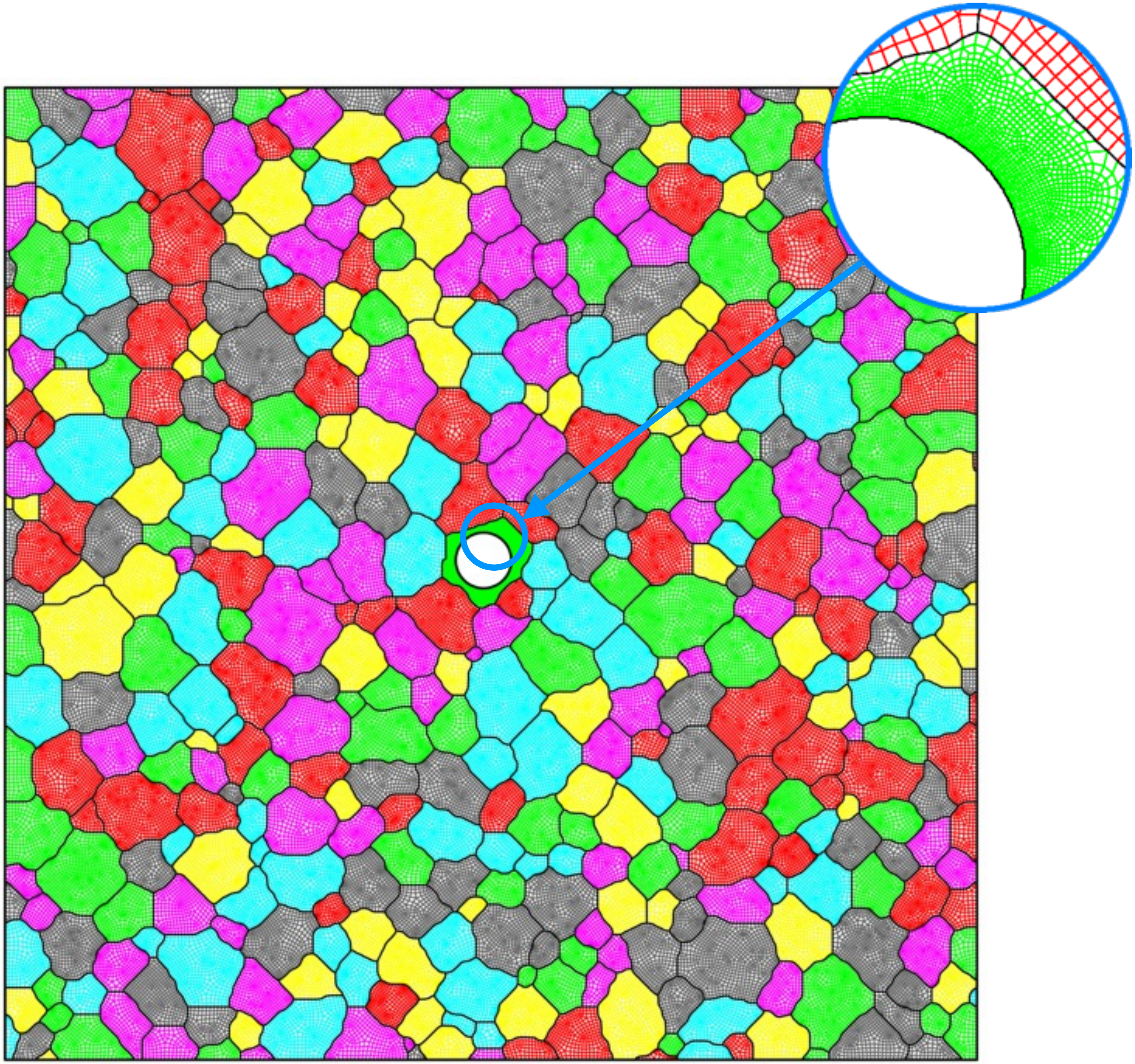
Punched Brass: Finite Element Mesh, R=7



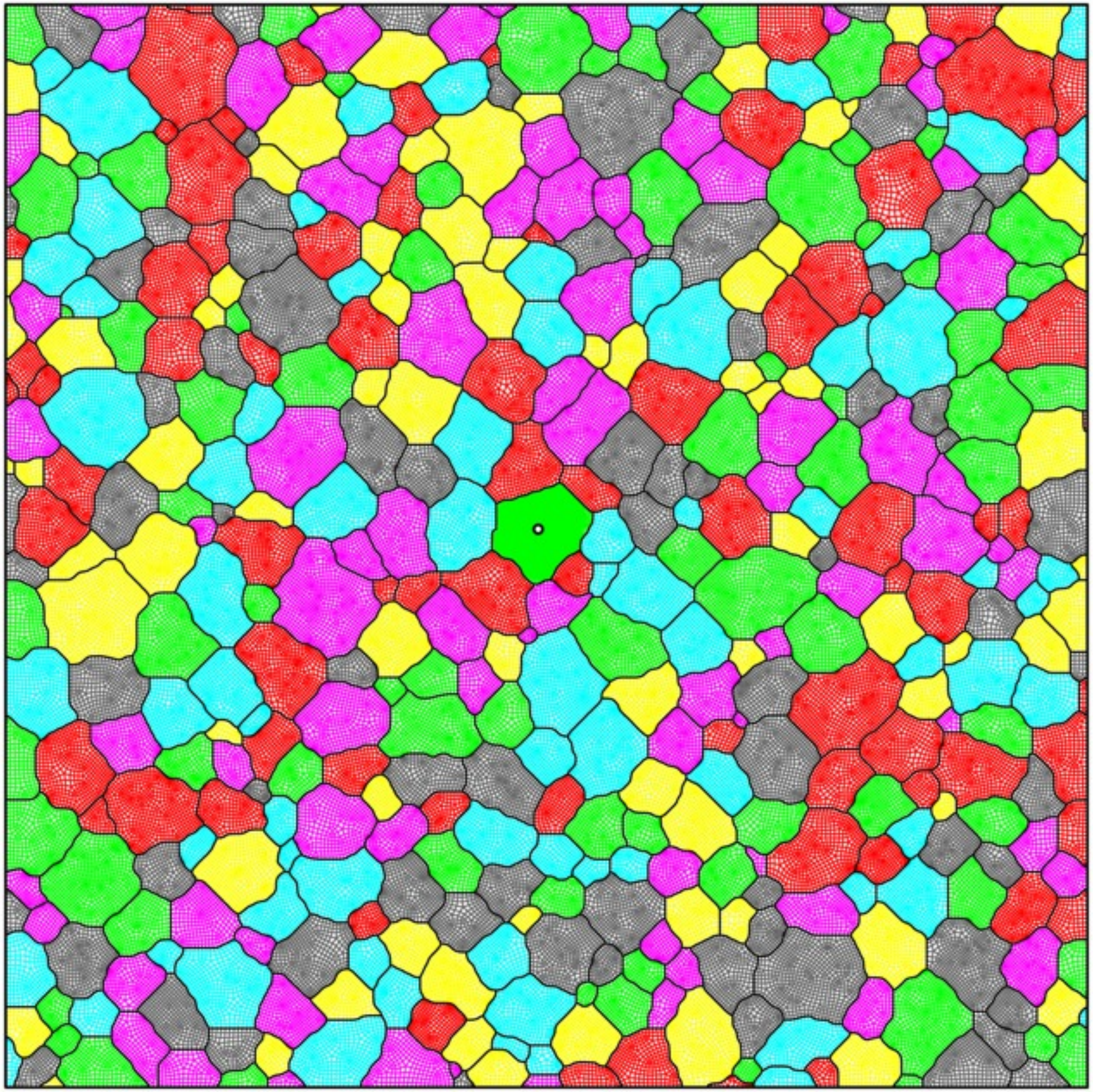
Punched Brass: Finite Element Mesh, R=1



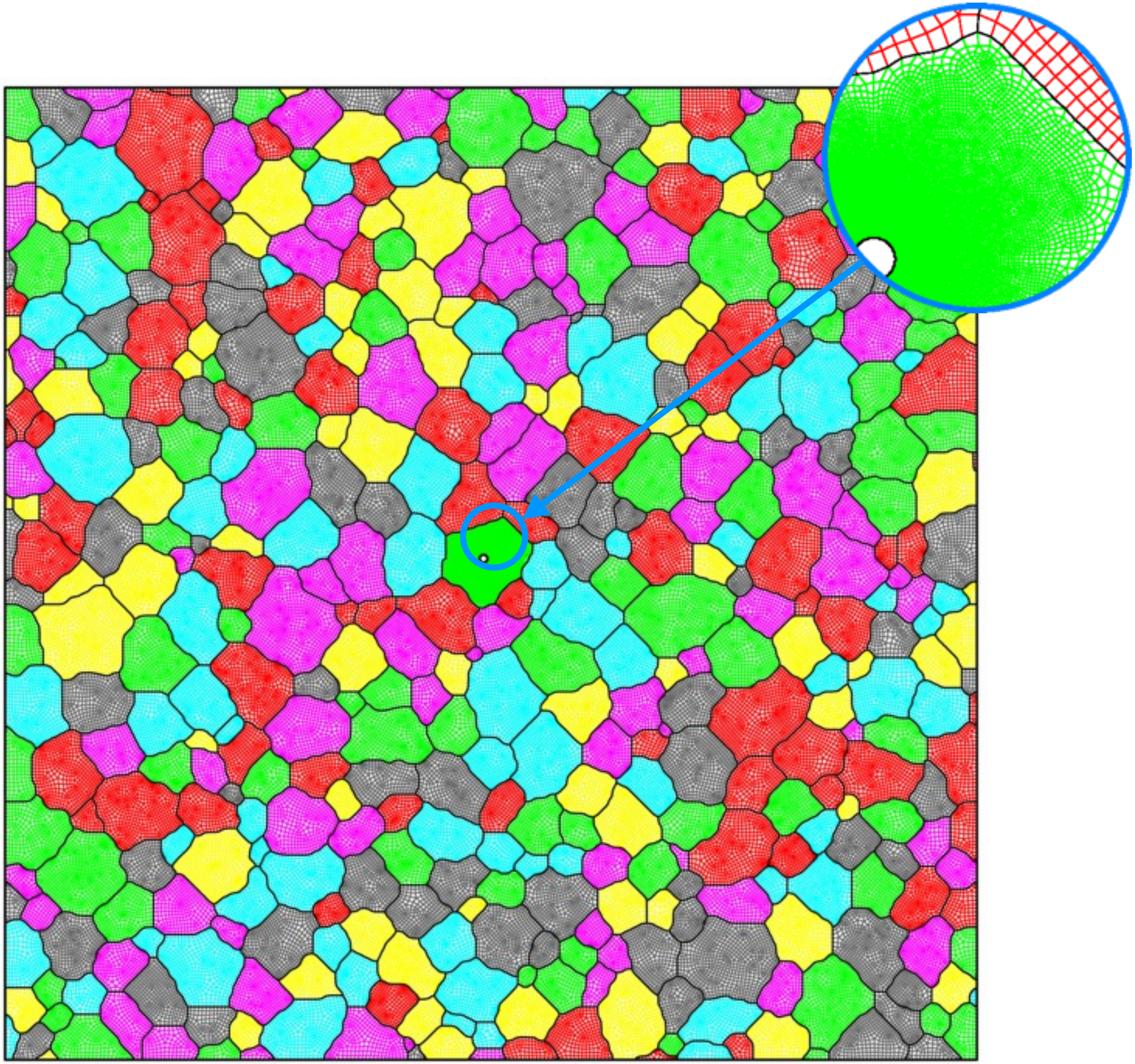
Punched Brass: Finite Element Mesh, R=1



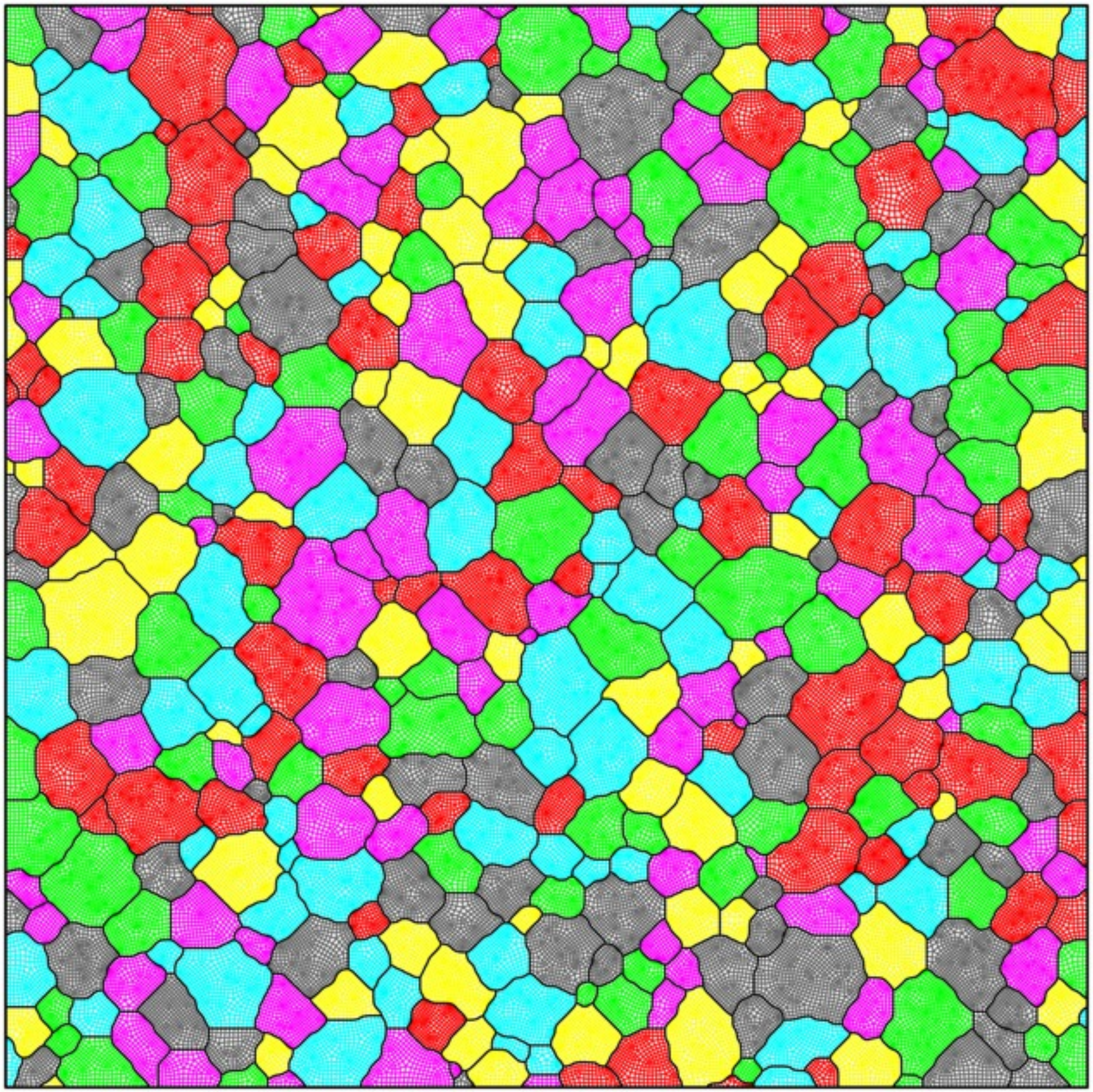
Punched Brass: Finite Element Mesh, R=1/7



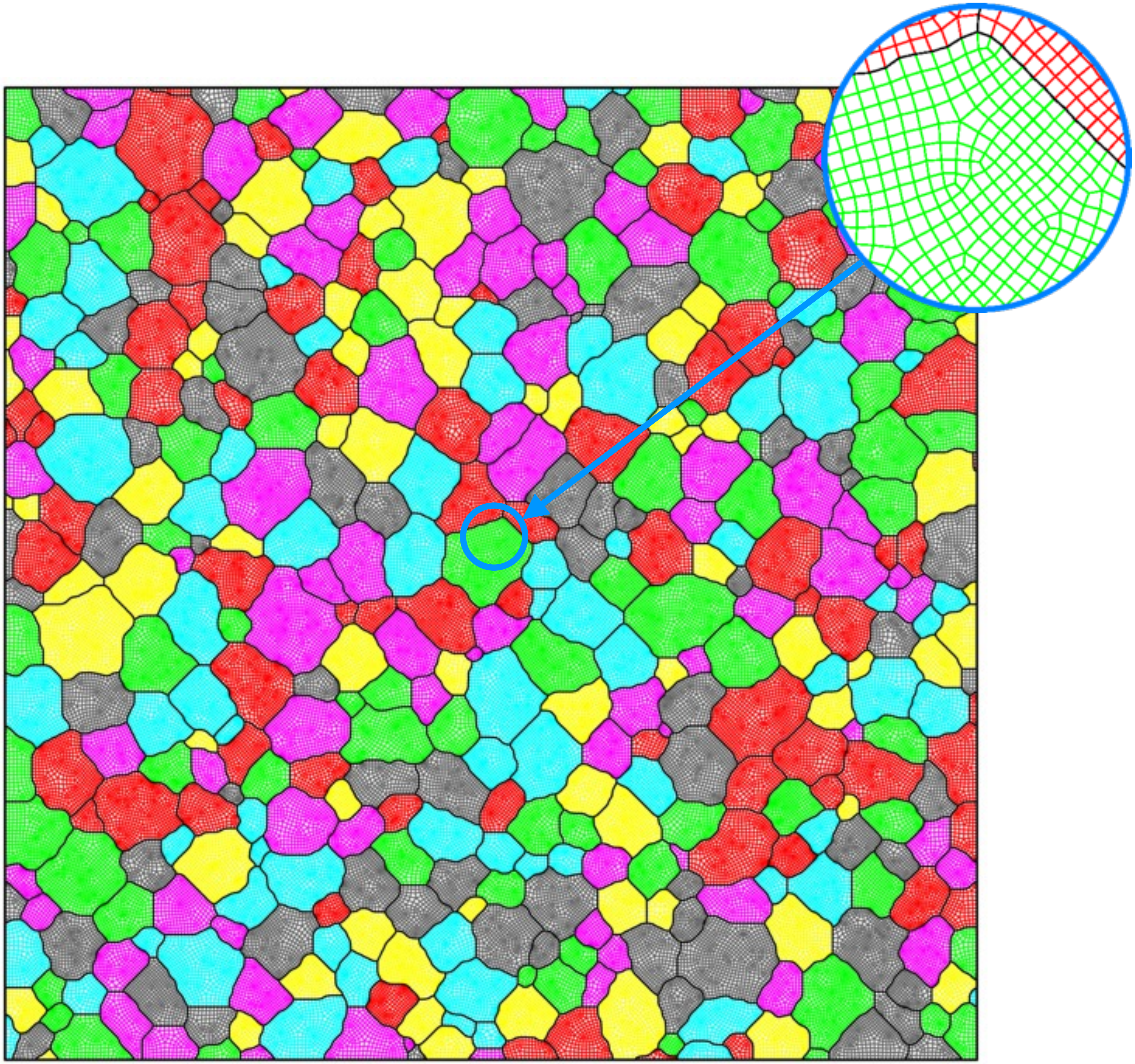
Punched Brass: Finite Element Mesh, R=1/7



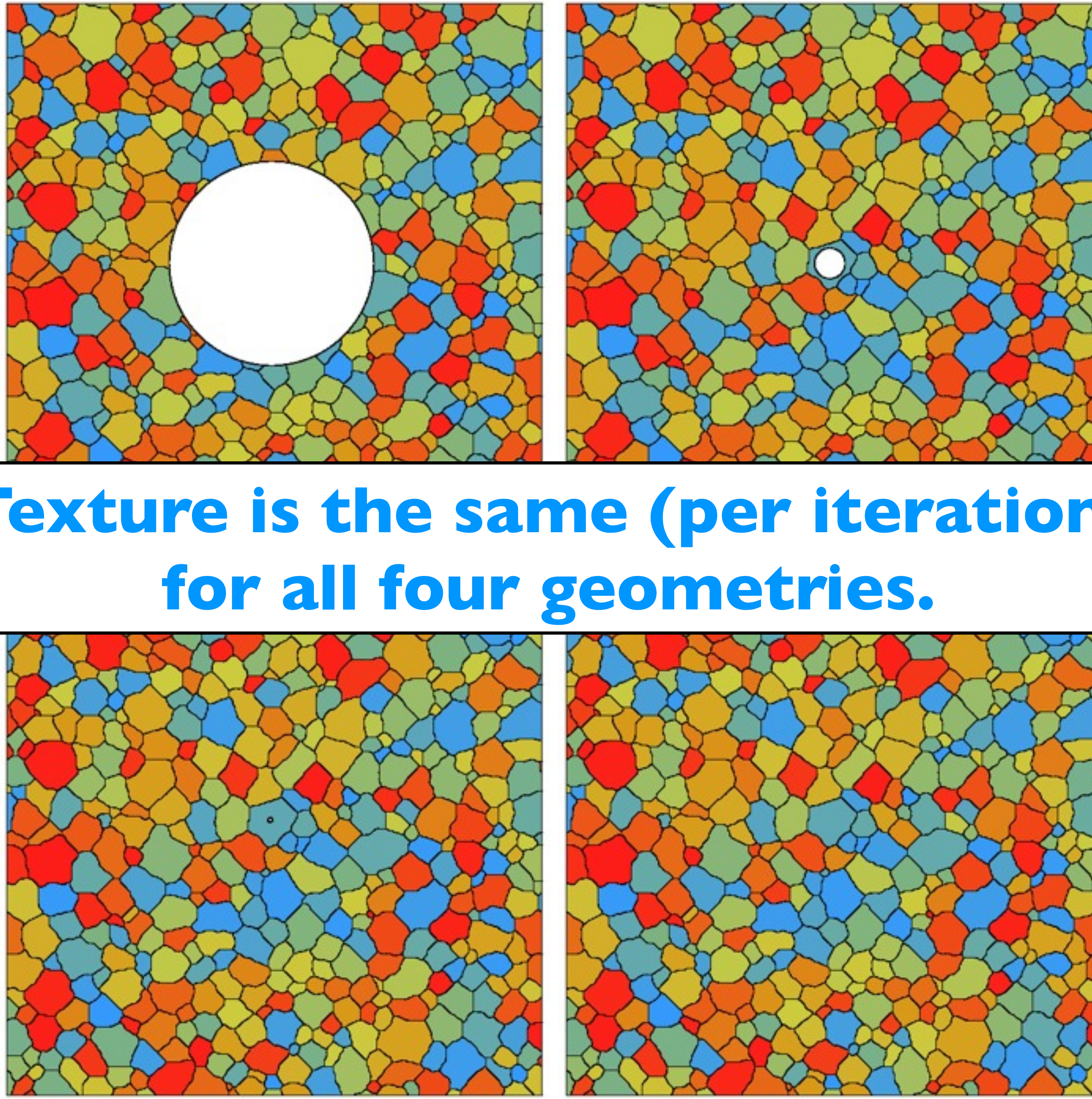
Punched Brass: Finite Element Mesh, R=0



Punched Brass: Finite Element Mesh, R=0

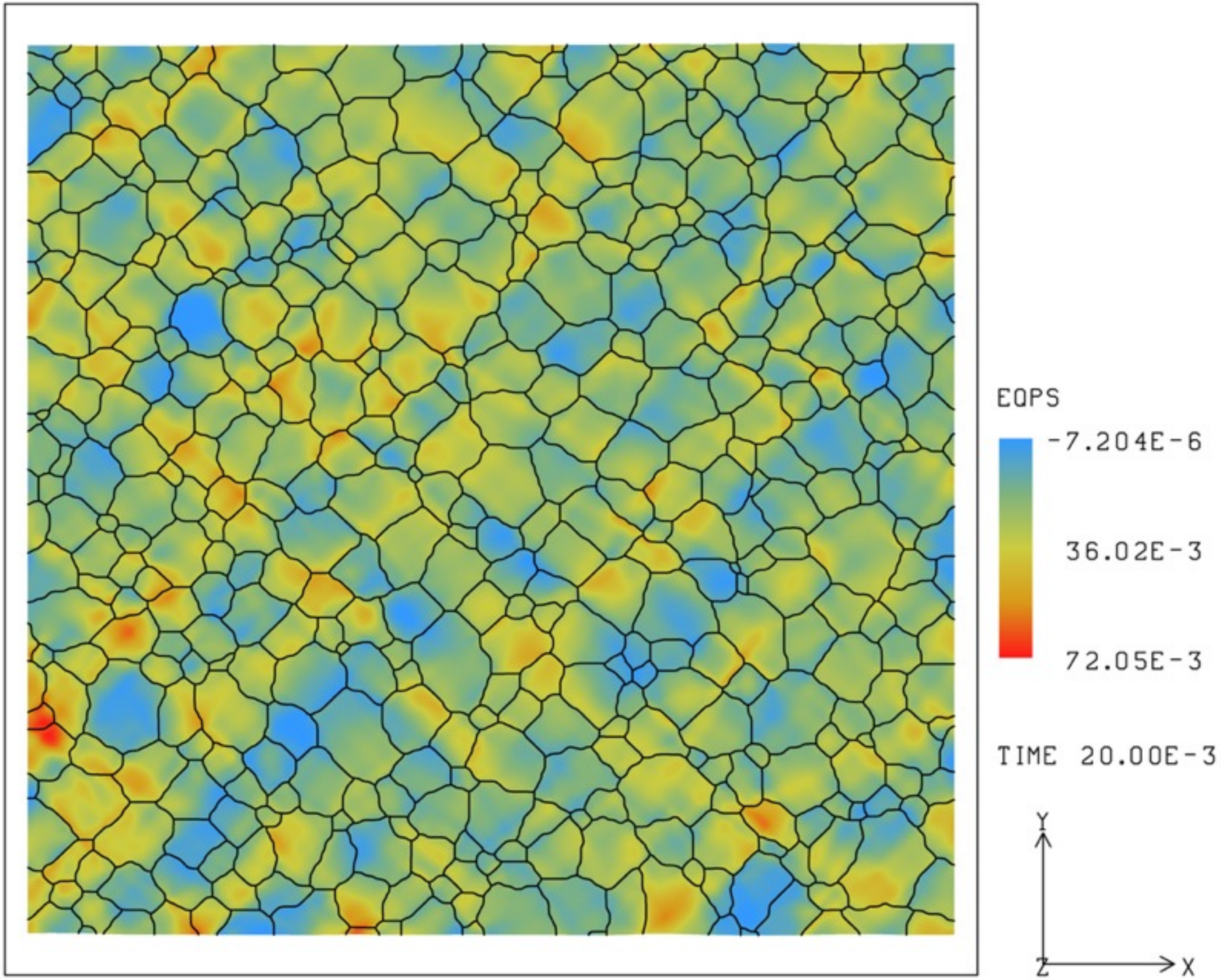


Punched Brass: Rotation Tensor Component, $\mathbf{T}_{11}$

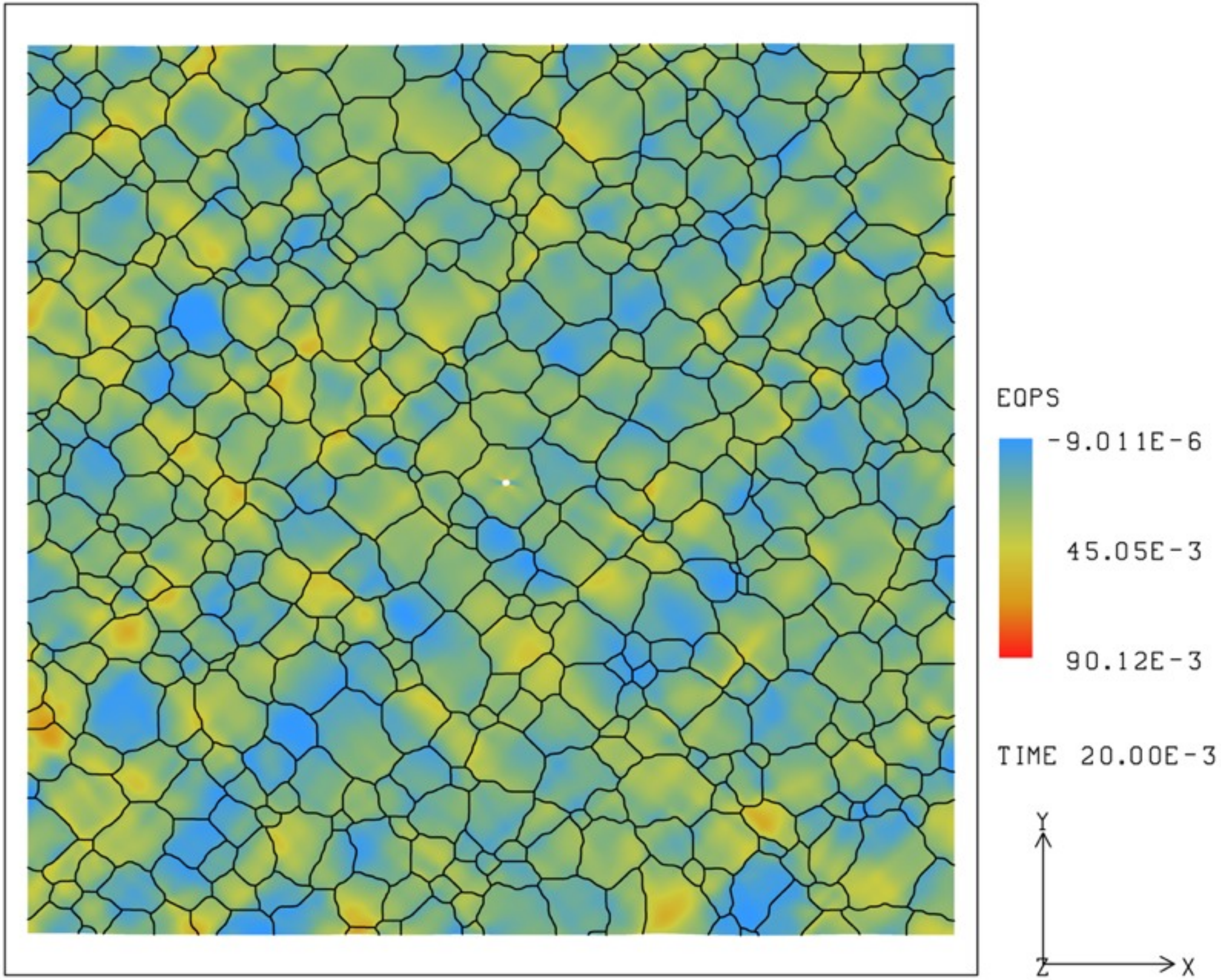


Texture is the same (per iteration) for all four geometries.

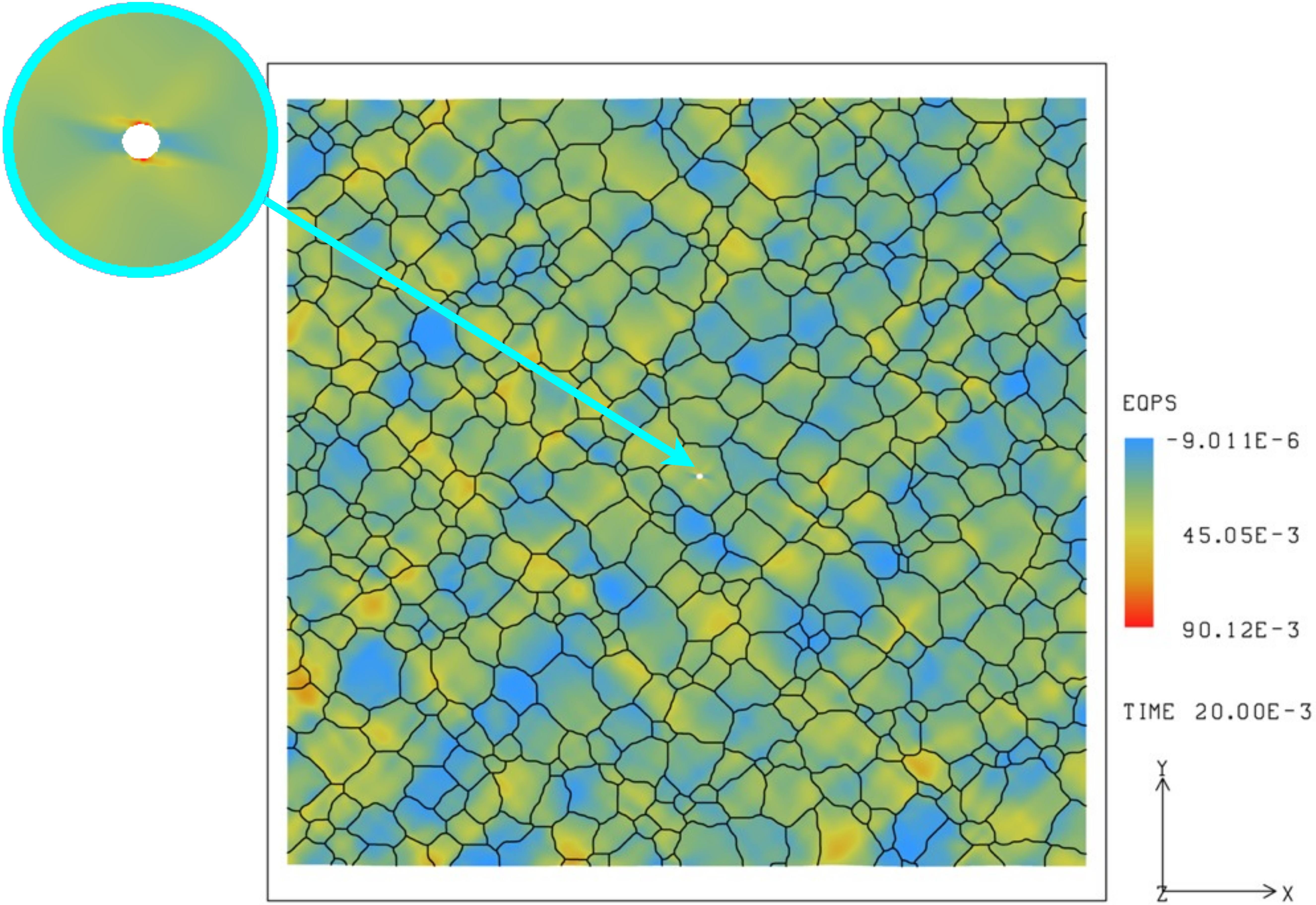
Punched Brass: Plastic Strain Map, R=0



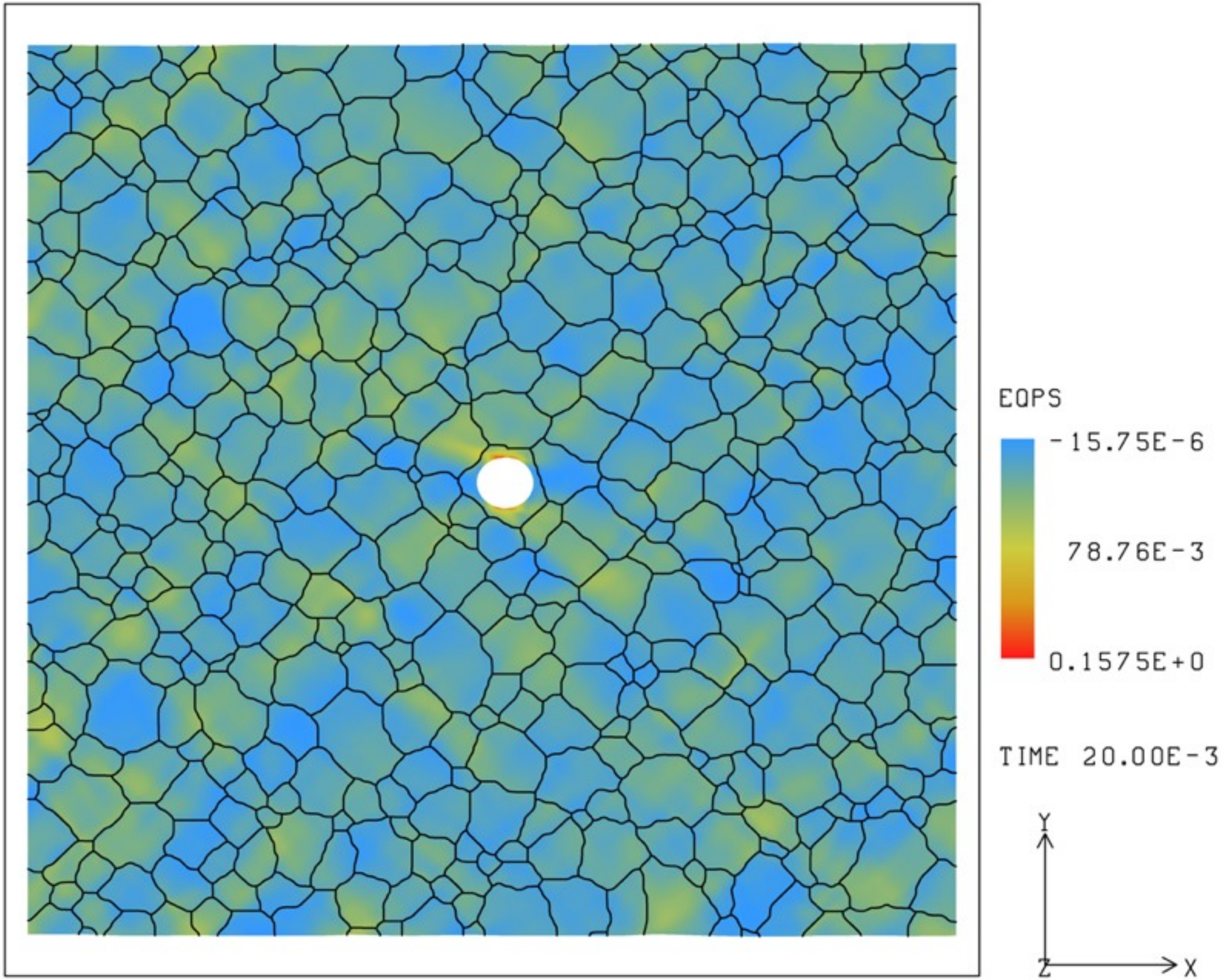
Punched Brass: Plastic Strain Map, R=1/7



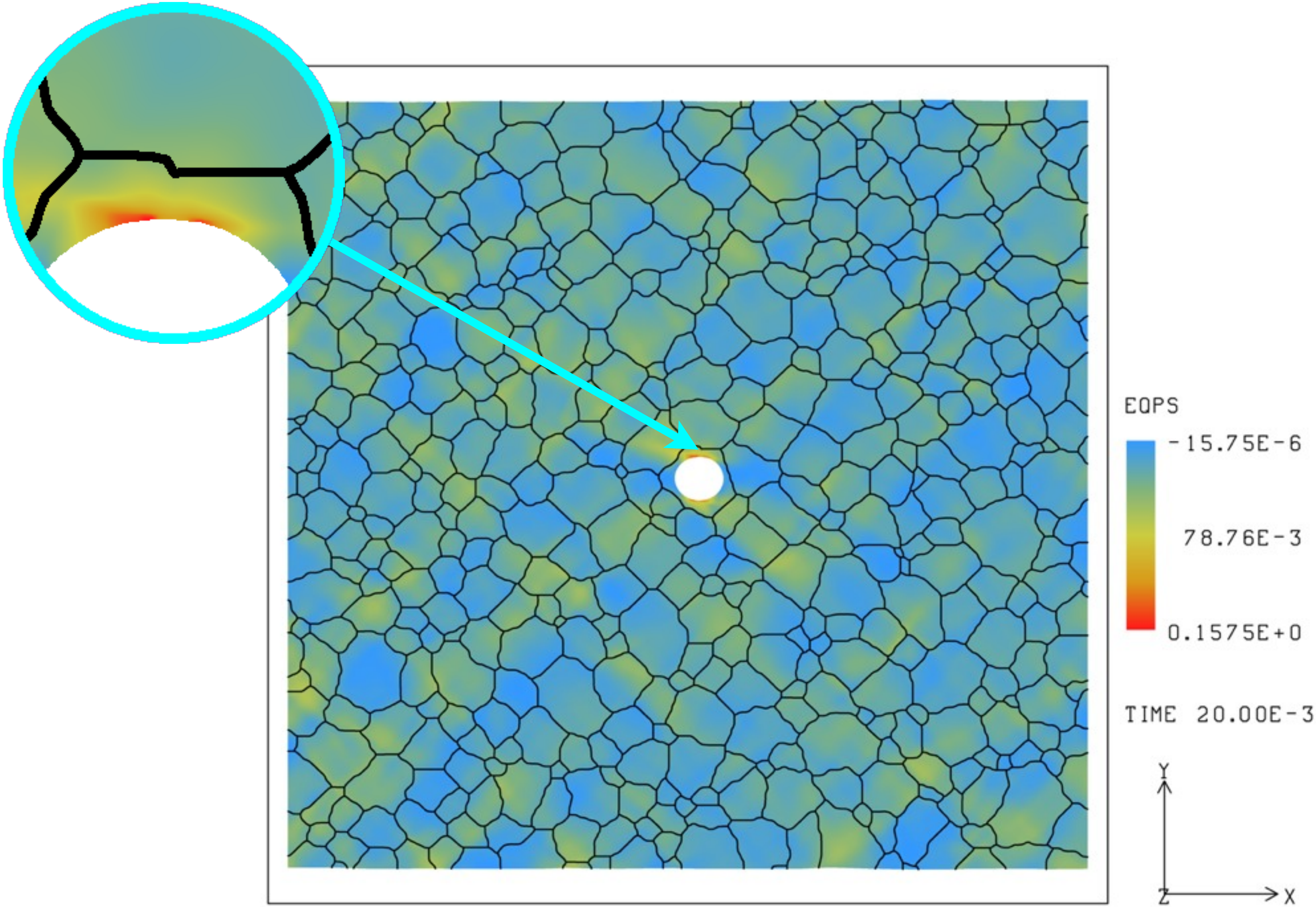
Punched Brass: Plastic Strain Map, R=1/7



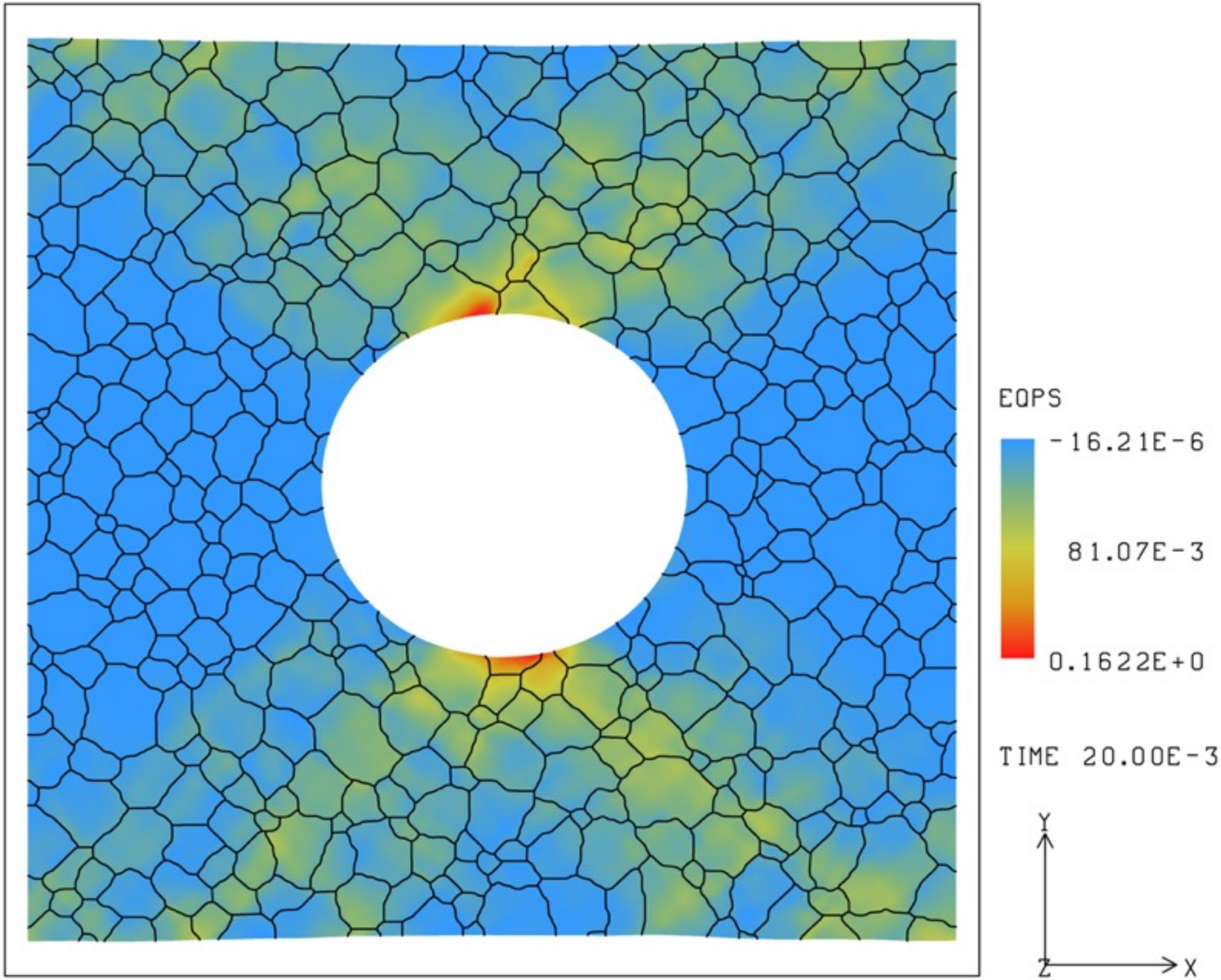
Punched Brass: Plastic Strain Map, R=1



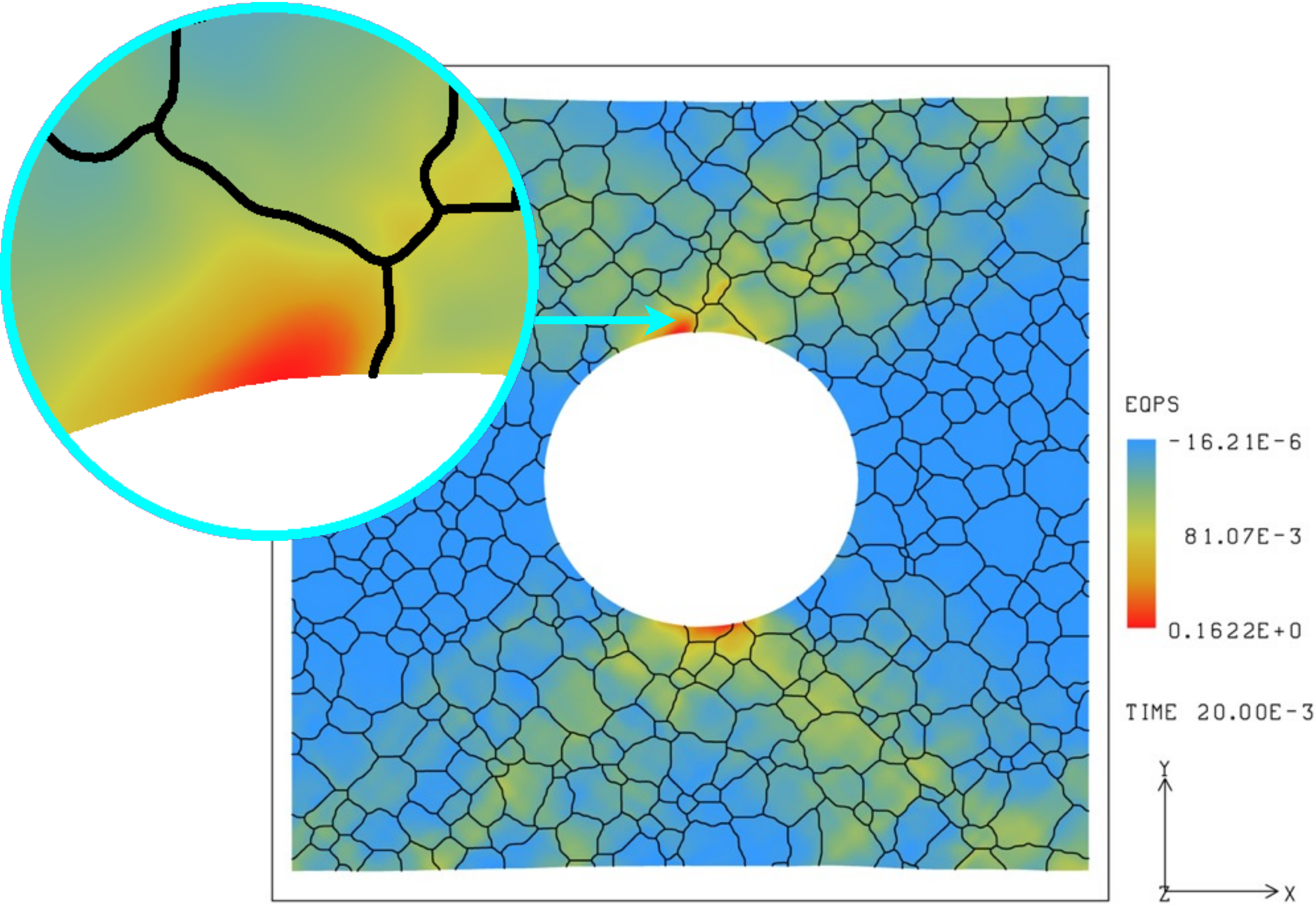
Punched Brass: Plastic Strain Map, R=1



Punched Brass: Plastic Strain Map, R=7



Punched Brass: Plastic Strain Map, R=7

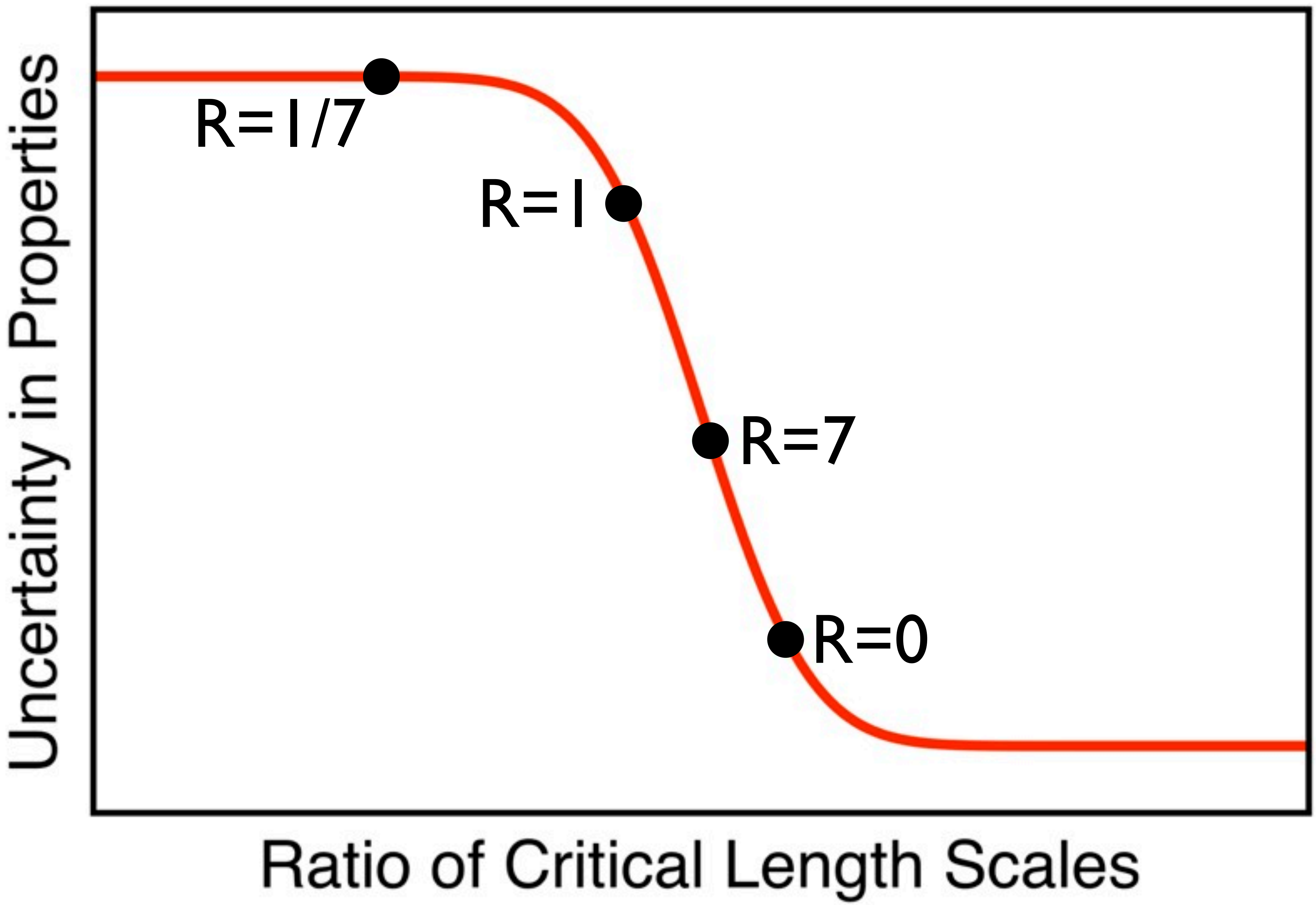


Punched Brass: Maximum Local Plastic Strain Statistics

	R=0	**R=7**	**R=1**	**R=1/7**
N	45	45	45	45
μ	0.0785	0.1601	0.1694	0.1337
σ	0.0075	0.0230	0.0392	0.0423
σ/μ	10%	14%	23%	**32%**

(2% Applied Strain)

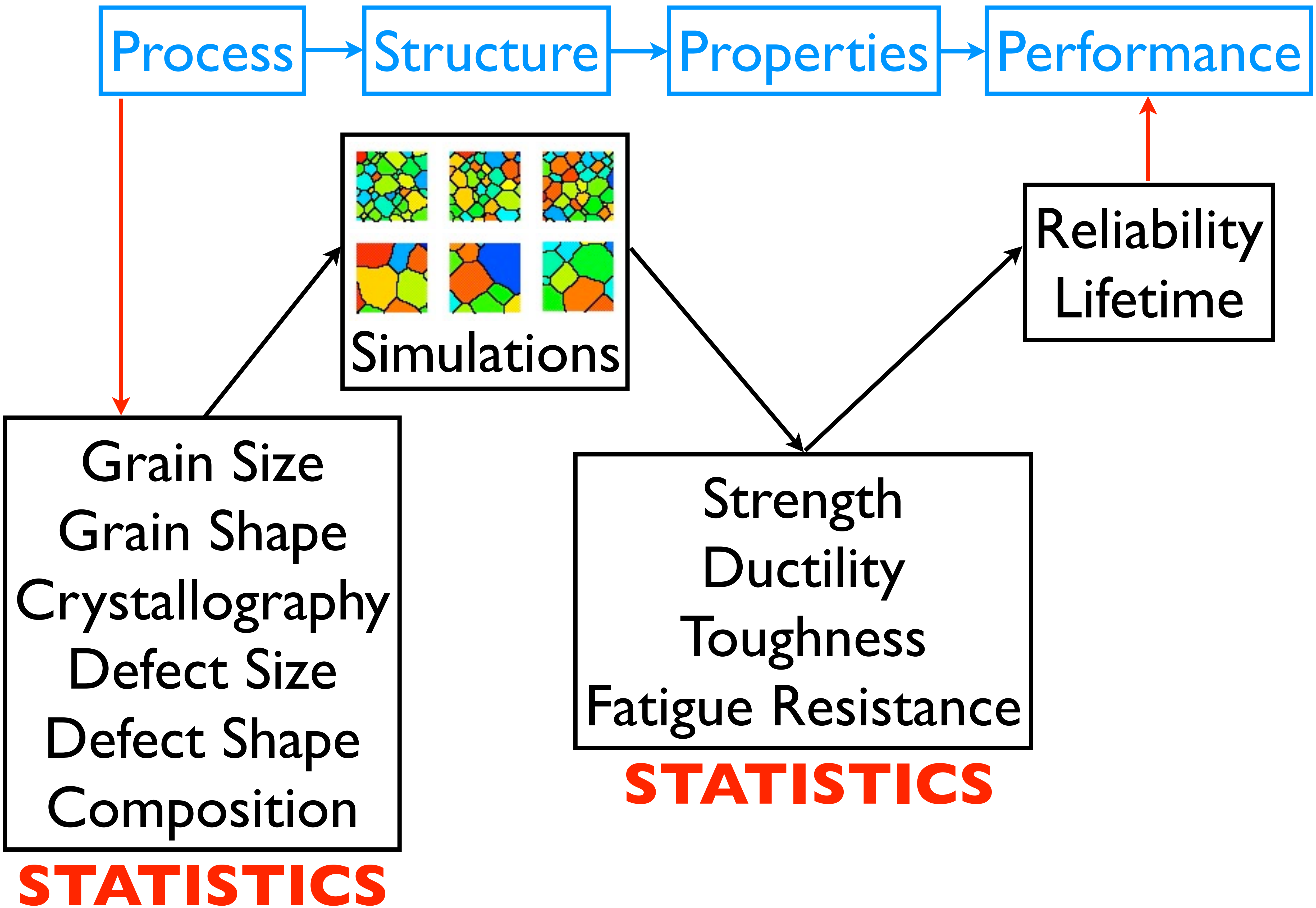
Punched Brass: Peak Plastic Strain Statistics



Outline

- **Introduction**
- **Strength and Ductility of 304L Welds**
  - Experiments
  - Simulations
- **Deformation near Holes in Brass**
  - Simulations
  - Experiments
- **Summary**

Summary: Variability Impacts All Levels of PSPP



Conclusions

- Most materials are inhomogeneous.

- Micro-structural and micro-geometry variability affects properties.

- Statistics are often required to accurately describe process-structure-properties-performance relationships.

- Computer simulation can be used to explore these large, statistical phase spaces.