Final Report for DOE Early Career Research Program Award
DE-SC0014232

Program Manager: Dr. John Vetrano
Sponsoring Program Office: U.S. Department of Energy, Office of Basic Energy Sciences,
Materials Science and Engineering Division

Doping Metallic Grain Boundaries to Control Atomic Structure and Damage Tolerance

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EXECUTIVE SUMMARY

The interfaces between crystals, known as grain boundaries, often act as sites for crack and void nucleation during plastic deformation of metallic materials. While it is known that interfacial character and structural state can greatly influence this damage nucleation process, the current level of control over such details is extremely limited. The objective of this project was to obtain a fundamental understanding of how metallic grain boundary structure can be controlled through intelligent doping, with the idea of inducing planned grain boundary phases or *complexions*. The effect of complexion structure on dislocation accommodation mechanisms was studied, to improve the field's understanding of damage nucleation at interfaces. While mechanical damage was the primary focus, the project showed that amorphous complexions can also improve a material's resistance to radiation damage, providing a single materials design concept that can address multiple important technological areas. This research used a combination of computational, experimental, and characterization techniques to isolate and understand the importance of nanoscale grain boundary structure and interfacial chemistry. The fundamental insights provided by this project enable the creation of advanced engineering metals with improved damage tolerance.

HYPOTHESES

This project was focused on understanding how grain boundary structure controls the damage resistance of metallic materials. Since even small changes to the structure of grain boundaries in single element systems can dramatically affect properties, **our major hypothesis was that the addition of amorphous complexions would improve the damage-tolerance of metallic alloys**. To systematically explore this topic, a number of additional hypotheses were put forth in our proposal and are listed below:

- Starting grain boundary character will affect complexion formation for a given set of thermodynamic conditions.
- Complexion type and structure can be controlled by manipulation of processing conditions such as temperature, quench rate, and alloy chemistry.
- Complexion type (ordered versus disordered) will determine the tolerance of a given boundary to mechanical and radiation damage.
- The formation of amorphous complexions will compete both with ordered complexions and the precipitation of bulk, wetting phases.

RESEARCH METHODS

To test the hypotheses listed above, we performed complementary experimental and computational research lines which ran in parallel but continually informed one another. Atomistic modeling with hybrid molecular dynamics/Monte Carlo simulations was used to study the formation and structure of different complexions in bicrystals and polycrystalline samples, while molecular dynamics was then used to probe damage resistance as well as crack nucleation and propagation. Sputter deposition was used to create films with targeted compositions, followed by annealing to induce segregation and complexion formation. Additional samples were created with mechanical alloying near the end of the project, to test new hypotheses about the importance of chemical complexity in the grain boundary region on interfacial amorphization. High resolution transmission electron microscopy allowed detailed boundary structure to be visualized and studied, while in situ experiments let us probe the mechanical behavior and radiation tolerance of amorphous complexions. As our work progressed and gained attention from our community, we also explored opportunities to access other unique capabilities through collaborations with Sandia National Laboratory.

ACCOMPLISHMENTS

(1) Fundamentals of segregation-induced complexion transitions

A major open question in this project was why different grain boundaries had different complexion structures, so we began our efforts by working to understand how grain boundary character influenced dopant segregation and complexion transitions. Thermodynamic theories for complexion formation that existed when we began this work treated all boundaries the same,

giving them the same energy or at best incorporating some small variation in grain boundary energy for a population of boundaries in a polycrystal. However, it is well-known that grain boundaries can have a wide range of energies and atomic structures, features which should alter segregation of dopants and subsequent complexion transitions. The tendency for the transition to a disordered interfacial structure was found to consistently depended on the relative solute excess, instead of the grain boundary energy or misorientation angle. Grain boundaries with high relative solute excess went through gradual disordering transitions, whereas those with low relative solute excess remained ordered until high global Zr concentrations but then abruptly transformed into thick disordered films. These results were published in ***Physical Review B*** [J2]. We then studied how complexion type could differ based on the elemental species that were segregating to the grain boundary region. Literature reports of nanometer-scale complexions in Cu-Ag, Cu-Zr, W-Ni, and Mo-Ni all show that such films are disordered. It was not clear if that was a foregone conclusion, with the abutting crystal frustrating crystallization of the intergranular film for nanoscale thicknesses, or if this observation is merely a function of the alloys that have been studied to date. Our work showed that, while Cu-Zr forms structurally disordered or amorphous films, ordered films comprised of a second phase usually precipitate in Cu-Nb, with a critical nucleation size of ~1 nm below which the ordered phase cannot form. We also found that free surfaces could compete with the grain boundaries as potential segregation sites, depending on the dopant element. These results have been published in ***Scripta Materialia*** [J4]. Next, we investigated whether nanoscale amorphous intergranular films with equilibrium thicknesses contain residual structural order from the lattices that surround them. We also explored the distribution of short-range order through the amorphous film, as this short-range order often controls the deformation of metallic glasses in a manner analogous to how long-range order determines the deformation mechanisms for crystalline materials. We found three distinct regions within the amorphous complexions: amorphous-crystalline interfaces, regions deep inside the films that mimic a bulk amorphous phase, and finally a transition region between the first two types of structure. The thickness of the transition region depends on film thickness at low temperature, but become thickness-independent at high temperature. Similarly, the interfacing crystal plane influences local order at low temperatures, but not at high temperatures near the melting point. These different regions and trends are important, because they should influence the physical mechanisms responsible for strength (related to the amorphous-crystalline interface) and ductility (related to the structure deep inside the film). These results were published in ***Computational Materials Science*** [J5].

Complexion formation should also be possible at other types of defects, like dislocations. Experimental observations of these "linear complexions" in Fe-Mn were first reported in recent articles by Prof. Dierk Raabe and his research group, using transmission electron microscopy and atom probe tomography. To improve the understanding of this new phenomenon, we used atomistic methods to simulate the segregation-induced formation of intermetallic linear complexions confined at edge dislocations, with an initial focus on α-Fe doped with Ni. The metastable B2-FeNi intermetallic phase is first nucleated near dislocations and then partially transformed to the stable $L1_0$-FeNi intermetallic compound. Nucleation of the $L1_0$-FeNi phase on dislocations occurs for a wide range of the global compositions and annealing temperatures outside of the two-phase coexistence region on the equilibrium Fe-Ni phase diagram. For some of these compositions and temperatures, homogeneous nucleation is thermodynamically-restricted and the final microstructure is determined by dislocation-assisted precipitation, which is limited by the amount of dopant segregation. For other cases, the solute segregation is strong enough to form

large, bulk-like precipitates at the dislocations. These results were published in ***Scripta Materialia*** [J9]. We have recently been able to provide a full thermodynamic description of linear complexion formation in Fe-Ni, uncovering the important role of interfacial energies in the formation of the metastable B2 phase. These results were published in ***Physical Review Letters*** [J12].

(2) Materials design rules for amorphous complexion formation

We originally showed that Cu-Zr can form amorphous complexions, but sought to gain a more universal understanding of which alloys can support such features. With this in mind, sputter deposition was used to synthesize Cu-rich binary metallic alloys characterized by different thermodynamic parameters such as atomic radius, enthalpy of segregation, and enthalpy of mixing. We found that both Cu-Zr and Cu-Hf form disordered complexions at high temperatures, while Cu-Nb and Cu-Mo retained ordered grain boundary structures under similar conditions. This contrast in interfacial structure was attributed primarily to differences in the enthalpy of mixing and its effect on the free energy penalty for a solid, amorphous complexion. With our new materials selection criteria, we then hypothesize binary alloy combinations that would be capable of sustaining amorphous complexions for a number of transition metal systems. For Ni-based alloys, we hypothesized and then proved that Ni-Zr can support thick amorphous intergranular films as well. This work was published in ***Acta Materialia*** [J7]. To connect these findings to materials theory, we explored which interatomic potentials were able to faithfully recreate the observed Zr segregation and interfacial premelting in Cu-Zr alloys using atomistic modeling. Using comparison with experimental evidence, we found that the functional form of the interatomic potential is less critical than the choice of properties chosen for fitting. Specifically, the enthalpy of mixing and the bond energies must be faithfully represented to predict the chemical segregation and transition to an amorphous intergranular complexion. This can be done multiple ways, as one of the reliable potentials was created by fitting the ab initio atomic forces from a variety of atomic configurations while the other was created by calibrating to the liquid enthalpy of mixing and diffraction data from amorphous alloys. These simulations also correctly predicted that Ni-Zr would sustain amorphous complexions, with this prediction then being confirmed in our sputtered films. This work was published in ***Computational Materials Science*** [J8].

Although we have shown that disordered complexions can form in binary metal alloys, the addition of a third element should in principle allow us to further reduce the free energy penalty for the amorphous phase, to increase complexion thickness and stability. To address this concept, hybrid Monte Carlo/molecular dynamics simulations were performed to investigate the behavior of dopants in two model ternary alloy systems (Cu-Zr-Ag and Al-Zr-Cu). In both systems, solutes segregate to the grain boundary and the grain boundary structure becomes disordered at high temperature and doping concentration. It is found that the various solutes occupy different sites at interface and there can be site competition if their promising segregation sites are the same. Moreover, when multiple solutes are present they can interact with each other and change the interfacial segregation behavior. Finally, a thicker amorphous intergranular film can be formed in multi-element system by controlling the concentration ratio of different solute elements, although this effect was relatively small in these simulations since the alloy choice was restricted by the available interatomic potentials. This work was published in ***Journal of Materials Science*** [J10], where the paper was chosen as a finalist for the Robert W. Cahn Best Paper Prize in that journal.

We next moved to test this hypothesis that chemical complexity at the grain boundary was a positive feature by exploring amorphous complexion formation in binary Cu-Zr and Cu-Hf as well as ternary Cu-Zr-Hf. We found an obvious thickening of the distribution of amorphous complexion thickness in the ternary alloy. These results demonstrate that design of the interfacial chemistry can be a powerful tool for controlling complexion structure. The work was published in ***Acta Materialia*** [J13].

(3) Stability of interfacial complexions

The complexion states that we have been exploring in this project require a great deal of segregation to the grain boundaries, which could potentially lead to other types of phase transformations within the system. To probe this competition, we studied the structural stability of sputtered Cu-Nb and Cu-Zr films, with the films annealed and studied with transmission electron microscopy. In both cases, microstructural evolution was dominated by the formation of Cu particles through a solid-state dewetting mechanism, damaging the structural stability of the films. Dopant concentration was observed to have the greatest impact on solid-state dewetting, where more dilute dopant concentrations limited the dewetting behavior. While more dilute alloys limit dewetting, low dopant concentrations can also result in decreased nanocrystalline stability, implying that ideal metallic thin film compositions must balance nanocrystalline and thin film structural stabilities. This work was published in ***Materialia*** [J16]. Transitions between different complexion states are also very important, as they demark the critical conditions where one complexion type is preferred by a confluence of thermodynamics and kinetics. To begin work in this area, the PI helped write a review article on the topic, with his contribution primarily focusing on the measurement of these transitions in direct and indirect ways in both experiments and simulations. The paper was published in the ***Annual Review of Materials Research*** [J14]. To continue on this topic, we performed a study of amorphous-to-ordered complexion transitions during cooling from the high temperatures needed for grain boundary premelting. Bulk Cu-Zr and Cu-Zr-Hf alloy samples were annealed to induce boundary premelting and then quenched through a procedure that induces a gradient of local cooling rate through the sample height. Amorphous complexion thickness distributions were found to be invariant to local cooling rate in the Cu-Zr-Hf alloy, demonstrating enhanced stability of the amorphous complexion structure compared to the Cu-Zr alloy, which had thinner amorphous complexions in the regions that were slowly cooled. The experimental results are used to construct time-temperature-transformation diagrams of the amorphous-to-ordered complexion transition for both the binary and ternary alloys, enabling a deeper understanding of the influence of cooling rate and grain boundary chemistry on complexion transitions. The critical cooling rate necessary to avoid complexion transitions in the ternary alloy was found to be at least three orders of magnitude slower than that for the binary alloy. This work has been submitted for publication as [J18].

Additional opportunities have arisen to explore the formation and stability of other complexion transitions. A collaborative opportunity arose to work with colleagues at the University of Virginia that were interested in ordered-disordered structural transitions in carbon nanotube wires. We found that the wires had a surface amorphous layer, analogous to what we observe at grain boundaries, which is a function of wire growth temperature. This work was published in *Physica Status Solidi A* [J6], with our main contribution being the characterization of the amorphous

surface films. We have also studied how faceting tranformations, another type of complexion transition, alter the migration of grain boundaries in a variety of pure and doped face centered cubic metals. These faceting transitions lead to unique temperature dependences of boundary mobility, which can be attributed to the emergence of new shuffling modes that relate to boundary structure. This work has been submitted for publication as [J17]

(4) Influence of complexion type on mechanical and radiation damage tolerance

A major class of materials which could be improved by the current project's results are nanocrystalline materials. To set the stage for the widespread implementation of our findings, the PI wrote an invited review article on this topic, with the idea that a robust theory for complexion formation would be a useful tool for describing the stabilization and properties of nano-grained materials. Specifically, we explained that disordered complexions can enable much improved ductility and thermal stability without degrading strength. This review paper was published at ***Current Opinion in Solid State & Materials Science*** [J3]. Jennifer Schuler, a Ph.D. student who was working on this project, was selected for a Department of Energy (DOE) Office of Science Graduate Student Research (SCGSR) award. This allowed her to spend approximately 6 months at Sandia National Laboratories collaborating with Dr. Brad Boyce and Dr. Khalid Hattar. One of her projects during this time was to perform in situ fatigue experiments on nanocrystalline thin films which had either (1) only order grain boundaries or (2) amorphous complexions dispersed throughout the grain boundary network. We discovered that nanocrystalline alloys containing disordered grain boundaries experience fatigue damage that has a ductile nature compared to the same alloy with only conventional, ordered grain boundaries. For example, the sample with amorphous intergranular films had a much larger plastic zone, leading to less fatigue damage. This enhanced ductility contributes to steady crack growth, whereas the same alloy containing only ordered grain boundaries had extensive nanocracking and unsteady crack growth. Including disordered grain boundaries in the alloy's grain boundary network can resist crack propagation and mitigate sudden, catastrophic failure. Both the ordered and disordered alloys also exhibited grain boundary bridging, which further enhances fatigue toughness. This work was published as part of a special issue in ***JOM*** [J11]. We also developed uniaxial tensile testing techniques to directly measure the mechanical behavior of nanocrystalline Cu-Zr with and without amorphous complexions, to isolate the effect of grain boundary structure. The sample with amorphous complexions showed evidence of extensive plastic flow, with ample necking in the gauge section. The cross-section was reduced by a great deal due to the local plastic strain. In contrast, the sample with ordered grain boundaries experienced catastrophic failure with little plastic strain, which is indicative of an extremely brittle material. These results are in the final stages of preparation for submission [J19].

We also hypothesized that disordered complexions would be beneficial for improving the radiation tolerance of interfaces. To test this hypothesis, we performed molecular dynamics simulations of collision cascades and analyzed residual point defects populations for a disordered amorphous intergranular film, an ordered boundary, and a single crystal. While ordered grain boundaries easily absorb interstitials, these interfaces are inefficient vacancy sinks. Alternatively, amorphous intergranular films act as ultra-efficient, unbiased defect sinks, providing a path for the creation of radiation-tolerant materials. These results were published in ***Scripta Materialia*** [J1]. To test this

theory directly with experiments, a combination of in situ and ex situ ion irradiation of ball milled Cu-Zr alloys was performed, with the heat treatment schedule again used to control grain boundary structure. We find that there are significantly fewer defects (dislocation loops, stacking fault tetrahedron, etc.) stored in the grains during irradiation for the sample with amorphous complexions. It is important to emphasize that the two materials are nearly identical, with the same grain size and composition. The only change is that some boundaries have transformed to an amorphous structure, yet this sample experiences only ~50% of the damage seen in the specimen with ordered boundaries. These results highlight that we now have experimental proof that amorphous intergranular films are efficient sinks for damage created by irradiation. We also find that the formation of the complexions stabilizes the microstructure against coarsening during irradiation. These results have been published in ***Acta Materialia*** [J15].

DISSEMINATION OF SCIENTIFIC RESULTS

The research results from this project have been distributed to the community in the form of invited talks and contributed presentations, as well as well as peer-reviewed journal articles. 38 invited talks and 11 contributed presentations were given, spread between conferences, universities, and national laboratories. These presentations are listed at the end of this document. 16 journal articles have been published to date on this project, including works appearing in top material science and engineering journals such as *Acta Materialia* and *Physical Review Letters*. In addition, 3 more papers are either already under external peer review or in the final stages of internal review. The details of these 19 journal articles are included at the end of this report. Copies of all journal articles resulting from this project have been uploaded to the arXiv.org repository, with PDF copies of the final articles also posted on the PI's website.

TRAINING AND PROFESSIONAL DEVELOPMENT

The project supported the effort of four Ph.D. students, as well as one M.S. student. Two postdoctoral scholars performed atomistic simulations for the project and received partial support. All trainees were mentored in the fields of Materials Science and Solid Mechanics, giving them multi-disciplinary skills that will help them in the workplace. The mixture of experimental, simulation, and theory found in this project also exposed all trainees to a broad range of skillsets to give them a deep appreciation for the field. Each met weekly with the PI to discuss research goals and career ambitions, while also presenting in front of the research group quarterly to develop presentation skills. Professional development included conference and workshop attendance, as well as career mentoring and counseling from the PI.

SCIENTIFIC PRODUCTS RELATED TO THIS PROJECT

All published journal articles, invited presentations, and contributed presentations acknowledged support from the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Science and Engineering Division under Award No. DE-SC0014232.

Journal Articles:

In Preparation

[J19] Wardini JL, Rupert TJ. "Complexion transitions alter the tensile failure of nanocrystalline Cu-Zr," (To be submitted to Materials Science and Engineering A).

Under Review

[J18] Grigorian CM, Rupert TJ. "Critical cooling rates for amorphous-to-ordered complexion transitions in Cu-rich nanocrystalline alloys," (Submitted to *Acta Materialia*).

[J17] McCarthy MJ, Rupert TJ. "Shuffling mode competition leads to directionally-anisotropic mobility of faceted Σ11 boundaries in face centered cubic metals," (Submitted to *Physical Review Materials*).

Published

[J16] Schuler JD, Copeland G, Hattar K, Rupert TJ, Briggs SA. "Solid-state dewetting instability in thermally-stable nanocrystalline binary alloys," *Materialia*, (2020) 9, 100618. (https://doi.org/10.1016/j.mtla.2020.100618)

[J15] Schuler JD, Grigorian CM, Barr CM, Boyce BL, Hattar K, Rupert TJ. "Amorphous intergranular films mitigate radiation damage in nanocrystalline Cu-Zr," *Acta Materialia*, (2020) 186, 341. (https://doi.org/10.1016/j.actamat.2019.12.048)

[J14] Cantwell PR, Frolov T, Rupert TJ, Krause AR, Marvel CJ, Rohrer GS, Rickman JM, Harmer MP. "Grain Boundary Complexion Transitions," *Annual Review of Materials Research*, (2020) 50, 465. (https://doi.org/10.1146/annurev-matsci-081619-114055)

[J13] Grigorian CM, Rupert TJ. "Thick amorphous complexion formation and extreme thermal stability in ternary nanocrystalline Cu-Zr-Hf alloys," *Acta Materialia*, (2019) 179, 172. (https://doi.org/10.1016/j.actamat.2019.08.031)

[J12] Turlo V, Rupert TJ. "Linear complexions: Metastable phase formation and coexistence at dislocations," *Physical Review Letters*, 122, 126102 (2019). (https://doi.org/10.1103/PhysRevLett.122.126102)

[J11] Schuler JD, Barr CM, Heckman NM, Copeland G, Boyce BL, Hattar K, Rupert TJ. "In situ high-cycle fatigue reveals the importance of grain boundary structure in nanocrystalline Cu-Zr," *JOM*, 74, 1221 (2019). (https://doi.org/10.1007/s11837-019-03361-7)

[J10] Hu Y, Rupert TJ. "Atomistic modeling of interfacial segregation and structural transitions in ternary alloys," *Journal of Materials Science*, 54, 3975 (2019). (https://doi.org/10.1007/s10853-018-3139-x)

[J9] Turlo V, Rupert TJ. "Dislocation-assisted linear complexion formation driven by segregation," *Scripta Materialia*, 154, 25 (2018). (https://doi.org/10.1016/j.scriptamat.2018.05.014)

[J8] Hu Y, Schuler JD, Rupert TJ. "Identifying interatomic potentials for the accurate modeling of interfacial segregation and structural transitions," *Computational Materials Science*, 148, 10 (2018). (https://doi.org/10.1016/j.commatsci.2018.02.020)

[J7] Schuler JD, Rupert TJ. "Materials selection rules for amorphous complexion formation in binary metallic alloys," *Acta Materialia*, 140, 196 (2017). (https://dx.doi.org/10.1016/j.actamat.2017.08.042)

[J6] Pham QN, Larkin LS, Lisboa CC, Saltonstall CB, Qiu L, Schuler JD, Rupert TJ, Norris PM. "Effect of Growth Temperature on the Synthesis of Carbon Nanotube Arrays and Amorphous Carbon for Thermal Applications," *Physica Status Solidi A*, 1600852 (2017). (http://dx.doi.org/10.1002/pssa.201600852)

[J5] Pan Z, Rupert TJ. "Spatial variation of short-range order in amorphous intergranular complexions," *Computational Materials Science*, 131, 62 (2017). (http://dx.doi.org/10.1016/j.commatsci.2017.01.033)

[J4] Pan Z, Rupert TJ. "Formation of ordered and disordered intergranular films in immiscible metal alloys," *Scripta Materialia*, 130, 91 (2017). (http://dx.doi.org/10.1016/j.scriptamat.2016.11.025)

[J3] Rupert TJ. "The role of complexions in metallic nano-grain stability and deformation," *Current Opinion in Solid State & Materials Science*, 20, 257 (2016). (http://dx.doi.org/10.1016/j.cossms.2016.05.005)

[J2] Pan Z, Rupert TJ. "Effect of grain boundary character on segregation-induced interface structural transitions," *Physical Review B*, 93, 134113 (2016). (http://dx.doi.org/10.1103/PhysRevB.93.134113)

[J1] Ludy JE, Rupert TJ. "Amorphous intergranular films act as ultra-efficient point defect sinks during collision cascades," *Scripta Materialia*, 110, 37 (2016). (http://dx.doi.org/10.1016/j.scriptamat.2015.07.040)

Invited Lectures:

[L38] "Moving closer to equilibrium but maintaining the defects (and the properties)," *The Minerals, Metals and Materials Society (TMS) Annual Meeting & Exhibition*, February 2020, San Diego, CA.

[L37] "Making strong, tough, thermally-stable, and radiation tolerant nanocrystalline materials in bulk form," *The Minerals, Metals and Materials Society (TMS) Annual Meeting & Exhibition*, February 2020, San Diego, CA.

[L36] "Optimizing the mechanical behavior of metals with grain boundary and dislocation complexions," *International Conference on Plasticity, Damage, and Fracture*, January 2020, Rivera Maya, Mexico.

[L35] "The thermodynamics and kinetics of defect-driven complexion formation," *International Conference on Plasticity, Damage, and Fracture*, January 2020, Rivera Maya, Mexico.

[L34] "Using TEM to isolate the importance of complexion transitions on the behavior of nanocrystalline materials," *Second International Symposium on Advanced Microscopy and Spectroscopy (ISAMS-2)*, December 2019, Irvine, CA.

[L33] "Coupled experimental and computational studies of amorphous grain boundary complexions," *Materials Science & Technology (MS&T) Conference and Exhibition*, September 2019, Portland, OR.

[L32] "Linear complexion formation driven by local stress concentrations near dislocations," *Dislocations 2019*, September 2019, Haifa, Israel.

[L31] "Probing nanoscale complexion transformations with computational techniques that complement experiments," *Recent Advances in the Modeling and Simulation of the Mechanics of Nanoscale Materials Workshop*, August 2019, Philadelphia, PA.

[L30] "Segregation-Induced Complexion Transitions: New Opportunities for Materials Design," *Gordon Research Conference – Physical Metallurgy*, July 2019, Manchester, NH.

[L29] "Amorphous intergranular films for improved performance under irradiation," *The Minerals, Metals and Materials Society (TMS) Annual Meeting & Exhibition*, March 2019, San Antonio, TX.

[L28] "Tailoring mechanical behavior with one- and two-dimensional complexions," *The Minerals, Metals and Materials Society (TMS) Annual Meeting & Exhibition*, March 2019, San Antonio, TX.

[L27] "Promoting beneficial complexion transitions: Tuning defect structure to make better materials," *University of California, Los Angeles – Department of Materials Science and Engineering*, March 2019, Los Angeles, CA.

[L26] "Promoting beneficial complexion transitions: Tuning defect structure to make better materials," *University of Illinois at Urbana-Champaign – Department of Materials Science and Engineering*, February 2019, Urbana, IL.

[L25] "Promoting beneficial complexion transitions: Using defects to make better materials," *Dartmouth College – Thayer School of Engineering*, January 2019, Hanover, NH.

[L24] "Enabling tough and stable nanocrystalline metals through the incorporation of amorphous complexions," *International Conference on Plasticity, Damage, and Fracture*, January 2019, Panama City, Panama.

[L23] "Decorating defects with segregating dopants to tailor mechanical properties," *Materials Science & Technology (MS&T) Conference and Exhibition*, October 2018, Columbus, OH.

[L22] "Dislocation-assisted linear complexion formation in body-centered cubic and face-centered cubic alloys," *Society of Engineering Science (SES) Annual Technical Meeting*, October 2018, Madrid, Spain. (KEYNOTE)

[L21] "Stabilization and toughening of nanocrystalline alloys through the incorporation of amorphous complexions," *THERMEC International Conference on Processing and Manufacturing of Advanced Materials*, July 2018, Paris, France.

[L20] "In situ mechanical testing of hierarchical and gradient nanostructures," *International Conference on Metallurgical Coatings and Thin Films (ICMCTF)*, April 2018, San Diego, CA.

[L19] "Promoting Beneficial Grain Boundary Phase Transitions with Segregation Engineering," *University of Pennsylvania – Department of Materials Science and Engineering*, April 2018, Philadelphia, PA.

[L18] "Manipulating the Structure and Properties of Nanocrystalline Metals using Segregation Engineering," *University of California, Berkeley – Department of Mechanical Engineering*, March 2018, Berkeley, CA.

[L17] "Modeling of complexion transitions at one- and two-dimensional defects," *The Minerals, Metals and Materials Society (TMS) Annual Meeting & Exhibition*, March 2018, Phoenix, AZ.

[L16] "Decorating defects with segregating dopants to tailor mechanical properties," *Materials Science & Technology (MS&T) Conference and Exhibition*, October 2017, Pittsburgh, PA.

[L15] "Complexion transitions in metals: Unique opportunities for mechanical behavior and materials processing," *The Minerals, Metals and Materials Society (TMS) Annual Meeting & Exhibition*, February 2017, San Diego, CA.

[L14] "Controlling Nanocrystalline Structure and Properties with Segregation Engineering," *California Institute of Technology – Department of Mechanical and Civil Engineering*, February 2017, Pasadena, CA.

[L13] "Promoting Beneficial Grain Boundary Phase Transitions with Segregation Engineering," *University of California, Santa Barbara – Materials Department*, November 2016, Santa Barbara, CA.

[L12] "Using Grain Boundary Complexion Transitions to Toughen Nanocrystalline Metals," *University of California, Irvine - Department of Chemical Engineering and Materials Science*, October 2016, Irvine, CA.

[L11] "Controlling Nanocrystalline Structure and Properties with Segregation Engineering," *Wuhan University of Technology*, September 2016, Wuhan, China.

[L10] "Adding Complexions to Nanostructured Metals to Achieve a Unique Combination of Strength and Ductility," *Functional and Nanomaterials 2025*, September 2016, Irvine, CA.

[L9] "Using Interfacial Structure to Control the Properties of Nanocrystalline Metals," *Sandia National Laboratories*, September 2016, Albuquerque, NM.

[L8] "Promoting Beneficial Grain Boundary Phase Transitions with Segregation Engineering," *University of Southern California – Materials Science and Engineering*, September 2016, Los Angeles, CA.

[L7] "Effect of Interfacial Doping and Complexion Formation on Nanocrystalline Mechanical Behavior," *Gordon Research Conference – Structural Nanomaterials*, July 2016, Hong Kong, China.

[L6] "Doping Nanocrystalline Alloys to Improve Strength and Toughness," *THERMEC International Conference on Processing and Manufacturing of Advanced Materials*, May 2016, Graz, Austria.

[L5] "Formation and Toughening Effects of Amorphous Interfacial Phases," *International Symposium on Plasticity*, January 2016, Kona, HI.

[L4] "Tuning Grain Boundary Structure to Control the Mechanical Behavior of Nanostructured Metallic Alloys," *Materials Research Society (MRS) Fall Meeting*, December 2015, Boston, MA.

[L3] "Controlling Grain Boundary Structure and Properties with Segregation Engineering," *University of Florida – Department of Materials Science and Engineering*, November 2015, Gainesville, FL.

[L2] "Nanoscale Amorphous Intergranular Films: Mechanical Properties and Interfacial Thermodynamics," *Materials Science & Technology (MS&T) Conference and Exhibition*, October 2015, Columbus, OH.

[L1] "Using amorphous complexions to tailor the mechanical behavior of nanostructured metals," *International Workshop on Interfaces*, September 2015, Bear Creek, PA.

Contributed Talks *(Presenter's name is in bold)***:**

[T11] **McCarthy MJ**, Rupert TJ. "Anisotropic mobility in faceted Σ11 <110> tilt FCC grain boundaries and the effect of subsequent doping," *The Minerals, Metals and Materials Society (TMS) Annual Meeting & Exhibition*, February 2020, San Diego, CA.

[T10] **Grigorian CM**, Rupert TJ. "Thick Amorphous Complexions Enabled by Compositional and Thermal Manipulation," *The Minerals, Metals and Materials Society (TMS) Annual Meeting & Exhibition*, February 2020, San Diego, CA.

[T9] **Turlo V**, Rupert TJ. "Discovery of a wide variety of linear complexions in metallic alloys," *Materials Science & Technology (MS&T) Conference and Exhibition*, September 2019, Portland, OR.

[T8] Schuler JD, Wardini JL, **Rupert TJ**. "Nanocrystalline Alloys with Disordered Complexions Probed by In Situ Mechanical Testing," *International Conference on Metallurgical Coatings and Thin Films (ICMCTF)*, May 2019, San Diego, CA.

[T7] **Schuler JD**, Barr C, Briggs S, Heckman NM, Hattar K, Boyce BL, Rupert TJ. "Irradiation and Mechanical Behavior of Nanocrystalline Alloys with Amorphous Intergranular Films," *The Minerals, Metals and Materials Society (TMS) Annual Meeting & Exhibition*, March 2019, San Antonio, TX.

[T6] **Hu Y**, Rupert TJ. "Atomistic modeling of interfacial segregation and structural transitions in ternary alloys," *Materials Science & Technology (MS&T) Conference and Exhibition*, October 2018, Columbus, OH.

[T5] **Rupert TJ**, McCarthy MJ. "Anisotropic mobility of faceted grain boundaries," *18th International Conference on the Strength of Materials (ICSMA)*, July 2018, Columbus, OH.

[T4] **Hu Y**, Rupert TJ. "Identifying interatomic potentials for the accurate modeling of interfacial segregation and structural transitions," *Materials Science & Technology (MS&T) Conference and Exhibition*, October 2017, Pittsburgh, PA. (poster)

[T3] **Schuler JD**, Rupert TJ. "Unambiguous Complexion Identification and Inspection in High Purity Binary Alloy Systems," *The Minerals, Metals and Materials Society (TMS) Annual Meeting & Exhibition*, February 2017, San Diego, CA.

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