Then and Now: Early Career Research Program (ECRP) Award Recipient in Solidification Science

Amy J. Clarke[1,2]

[1]Scientist 5, Sigma Manufacturing Science Division, Los Alamos National Laboratory
[2]Faculty Joint Appointment, Department of Metallurgical and Materials Engineering, Colorado School of Mines

Presentation to the Basic Energy Sciences Advisory Committee (BESAC)
September 25, 2024

In-situ Visualization and Modeling of Microstructure Evolution in Metallic Alloys under Additive Manufacturing Conditions
In-situ Visualization of Microstructure Evolution in Metallic Alloys under Additive Manufacturing Conditions
In-situ Monitoring of Dynamic Phenomena during Solidification, U.S. DOE Office of Science ECRP Award

U.S. DOE Office of Science, Synthesis and Processing Science

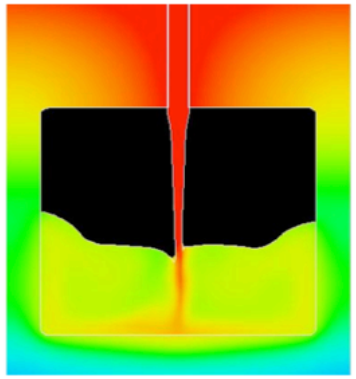
Los Alamos NATIONAL LABORATORY

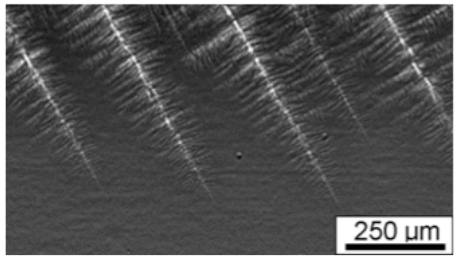
COLORADO SCHOOL OF MINES @150 | 1874-2024

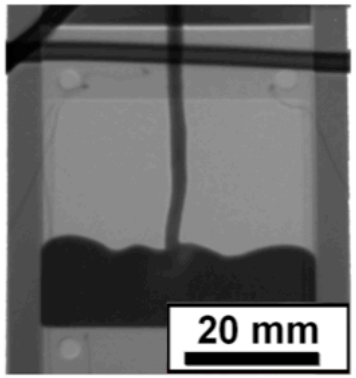
U.S. DEPARTMENT OF ENERGY | Office of Science

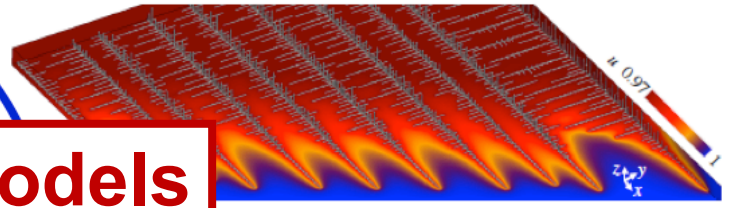
National Nuclear Security Administration

Multiscale Prediction and Control of Metallic Alloy Solidification Dynamics









Model Predictions

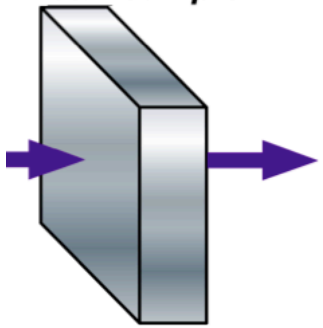
Experiments ↔ Models

In-situ Characterization

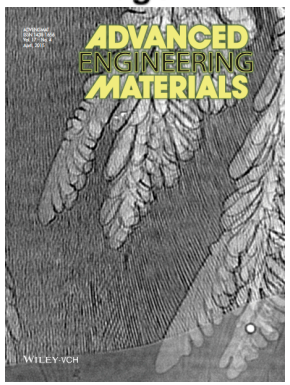
Controlled Processing

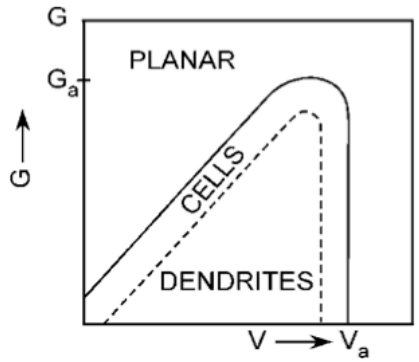
Metal Sample

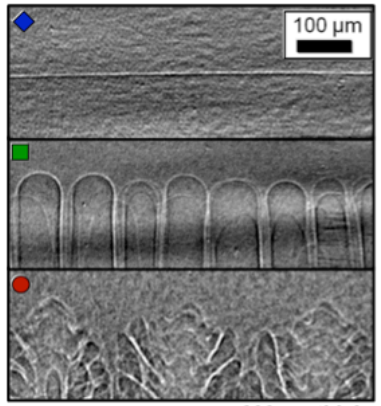
X-rays
Protons
Electrons



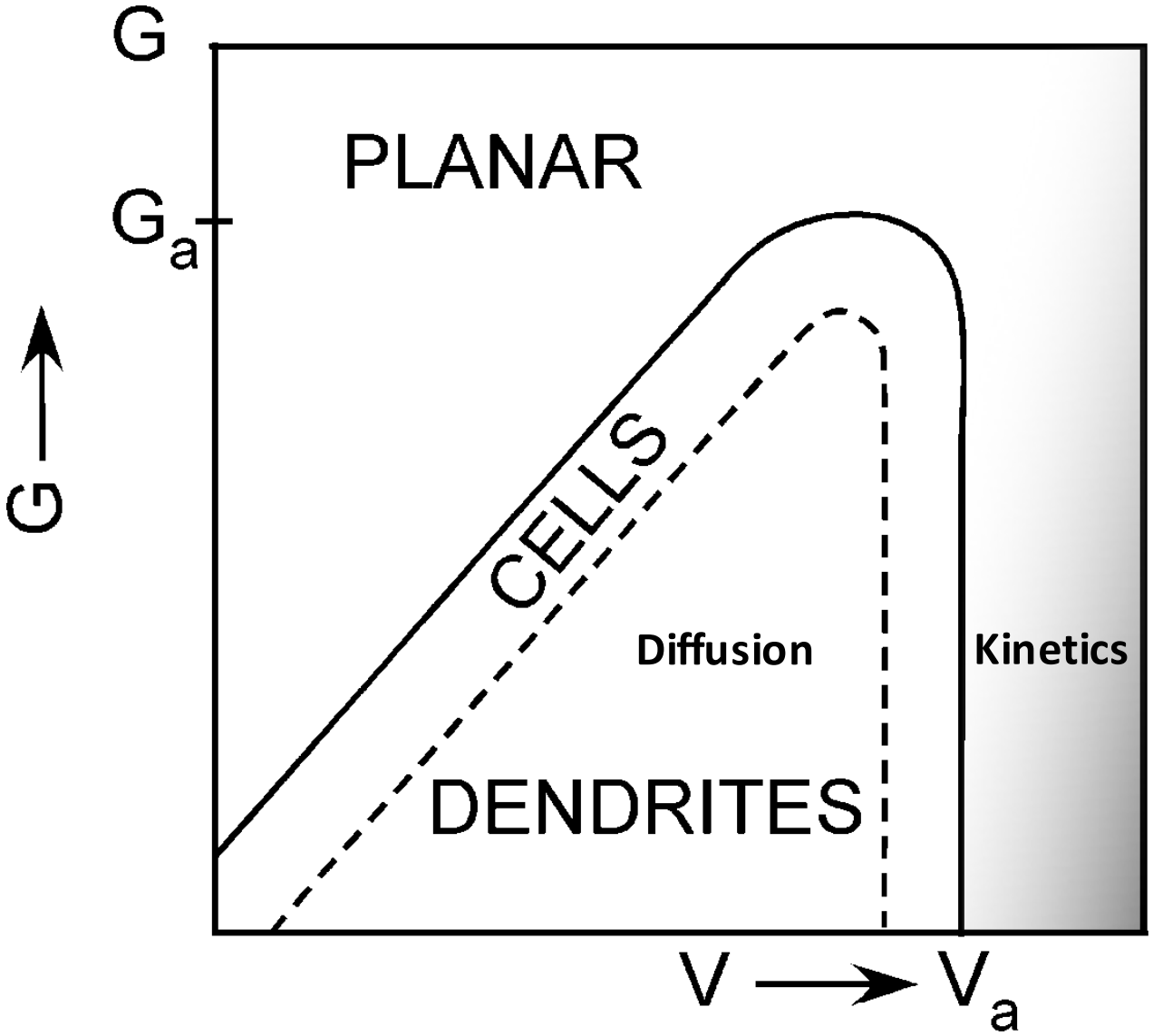
Image



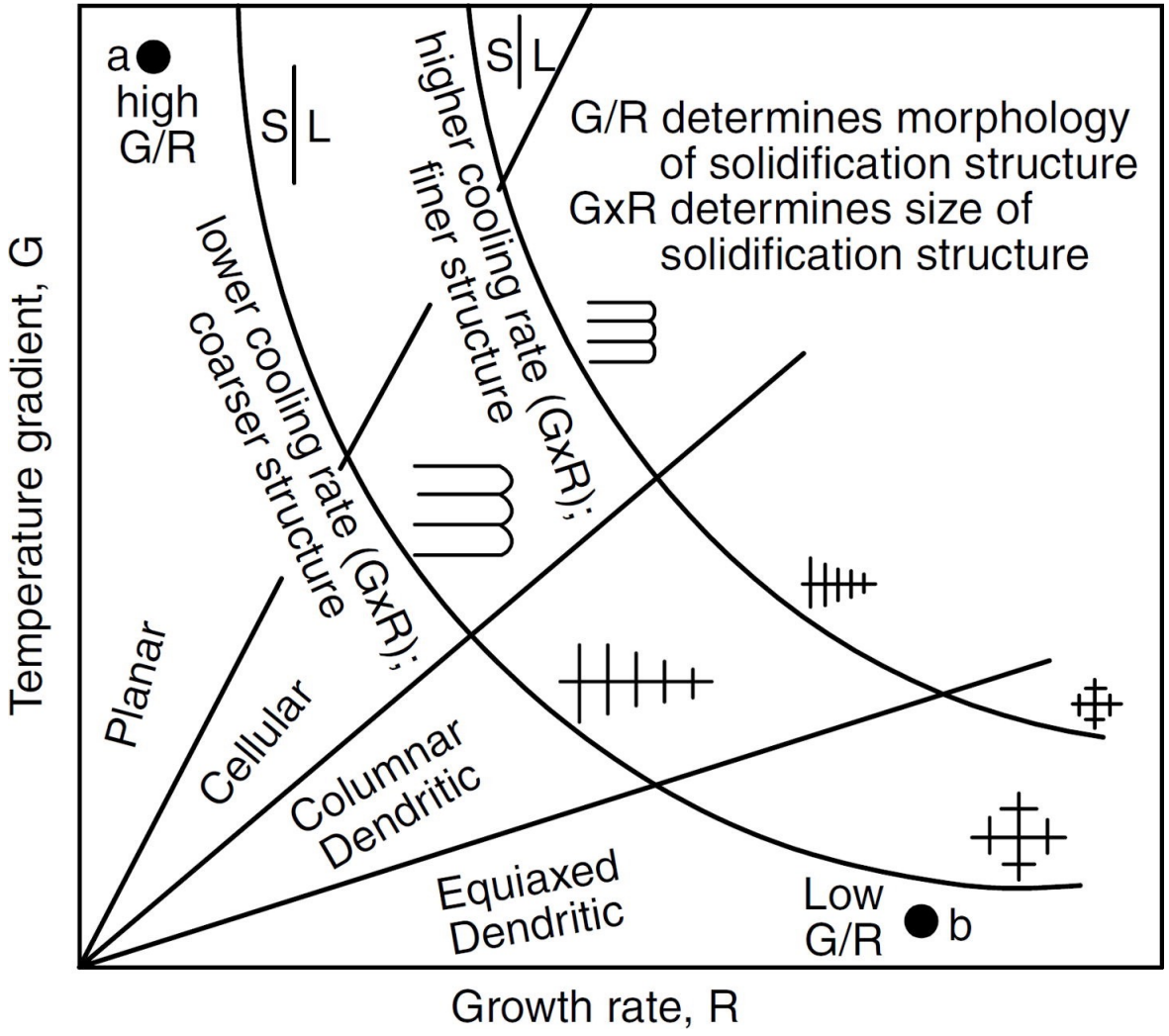




Thermal Gradient (G) and Interface Velocity (V) or Growth Rate (R) Control Microstructure Development

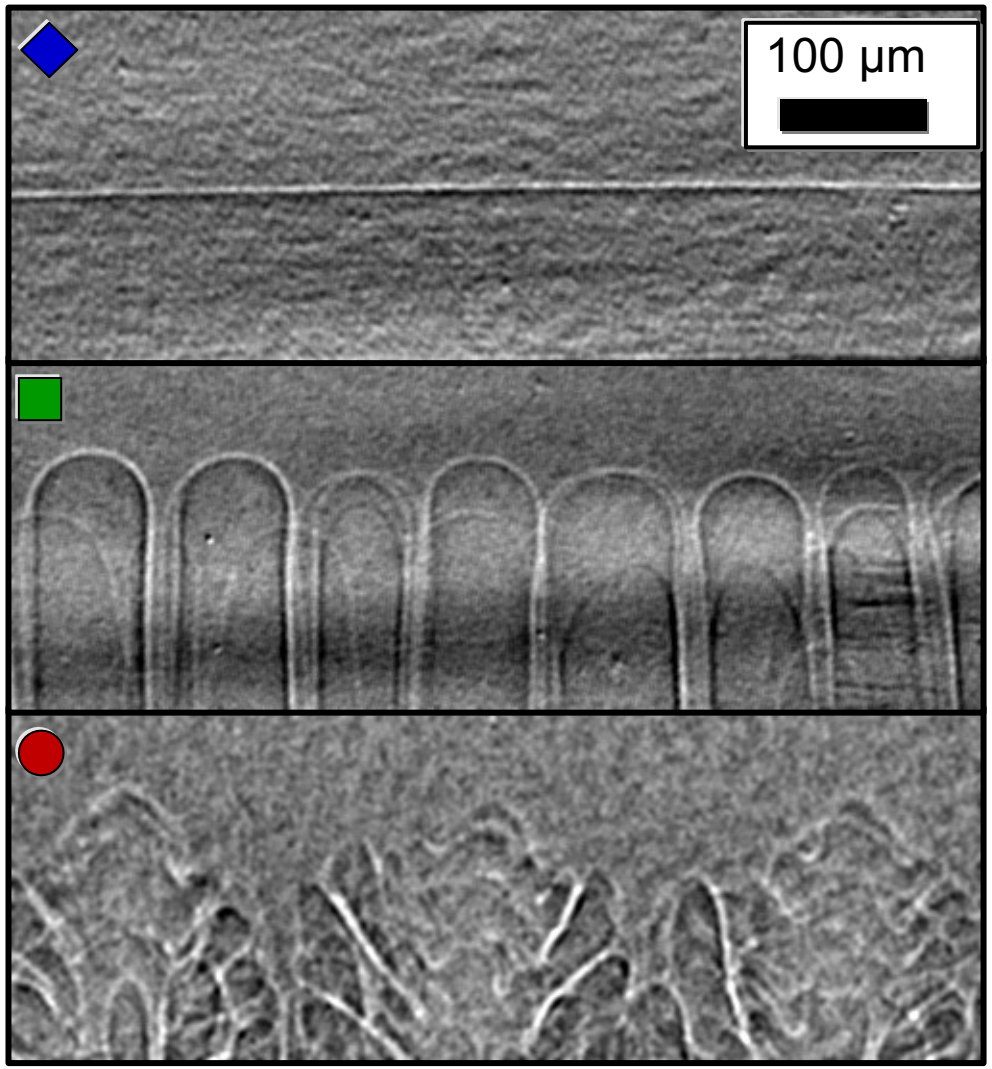


(e.g. [Kurz, Fisher, *Fundamentals of Solidification*])

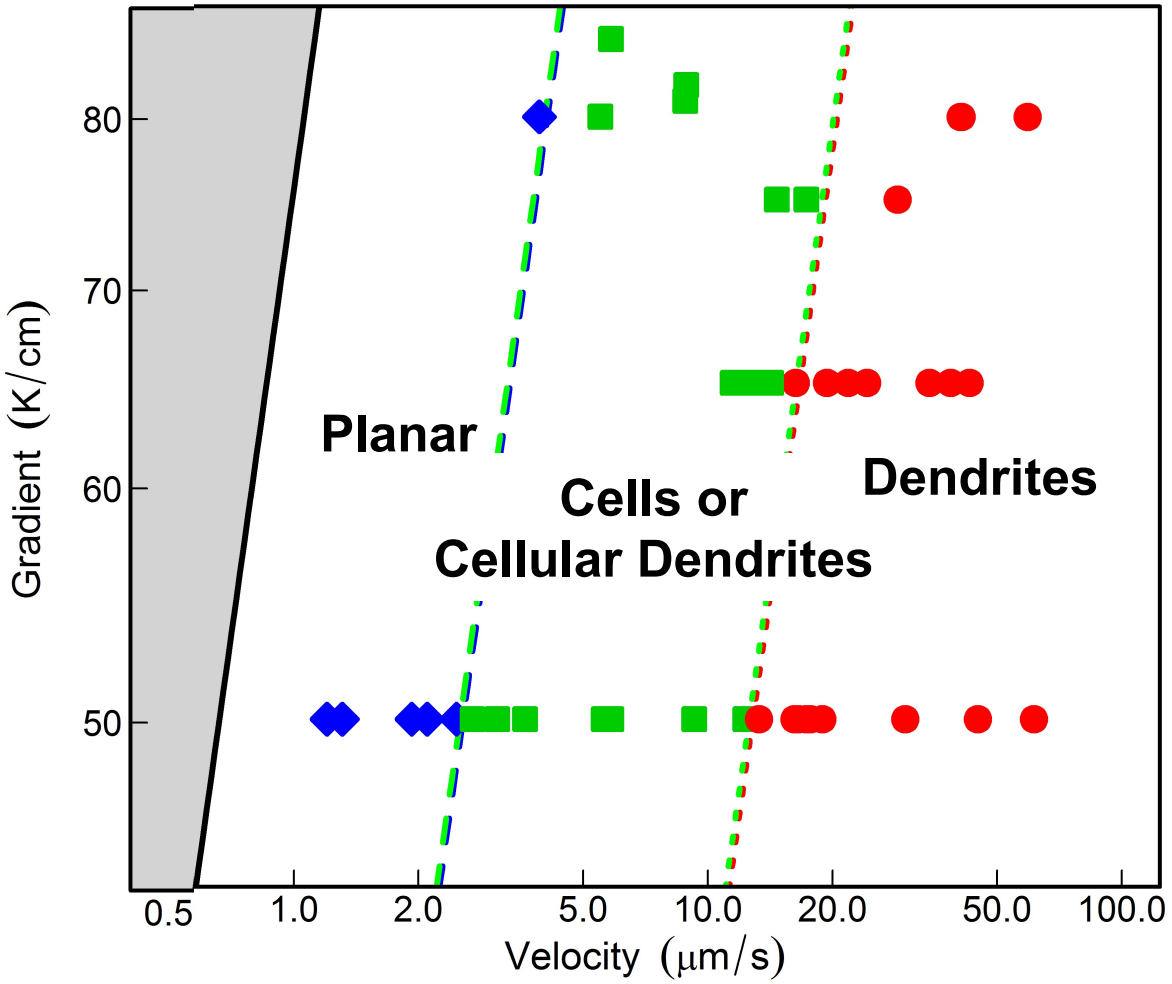


T. DebRoy, et al., Progress in Materials Science, 2018, 92:112-224

Controlled Growth and Solidification Pattern and Regime Transitions in Dilute Al-0.6at.%Cu



~200 μm thick

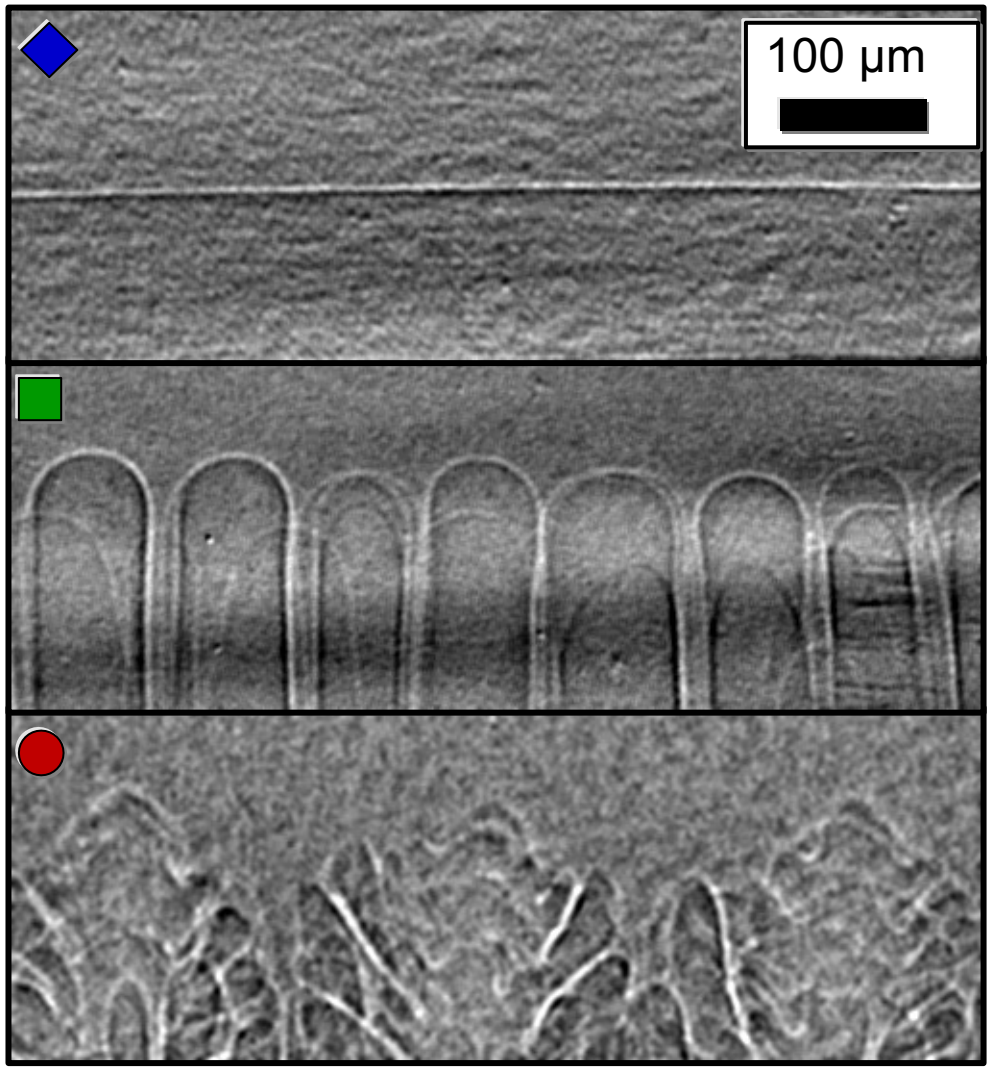


- G varies from ~85 K/cm to ~ 50 K/cm
- V varies from < 2μm/s to > 100 μm/s

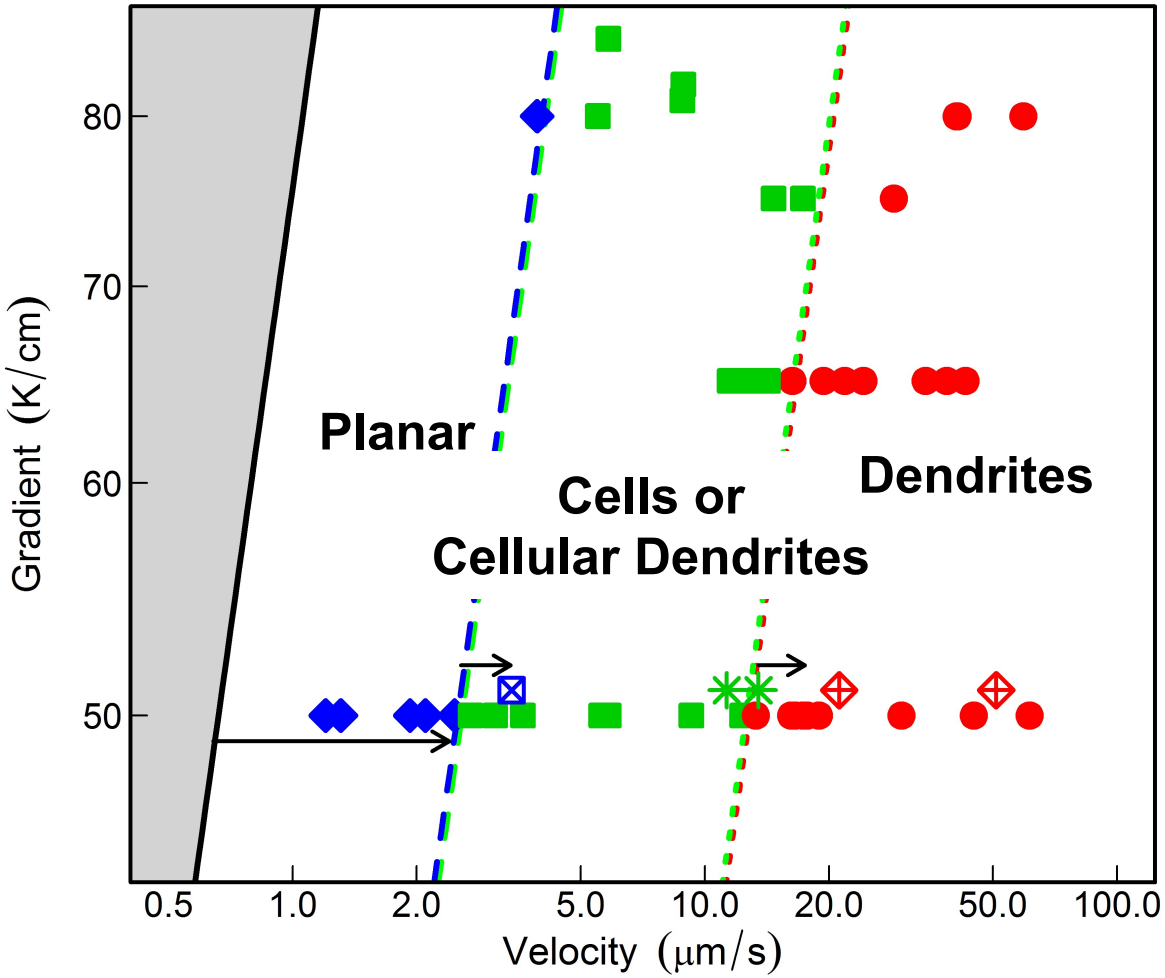
A.J. Clarke et al., Acta Materialia, 2017, 129:203-216

Northeastern Los Alamos NATIONAL LABORATORY U.S. DEPARTMENT OF ENERGY Office of Science Argonne NATIONAL LABORATORY

Controlled Growth and Solidification Pattern and Regime Transitions in Dilute Al-0.6at.%Cu

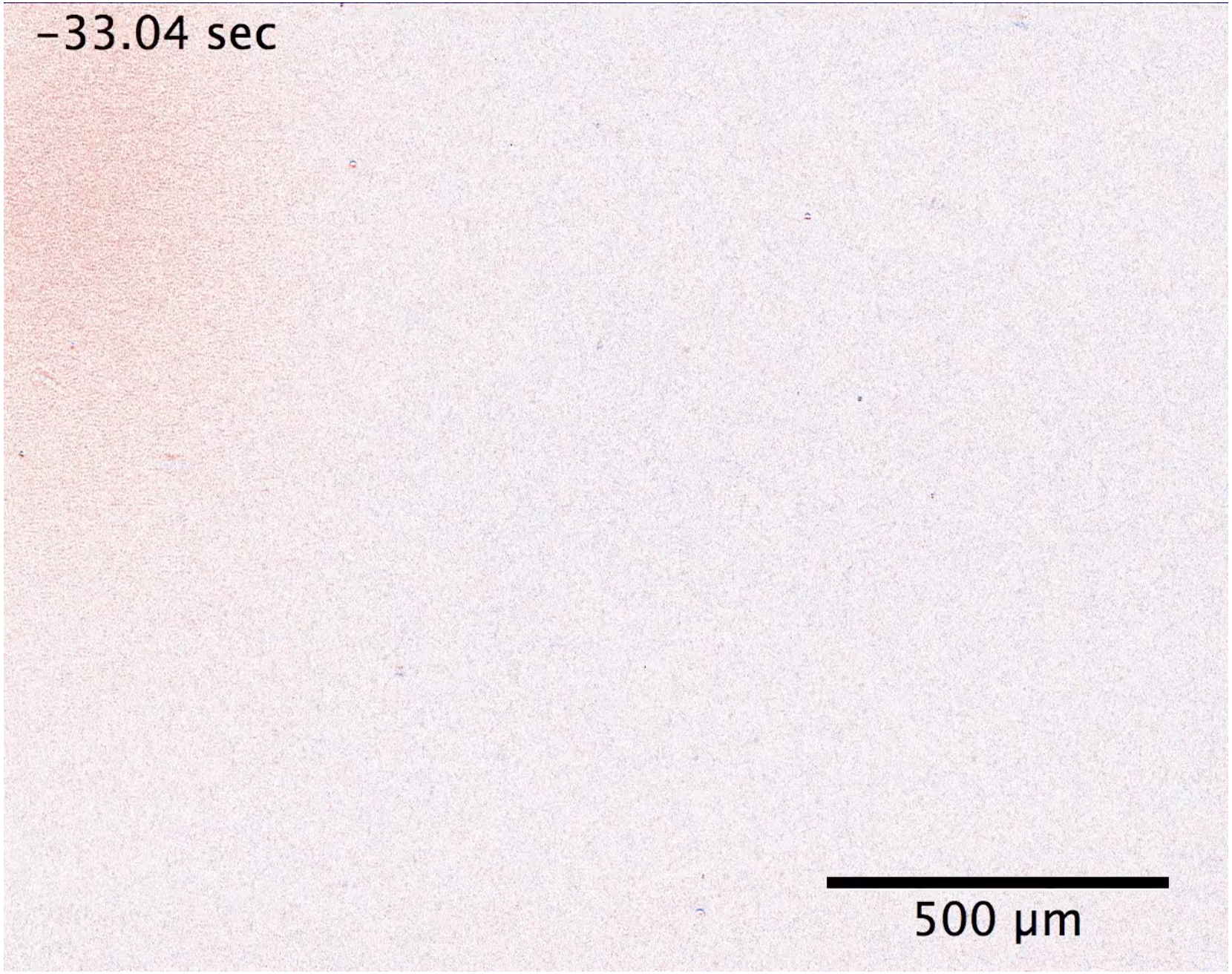


~200 μm thick



- G varies from ~85 K/cm to ~ 50 K/cm
- V varies from < 2μm/s to > 100 μm/s

A.J. Clarke et al., Acta Materialia, 2017, 129:203-216



J.W. Gibbs et al., JOM, 2016, 68:170-177

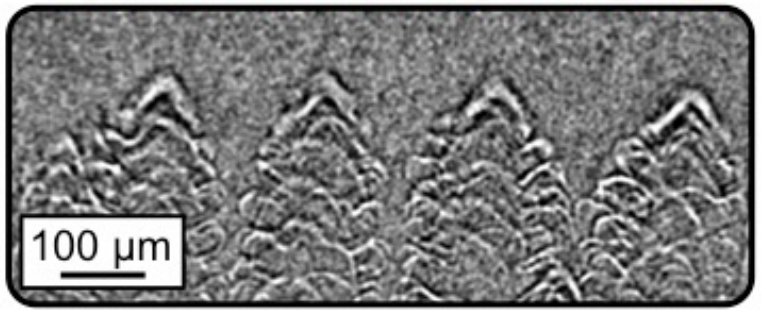
Sn-27at.%Bi, G= 28 K/cm, V= 46 µm/s

Northeastern Los Alamos NATIONAL LABORATORY U.S. DEPARTMENT OF ENERGY Office of Science Argonne NATIONAL LABORATORY

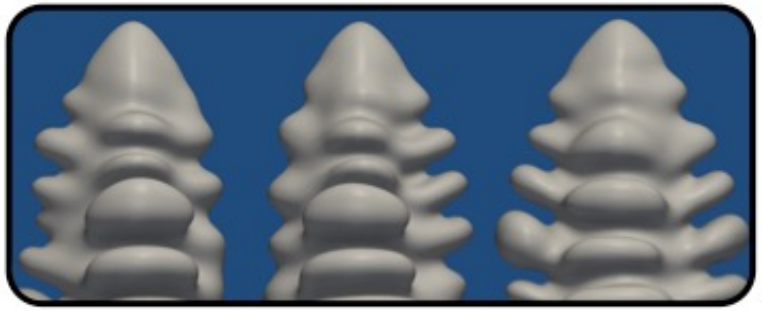
Microscopic Structural Evolution in Metal Alloys during Solidification

A.J. Clarke et al., Acta Materialia, 2017, 129:203-216

Synchrotron X-ray Imaging

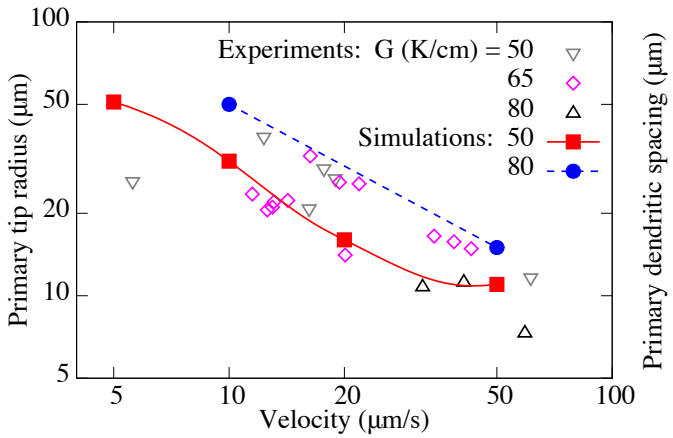


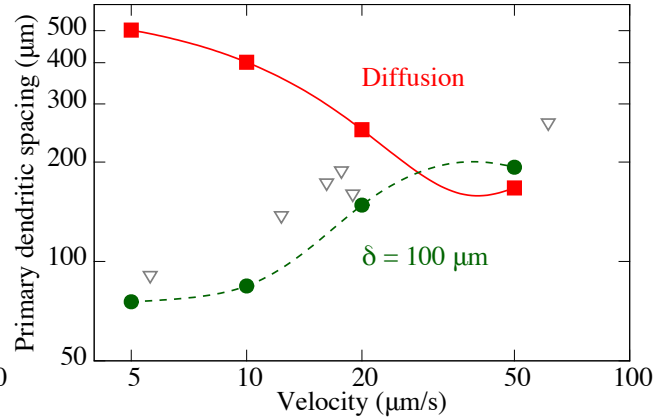
3D Phase-field Simulation

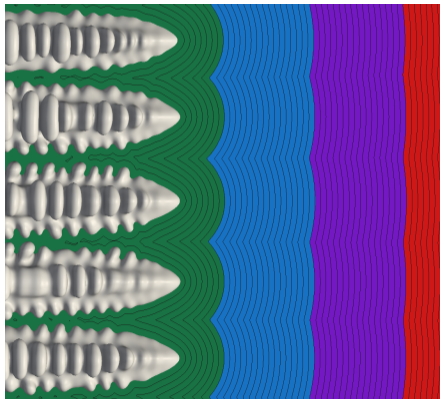


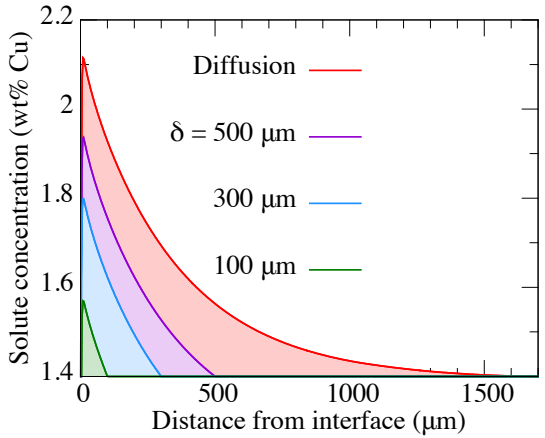
Al-0.6at.%Cu, ≈ 200 µm thick,
G = 80 K/cm, V ≈ 40-50 µm/s

Experiments inform modeling









Boundary layer analysis to study mixed diffusive-convective regime in the liquid

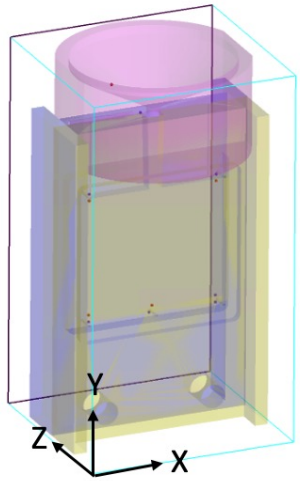
δ, boundary layer width

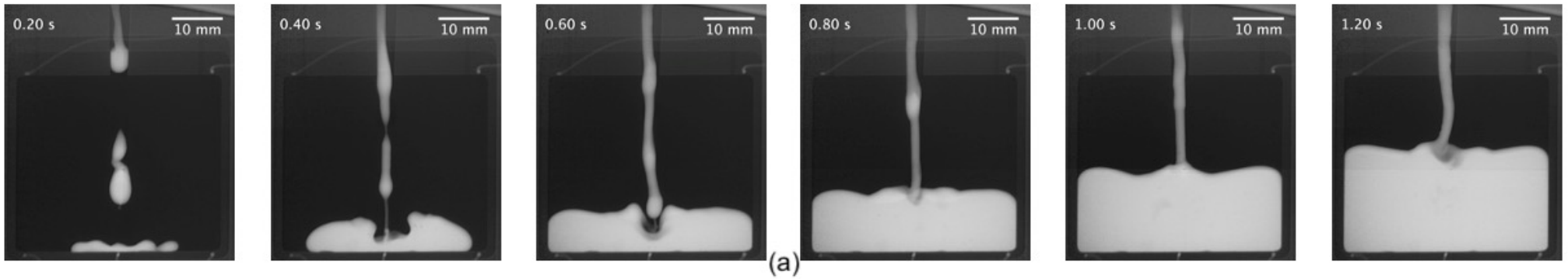
A.J. Clarke et al., Acta Materialia, 2017, 129:203-216

Northeastern Los Alamos NATIONAL LABORATORY U.S. DEPARTMENT OF ENERGY Office of Science Argonne NATIONAL LABORATORY

800 MeV Proton Radiography (pRad) of Sn-Bi Alloy Casting: Experimentally-Informed Fluid Flow Modeling

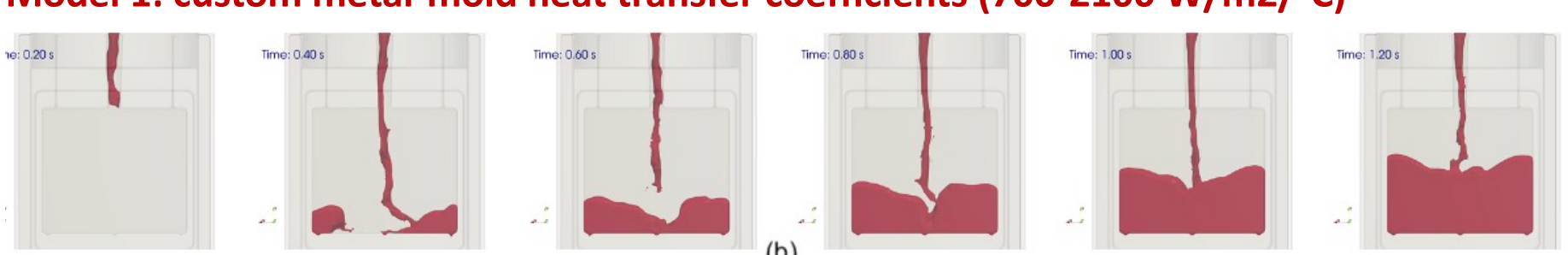
800 MeV pRad (0.2 s timestep after pour time until 1.2 s)





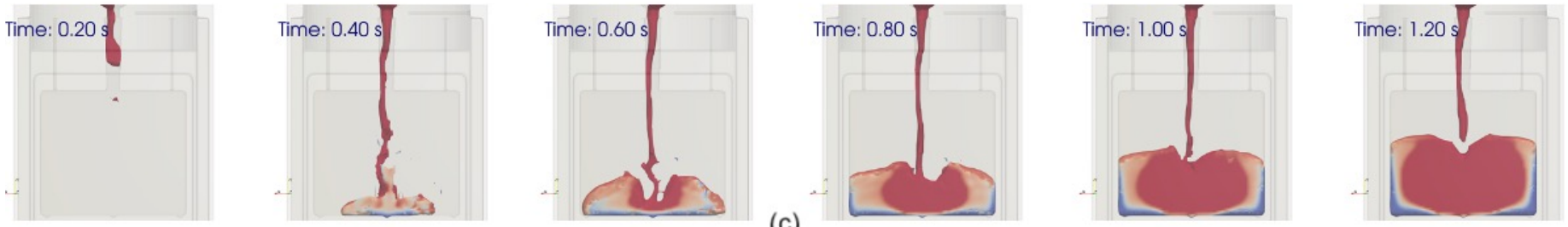
(a)

Model 1: custom metal-mold heat transfer coefficients (700-2100 W/m2/°C)

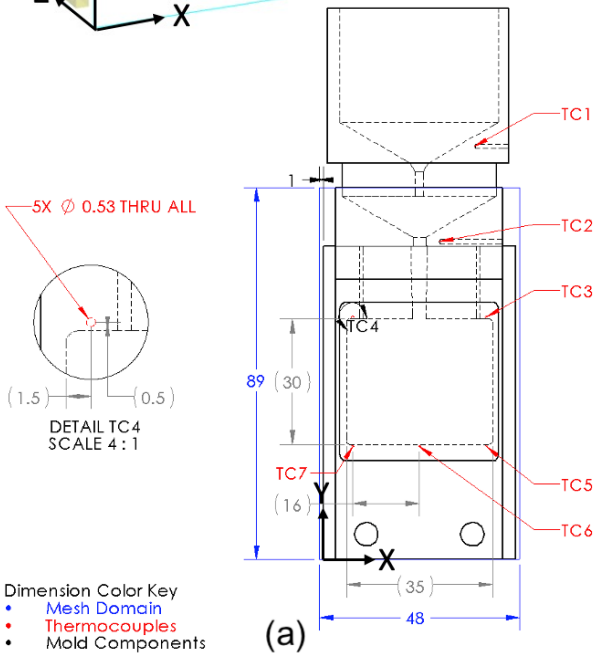


(b)

Model 2: Flow-3D calculated metal-mold heat transfer coefficients (10^4-10^5 W/m^2/°C)



(c)

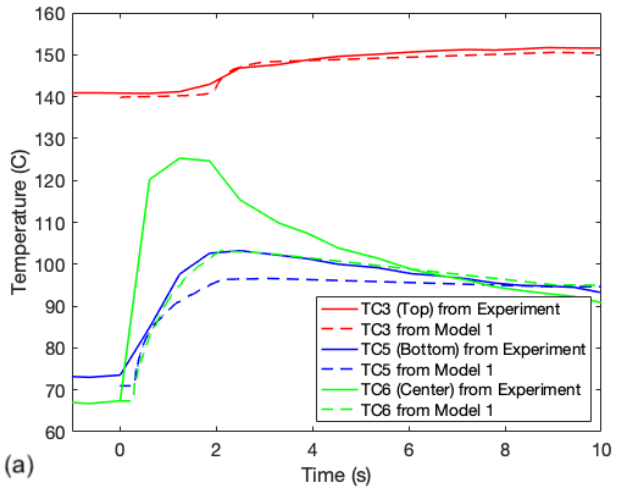


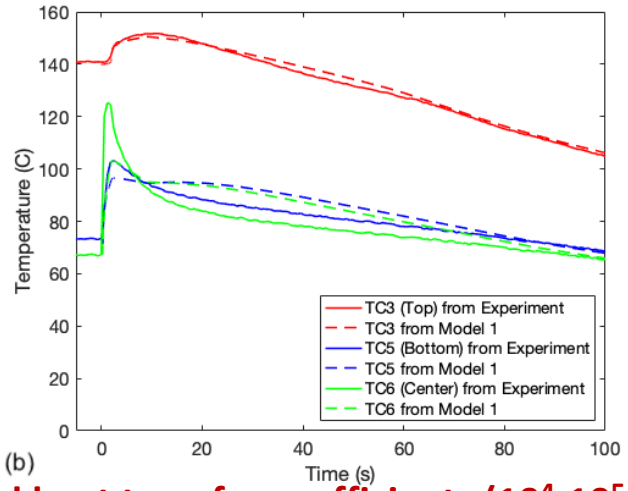
N. Surghani et al., 2024, in preparation

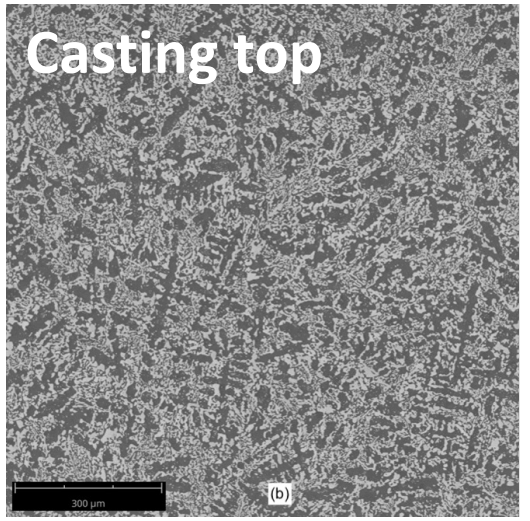
COLORADO SCHOOL OF MINES @150 | 1874-2024 · Lawrence Livermore National Laboratory · PROTON RADIOGRAPHY · U.S. DEPARTMENT OF ENERGY · Office of Science · LDRD innovation for our nation

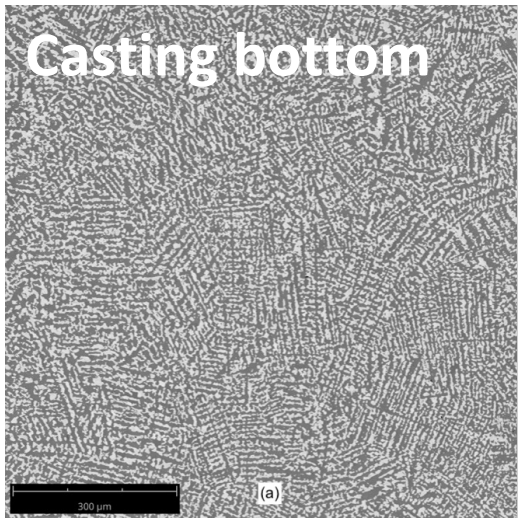
800 MeV pRad of Sn-Bi Alloy Casting: Temperatures, Microstructures, and Solidification Modeling

Model 1: Custom metal-mold heat transfer coefficients (700-2100 W/m2/°C)

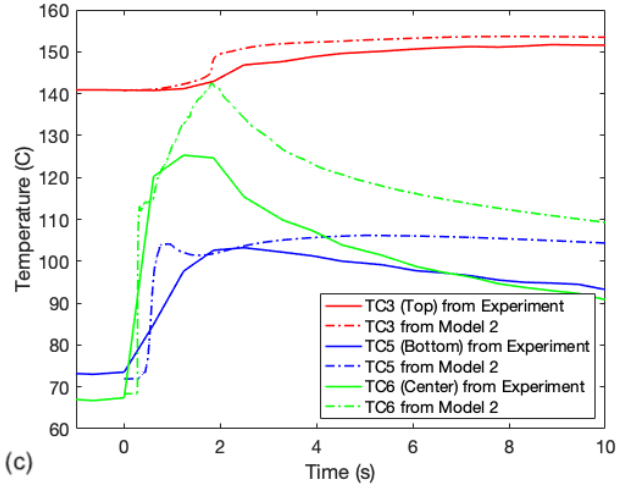


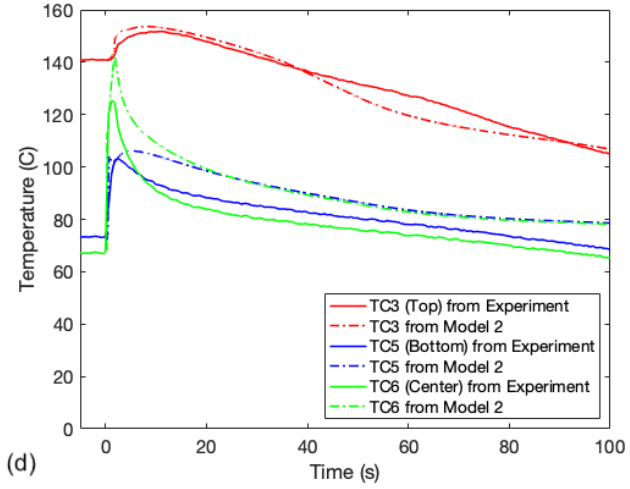


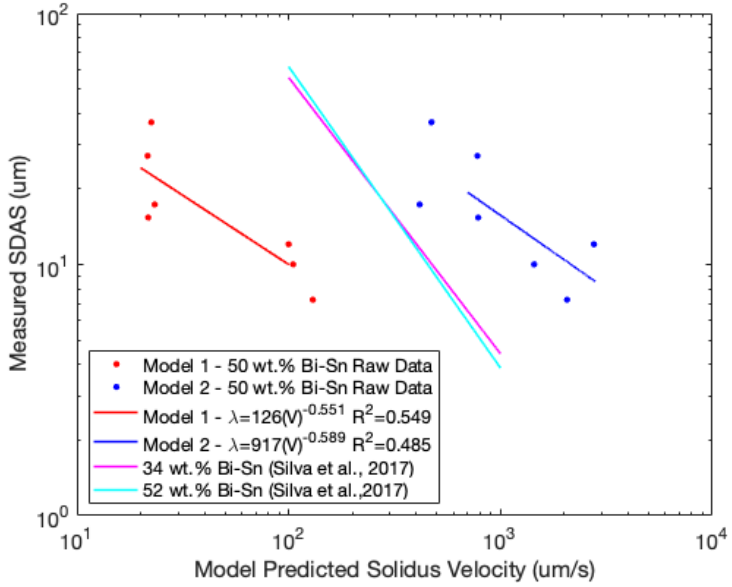




Model 2: Flow-3D calculated metal-mold heat transfer coefficients (10^4-10^5 W/m^2/°C)





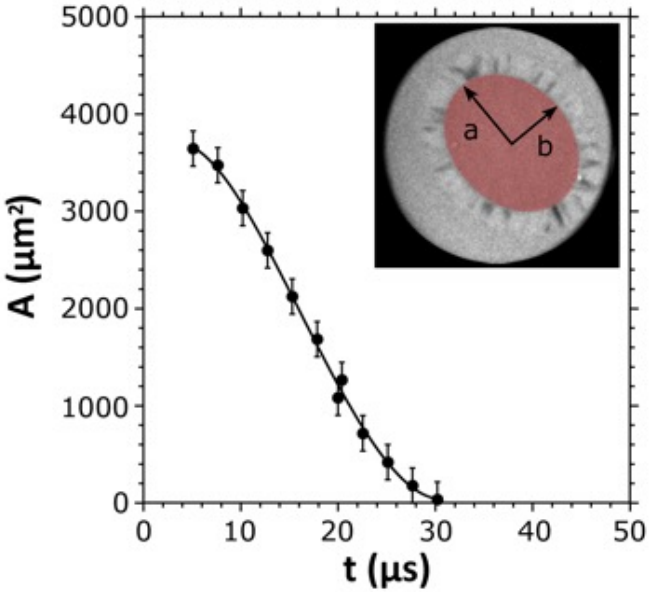


N. Surghani et al., 2024, in preparation

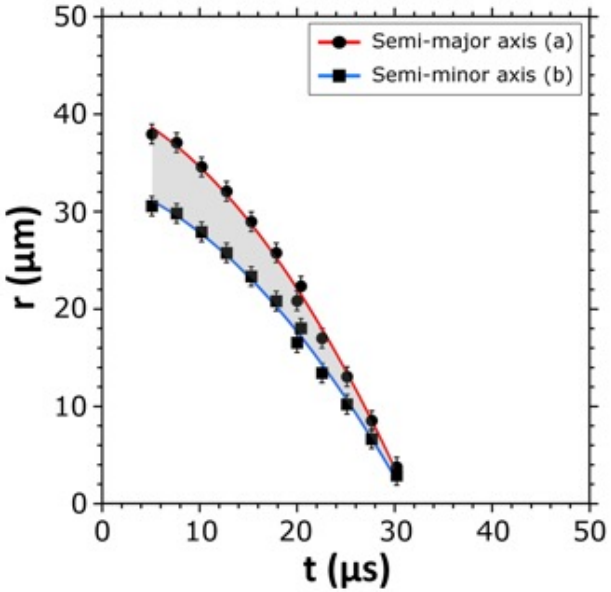
COLORADO SCHOOL OF MINES @150 | 1874-2024 · Lawrence Livermore National Laboratory · PROTON RADIOGRAPHY · U.S. DEPARTMENT OF ENERGY · Office of Science · LDRD innovation for our nation

Dynamic Transmission Electron Microscopy (DTEM): Al-4at.%Cu Rapid Solidification Interface Velocity Measurements

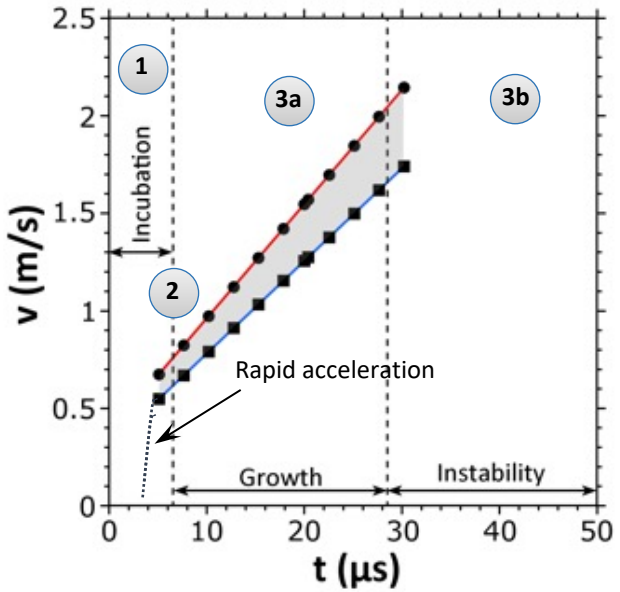
Melt pool area

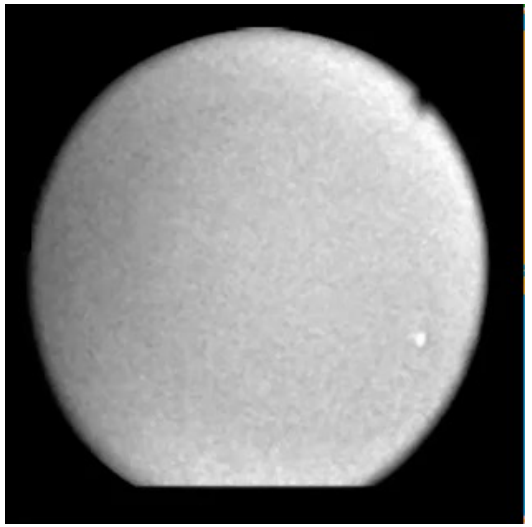


Melt pool axes



Interface velocity evolution





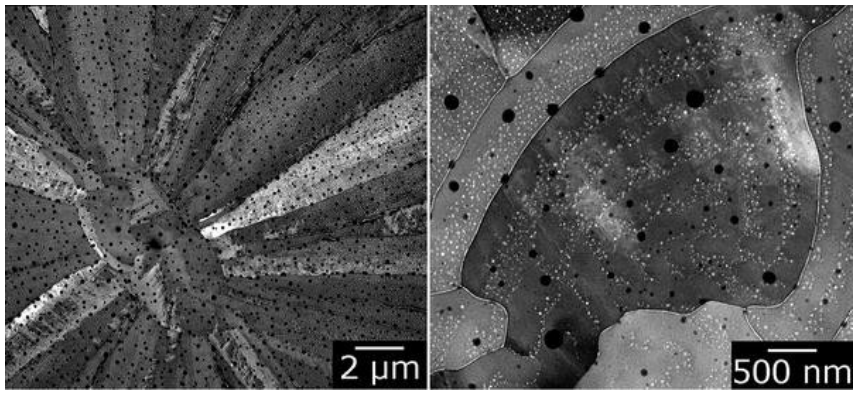
Solidification regimes

1. ***Incubation:*** Mushy zone evolution

2. ***Transition:*** Directional RS begins, rapid acceleration

3a. ***Growth:*** Columnar growth with accelerating solid-liquid interface

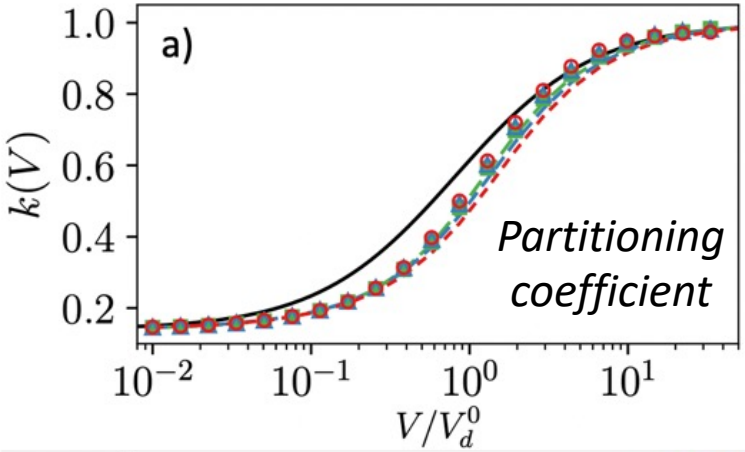
3b. ***Instability:*** Banded growth morphology, acceleration to critical velocity, v_a



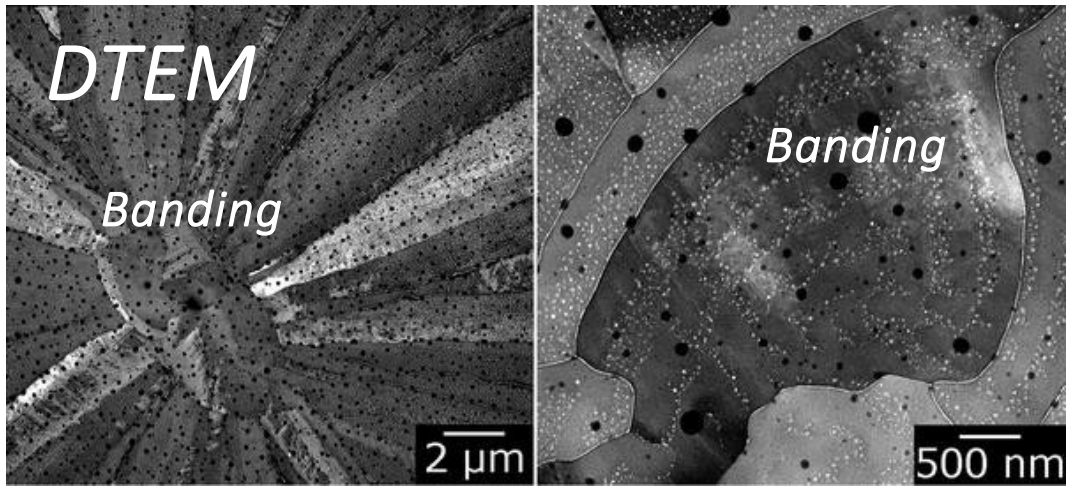
J.T. McKeown et al., JOM, 2016, 68:985-999

Los Alamos NATIONAL LABORATORY | Lawrence Livermore National Laboratory | University of Pittsburgh | U.S. DEPARTMENT OF ENERGY | Office of Science | NSF

Quantitative Phase Field Modeling of Microstructural Evolution Under Rapid Solidification Conditions

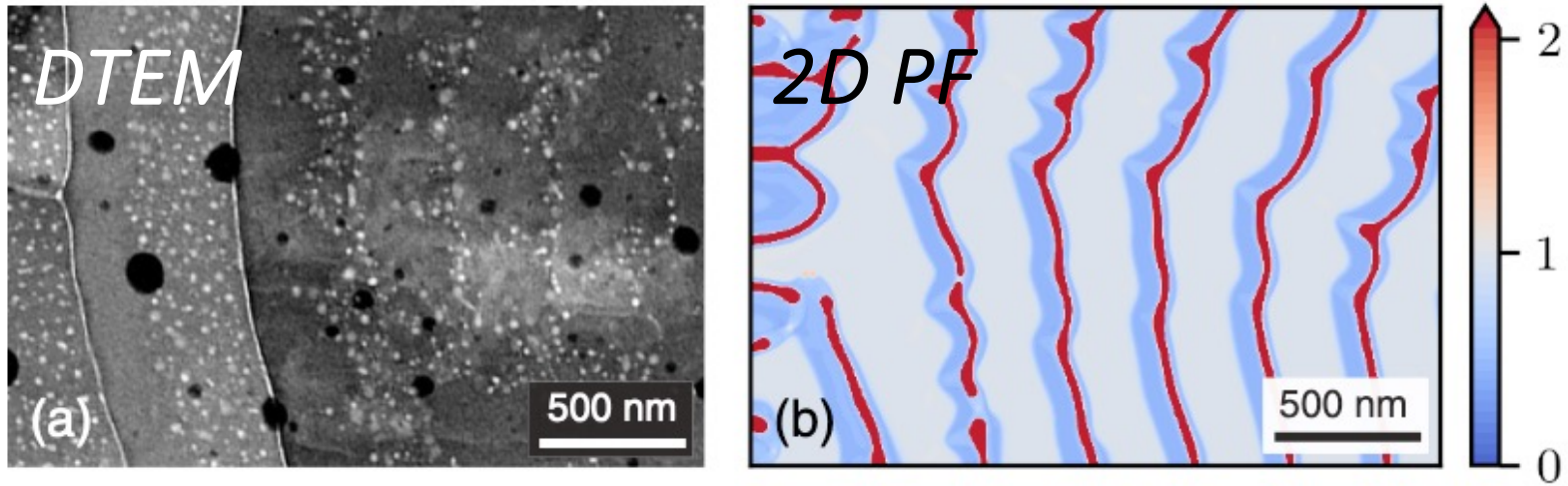


Prediction of velocity dependent properties



J.T. McKeown et al., JOM, 2016, 68:985-999

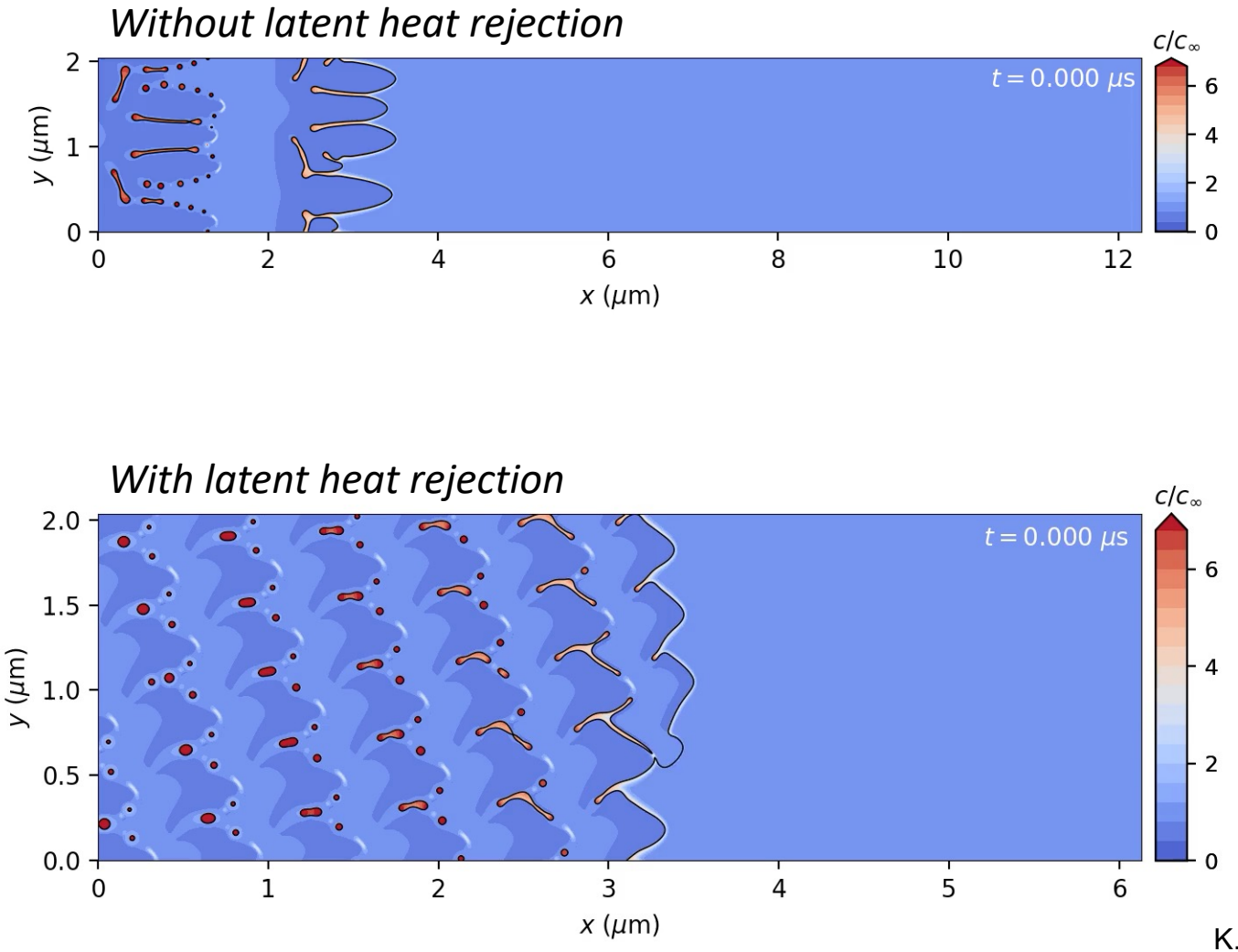
Banded microstructures in Al-9 Cu (wt.%) of late-stage, thin film solidification and a 2D PF simulation with latent heat and thermal gradient G = 5 x 10^6 K/m

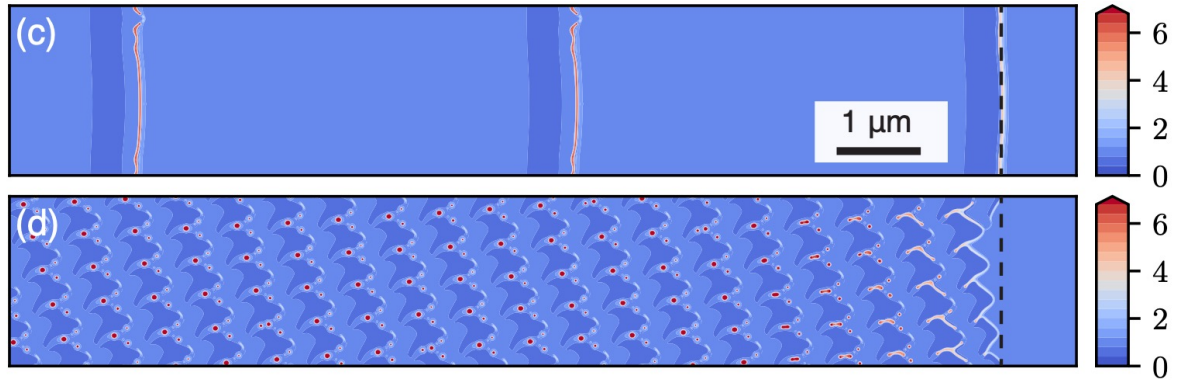


K. Ji, E. Dorari, A.J. Clarke, A. Karma, Physical Review Letters, 2023, 130:026203
K. Ji, A.J. Clarke, J.T. McKeown, A. Karma, MRS Bulletin, 2024, 49:556-567

Los Alamos NATIONAL LABORATORY | COLORADO SCHOOL OF MINES @150 | 1874-2024 | Lawrence Livermore National Laboratory | Northeastern | U.S. DEPARTMENT OF ENERGY | Office of Science

Strong Effect of Latent Heat Rejection





Al-3wt% Cu alloy, G = 5×10^6 K/m, V_p = 0.96 m/s

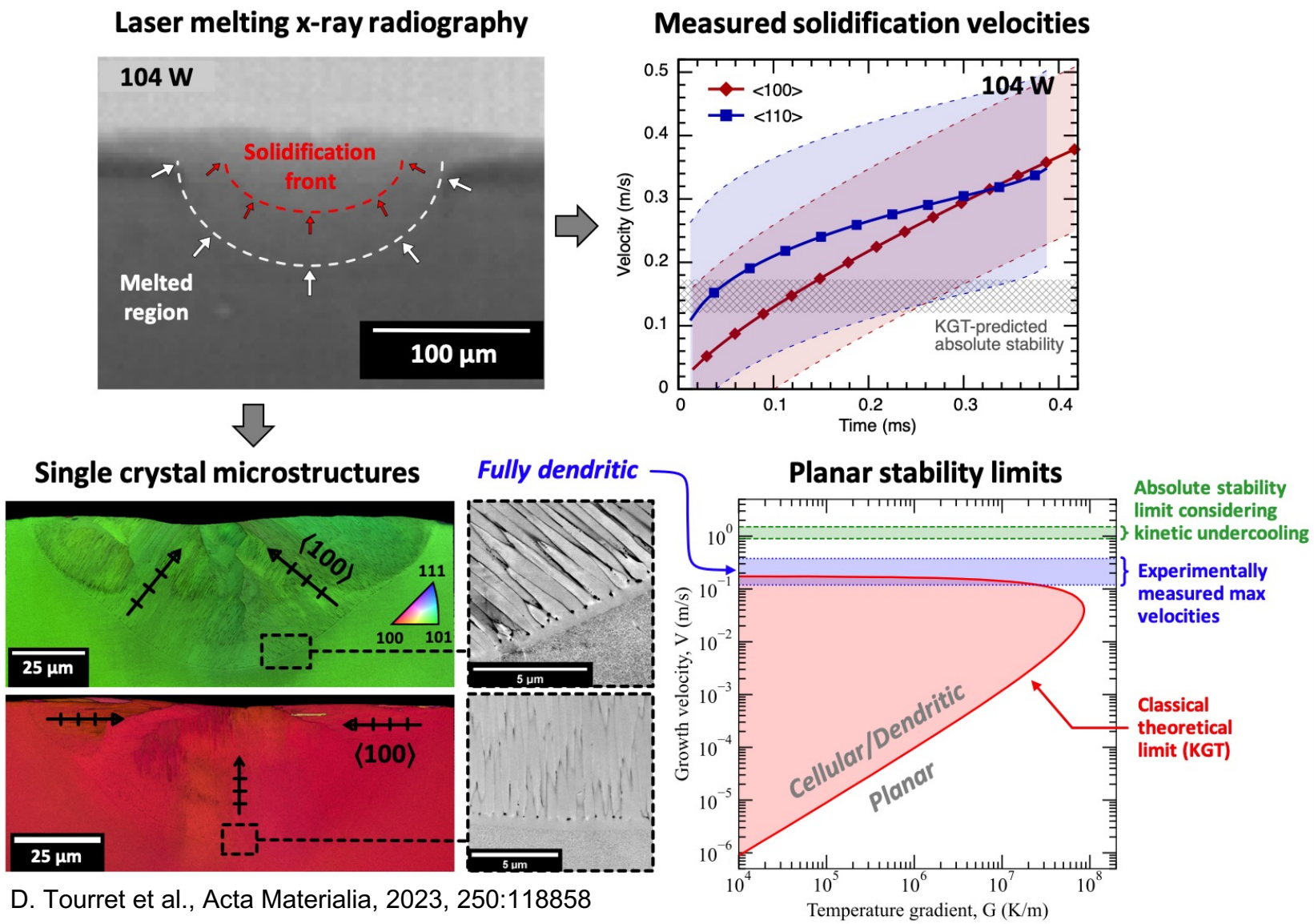
K. Ji, E. Dorari, A.J. Clarke, A. Karma, Physical Review Letters, 2023, 130:026203
K. Ji, A.J. Clarke, J.T. McKeown, A. Karma, MRS Bulletin, 2024, 49:556-567

Los Alamos NATIONAL LABORATORY
COLORADO SCHOOL OF MINES @150 | 1874-2024
Lawrence Livermore National Laboratory
Northeastern
U.S. DEPARTMENT OF ENERGY | Office of Science

Microstructure Selection during Additive Manufacturing: Need for Improved Models

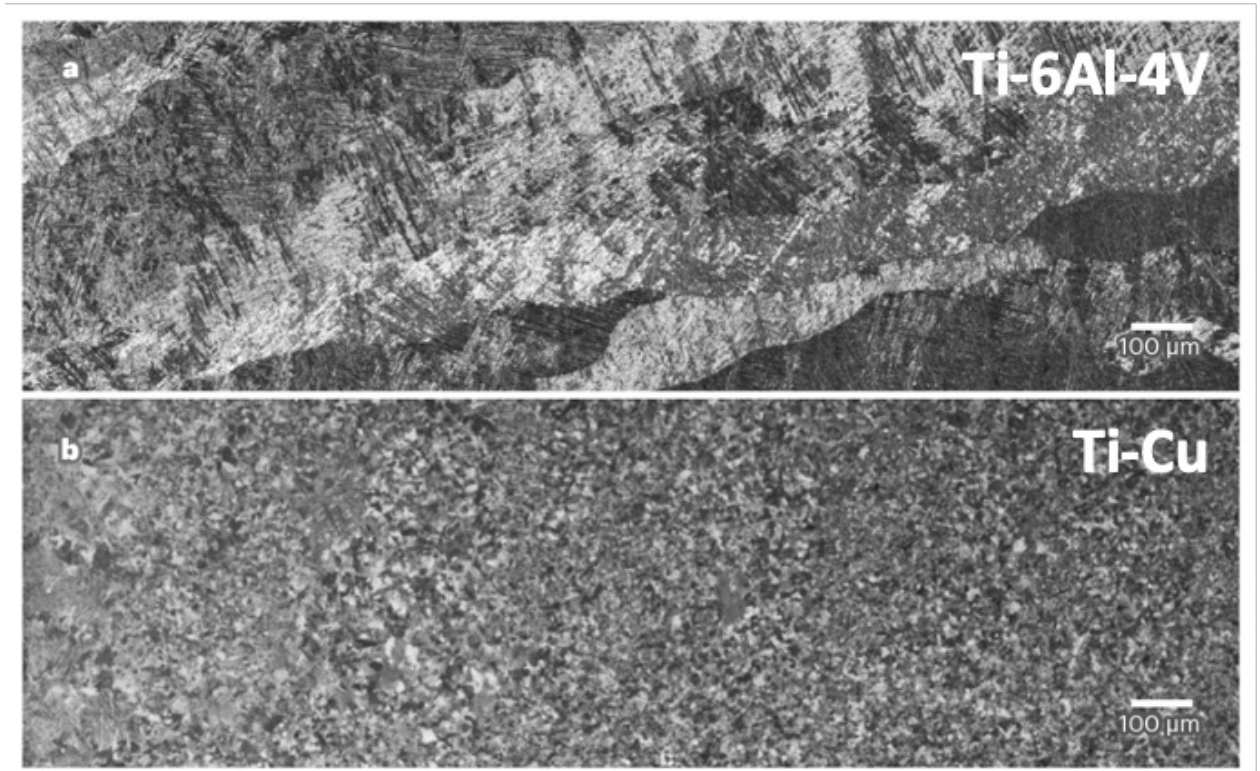
- Measured S-L interface velocities and microstructure characterization reveal discrepancies with classical theories regarding the onset velocity for absolute stability of a planar S-L interface

- Cellular/dendritic microstructures persist beyond the expected absolute stability limit, where banded structures should theoretically appear

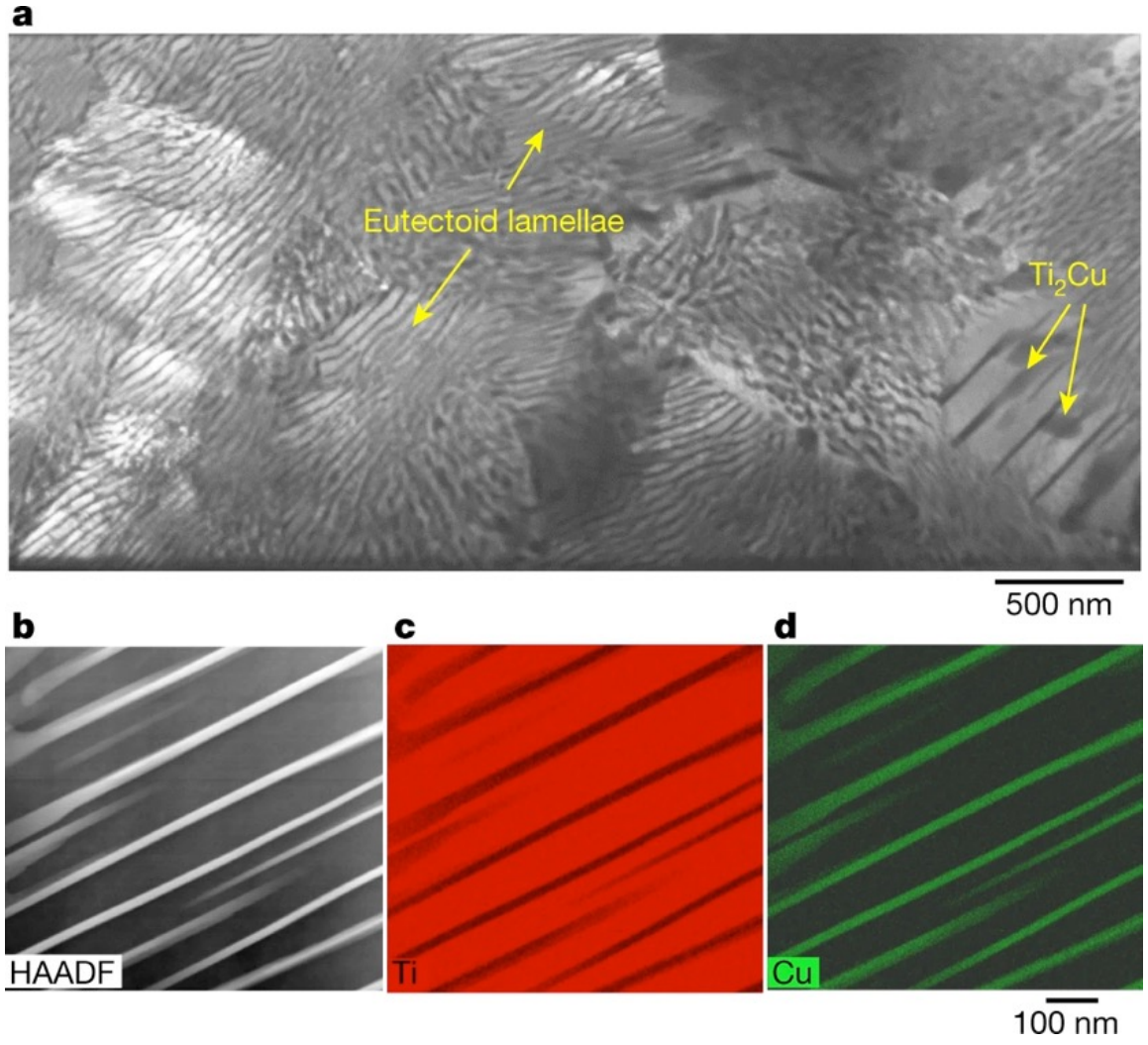


D. Tourret et al., Acta Materialia, 2023, 250:118858

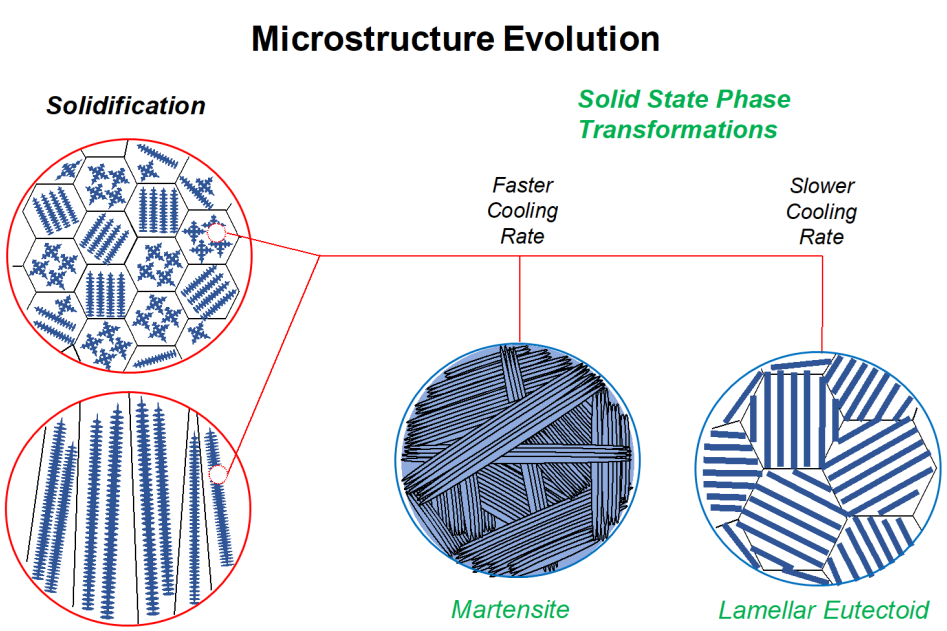
Fine-Grained Ti-Cu Microstructures Produced by AM

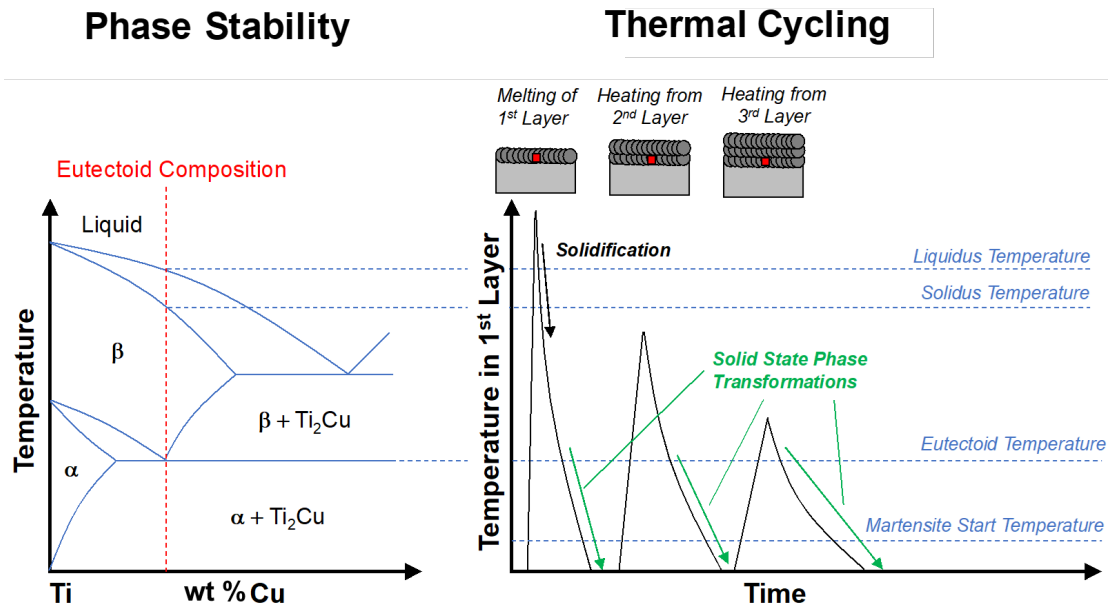


D. Zhang et al., Nature, 2019, 576:91-95
A.J. Clarke, Nature, 2019, 576:41-42



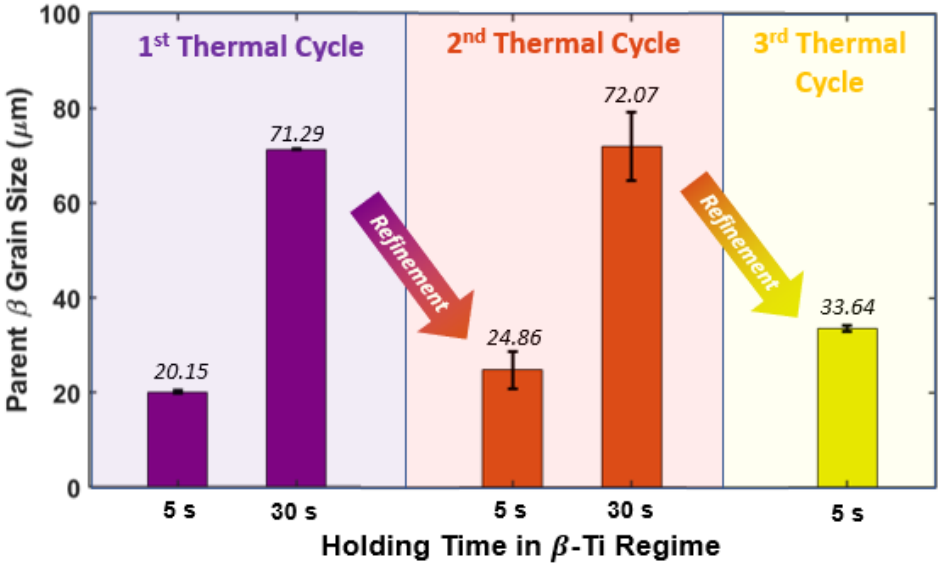
Grain Refinement by Solid State Thermal Cycling

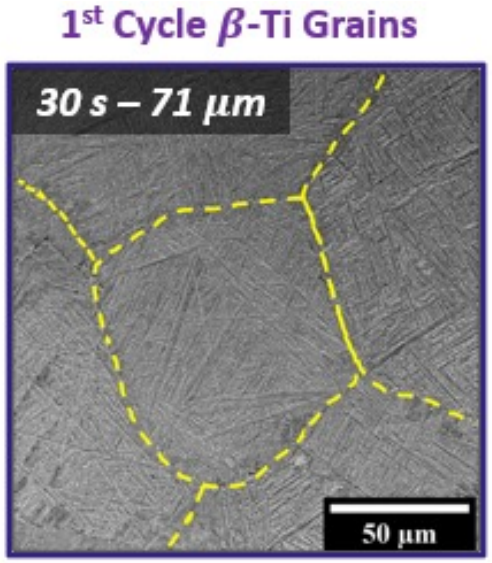


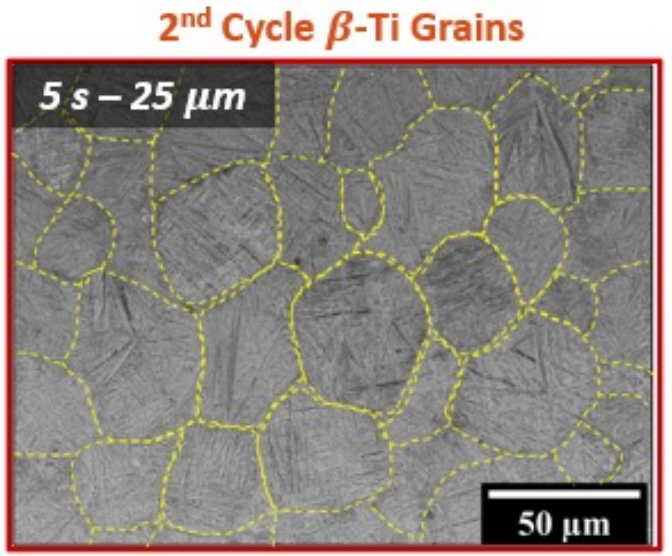


A.J. Clarke, Nature, 2019, 576:41-42

A. Saville et al., Additive Manufacturing, 2023, 75:103747







Solid state thermal cycling, inherent to AM processes, refines β-Ti grain size

Northeastern
COLORADO SCHOOL OF MINES @150 | 1874-2024
U.S. DEPARTMENT OF ENERGY
Office of Science

Selected Honors/Awards (Beyond U.S. DOE ECRP Award):

- 2024: National Academies of Sciences, Engineering, and Medicine's Panel on Assessment of Sciences of Extreme Materials; provides input to the Army Research Laboratory Technical Assessment Board on scientific and technical quality of the Army Research Laboratory
- 2022-2023: Colorado School of Mines (Mines) Excellence in Research Award (Senior)
- 2021-present: The Minerals, Metals & Materials Society (TMS) Foundation Board of Trustees
- 2021-2023: John Henry Moore Distinguished Professor of Metallurgical and Materials Engineering at Mines
- 2020: TMS Brimacombe Medalist
- 2018: Fellow of ASM International
- 2017-present, Editor, Metallurgical and Materials Transactions A
- 2018-2021: Office of Naval Research (ONR) Young Investigator Program (YIP) Award
- 2015-2019: TMS Board of Directors
- 2015-2018: Chair/Vice Chair, Advanced Photon Source Users Organization Steering Committee (APSUO) at Argonne National Laboratory
- 2014: National Academy of Sciences 26th Annual Kavli Frontiers of Science Symposium Fellow
- 2013: MTU Alumni Association's Outstanding Young Alumni Award
- 2013, TMS/Federation of European Materials Societies (FEMS) Young Leader International Scholar
- 2014-2016: Association for Iron & Steel Technology (AIST) Board of Directors
- 2011: Presidential Early Career Award for Scientists and Engineers (PECASE)

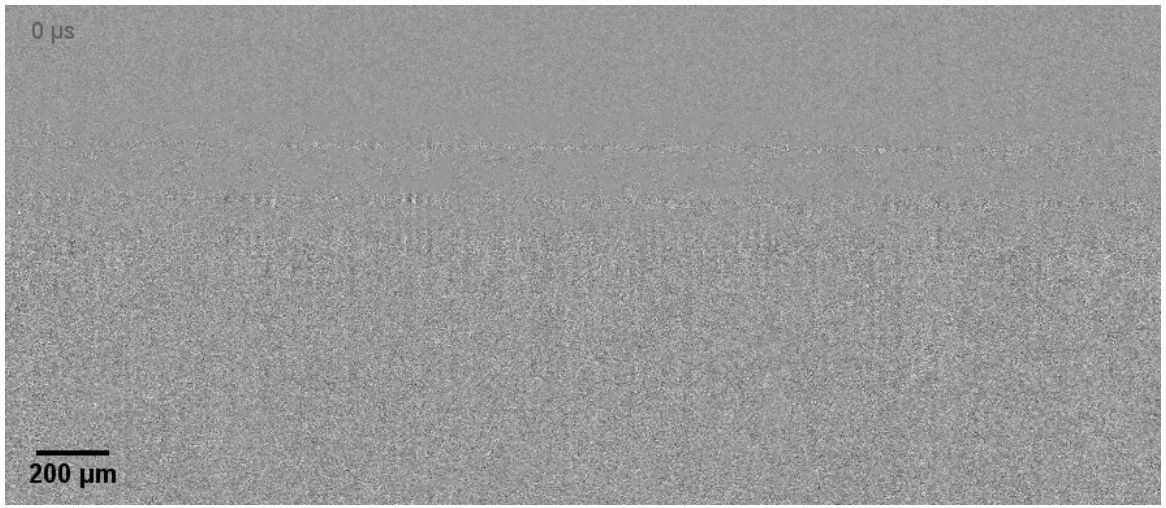
Example Synergistic Activities

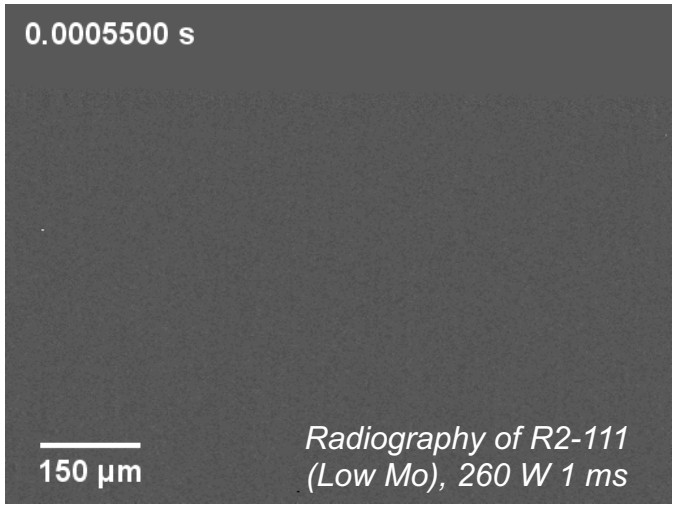
- 2024-2027, PI (Co-PIs: LLNL, SNL), Refractory Additive Manufacturing: Alloys to Z Pulsed Power Facility (RAM: A to Z), Laboratory Directed Research and Development (LDRD) FY24 Interlaboratory Collaboration, LANL, $3M ($1M to LANL)
- 2024-2025, PI, Additive Manufacturing for Earth Penetrators (AM for EP), LDRD Director's Initiative (DI), LANL, $4.5M
- 2022-2025, PI, Microstructure Control of Additively Manufactured Metals of Interest to the NNSA Weapons Complex, NNSA Stewardship Science Academic Alliance (SSAA), $900K
- 2018-2024, Co-PI, Rationalization of Liquid/Solid and Solid-Solid Interphase Instabilities during Thermal-Mechanical Transients of Metal Additive Manufacturing, ONR Multidisciplinary University Research Initiative (MURI), ~$7.5M
- 2023-2028, PI/Director, Advanced Characterization of Metals under Extreme Environments (ACME^2), NNSA SSAA Center of Excellence, led by Mines, $12.5M
- 2020-2025, Co-PI/Co-Director, Center for Micromorphic Multiphysics Porous and Particulate Materials Simulations within Exascale Computing Workflows, NNSA Predictive Science Academic Alliance Program III Multidisciplinary Simulation Center, led by CU Boulder, ~$13.2M
- 2021-2025, PI, Thermomechanical Processing of Refractory Multi-Principal Element Alloys for Ultrahigh Temperature Performance, ONR, ~$560K

Students and Postdocs

- Advise(d) 11 postdocs, 39 graduate students, 6 non-thesis graduate students, 6 visiting international graduate students, 18 undergraduate students, and 18 undergraduate researchers since 2016 at Mines. Serve(d) on 66 thesis committees (53 have graduated to date), and as an external examiner for 8 students in Australia, Brazil, Canada, Finland, Spain, and Sweden
  - John Copley, NNSA SSGF Stewardship Science Graduate Fellowship (SSGF), now at Princeton University
  - Chris Jasien, DOE NNSA Stewardship Science Graduate Fellowship (SSGF), now at Fortius Metals
  - Virginia Euser, Spring 2020 Dr. Bhakta Rath and Sushama Rath Research Award for Outstanding Graduate Thesis from Mines, now at LANL
  - Brian Rodgers, NNSA Laboratory Residency Graduate Fellowship (LRGF)
  - Alec Saville, NSF Graduate Research Fellowship Program (GRFP), now a National Research Council (NRC) postdoc at the National Institute of Standards and Technology, NIST in Boulder, CO
- At LANL, mentor(ed) 8 postdocs, 3 students, and served as an industrial mentor for 5 students, including 2 prestigious Director's funded postdocs and 1 G.T. Seaborg Institute Postdoctoral Fellow
  - John Gibbs, Director's Fellow Postdoctoral Appointment, now a Program Manager at LANL
  - Damien Tourret, Director's Fellow Postdoctoral Appointment, now a Researcher at Institute IMDEA Materials, Spain
  - Nathan Peterson, G.T. Seaborg Postdoctoral Research Fellow, now at LANL

Collaborators, Facilities, Funding Agencies…





Thank You!

Amy J. Clarke
aclarke@lanl.gov , amyclarke@mines.edu