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George Mason University
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a. REPORT	b. ABSTRACT	c. THIS PAGE			Yuri Mishin
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RPPR Final Report
as of 03-Jan-2023

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Proposal Number: 73001SM **Agreement Number: W911NF-18-1-0110**
INVESTIGATOR(S):

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Title: Stabilization and strengthening of nano-crystalline materials by alloying
Begin Performance Period: 12-Mar-2018 **End Performance Period:** 11-Sep-2022
Report Term: 0-Other

Submitted By: Yuri Mishin Email: ymishin@gmu.edu
Phone: (703) 993-3984

Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 0 **STEM Participants:**

Major Goals: The goal of the project was to advance the fundamental understanding of the thermodynamic and kinetic mechanisms of grain stabilization in nano-materials. The model systems chosen for this project are Cu-Ta alloys stabilized by Zener pinning of grain boundaries (GBs) (kinetic mechanism), and Cu-Bi alloys stabilized by reduction of the GB free energy (thermodynamic mechanism). A wide range of atomistic computer simulation methods were applied to investigate the thermodynamics and kinetics of GBs in the chosen alloys and the effect of GB segregation on their mechanical behavior. This required the development of a new interatomic potentials and computationally efficient algorithms for GB free energy calculations in the high-throughput mode. The simulations were performed on both polycrystalline samples, representing collective behavior of multiple GBs, and on individual, crystallographically characterized boundaries. In the latter case, the goal was to establish a link between GB structure, bicrystallography, and thermodynamic and kinetic factors of thermal stability. This project contributed to the fundamental knowledge base needed for the optimization of synthesis and processing routes and discovery of new thermally stable nanocrystalline alloys. This research was synergistic with experimental work on stabilized nanocrystalline alloys conducted at the Army Research Laboratory.

Accomplishments: The accomplishments are described in detail in the PDF file attached.

Training Opportunities: The postdoc and PhD student supported by this grant have been trained in a large spectrum of atomistic simulation methods, ranging from the construction of classical interatomic potentials to the implementation of large-scale MD and Monte Carlo simulations of structural evolution, diffusion and mechanical behavior of alloys. They further expanded their knowledge of the field by attending a number of workshops and conferences and giving presentations.

In particular, they attended the TMS-2018 Conference. The student has also attended the LAMMPS Workshop at Sandia National Labs (2019).

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Results Dissemination: The results obtained in this project have been presented in the following journal publications:

R. K. Koju, K. A. Darling, K. N. Solanki and Y. Mishin: Atomistic modeling of capillary-driven grain boundary motion in Cu-Ta alloys, Acta Materialia, 148, 311-39119 (2018). ?
Y. Mishin: Solute drag and dynamic phase transformations in moving grain boundaries, Acta Materialia 179, 383-395 (2019). ?
M. Rajagopalan, K.A. Darling, C. Kale, S.A. Turnage, R.K. Koju, B.C. Hornbuckle, Y. Mishin, K.N. Solanki: Nanotechnology enabled design of a structural material with extreme strength as well as thermal and electrical properties, Materials Today 31, 10-20 (2019).

C. Kale, S. Srinivasan, B.C. Hornbuckle, R.K. Koju, K. Darling, Y. Mishin, K.N. Solanki: An experimental and modeling investigation of tensile creep resistance of a stable nanocrystalline alloy, Acta Materialia 199, 141-154 (2020).

K. Darling, S. Srinivasan, R.K. Koju, B.C. Hornbuckle, J. Smeltzer, Y. Mishin, K.N. Solanki: Stress-driven grain refinement in a microstructurally stable nanocrystalline binary alloy, Scripta Materialia 191, 185-190 (2021).

Honors and Awards: Y. Mishin was elected Fellow of the American Physical Society (2020).

Protocol Activity Status:

Technology Transfer: Work on this project was conducted in close collaboration wth ARL. Atomistic simulations performed at GMU guide the experimental studies at ARL and at two other experimental groups (UNT and ASU). At the same time, the modeling and simulation work at GMU was driven by the goal of explaining and better understanding the experimental observations. The collaboration with the experimental groups also allowed us to focus on models and situations that were most relevant to experimental conditions and technological applications. Most of our publications were co-authored with ARL collaborators, some with UNT and ASU collaborators. The collaboration with ARL kept our work aligned with the Army missions.

The following patent application has been approved:

“Extreme Creep Resistant Nano-Crystalline Metallic Materials”, Inventors: L. J. Kecskes, K. A. Darling, R. S. Mishra, Y. Mishin, K. N. Solanki, and M. Rajagopalan. U.S. Patent 10,766,071.

PARTICIPANTS:

Participant Type: PD/PI
Participant: Yuri Mishin
Person Months Worked: 3.00 **Funding Support:**
Project Contribution:
National Academy Member: N

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Raj K Koju
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Publication Location:
Article Title: Atomistic modeling of capillary-driven grain boundary motion in Cu-Ta alloys
Authors: R.K. Koju, K.A. Darling, K.N. Solanki, Y. Mishin
Keywords: Atomistic modeling, Grain boundary, Zener pinning, Cluster precipitation
Abstract: Nanocrystalline Cu-Ta alloys are emerging as a new class of structural materials preserving the nano-scale grain size up to the melting point of Cu. This extraordinary structural stability is caused by the strong pinning of grain boundaries (GBs) by Ta nano-clusters precipitating from the unstable solid so- lution after mechanical alloying. Many aspects of the Ta stabilization effect remain elusive and call for further experimental and simulation work. In previous atomistic computer simulations of stress-driven GB migration [JOM 68, 1596 (2016)], the GBecluster interactions in Cu-Ta alloys have been studied for several different compositions and GB velocities. The results have pointed to the Zener pinning as the main mechanism responsible for the grain stabilization. This paper extends the previous work to the motion of individual GBs driven by capillary forces whose magnitude is similar to that in real nano- crystalline materials. Both the impingement of a moving GB on a set of Ta cl
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Article Title: Solute drag and dynamic phase transformations in moving grain boundaries
Authors: Y. Mishin
Keywords: Modeling and simulation, Grain boundary, Solute drag, Interface phases
Abstract: A discrete model and the regular solution approximation are applied to describe the effect of grain boundary motion on grain boundary phase transformations in a binary alloy. The model predicts all thermodynamic properties of the grain boundary and the solute drag force, and permits a broad exploration of the parameter space and different dynamic regimes. The grain boundary phases continue to exist in the moving grain boundary and show a dynamic hysteresis loop, a dynamic critical line, and other features that are similar to those for equilibrium phases. Grain boundary motion strongly affects the relative stability of the phases and can even stabilize phases that are absolutely unstable under equilibrium conditions. Grain boundary phase transformations are accompanied by drastic changes in the boundary mobil- ity. The results are analyzed in the context of non-equilibrium thermodynamics. Unresolved problems and future work are discussed.
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Article Title: Nanotechnology enabled design of a structural material with extreme strength as well as thermal and electrical properties
Authors: M. Rajagopalan, K.A. Darling, C. Kale, S.A. Turnage, R.K. Koju, B.C. Hornbuckle, Y. Mishin, K.N. Solan
Keywords: Materials design, nanotechnology, extreme strength
Abstract: The potential benefits of nanocrystalline (NC) alloys for use in various structural applications stem from their enhanced mechanical strengths. However, deformation-induced grain growth in NC materials reduces the strength and is a widely reported phenomenon occurring even at low- temperatures. Controlling such behavior is critical for the maturation of bulk nanocrystalline metals in various advanced engineering applications. Here, we disclose the mechanism by which grain boundary sliding and rotation are suppressed when a NC material is truly thermo-mechanically stabilized against grain growth. Unlike in any other known nanocrystalline metals, the absence of sliding and rotation during loading, at extreme temperatures, is related to short-circuit solute diffusion along the grain boundaries causing the formation of solute clusters and thus a significant change of the grain boundary structures. The departure of this unusual behavior from the well-established norm leads to a strong enhan
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Volume: 199 Issue: First Page #: 141
Date Submitted: 8/31/20 12:00AM Date Published: 10/1/20 4:00AM
Publication Location:
Article Title: An experimental and modeling investigation of tensile creep resistance of a stable nanocrystalline alloy
Authors: C. Kale, S. Srinivasan, B.C. Hornbuckle, R.K. Koju, K. Darling, Y. Mishin, K.N. Solanki
Keywords: Nanocrystalline Tensile creep Transmission electron microscopy Atomistic simulations
Abstract: Nanocrystalline (NC) materials possess excellent room temperature properties, such as high strength, wear resistance, and toughness as compared to their coarse-grained counterparts. However, due to the excess free energy, NC microstructures are unstable at higher temperatures. Significant grain growth is observed already at moderately low temperatures, limiting the broader applicability of NC materials. Here, we present a design approach that leads to a significant improvement in the high temperature tensile creep resistance (up to 0.64 of the melting temperature) of a NC Cu-Ta alloy. The design approach involves alloying of pure elements to create a distribution of nanometer sized solute clusters within the grains and along the grain boundaries. We demonstrate that the addition of Ta nanoclusters inhibits the migration of grain boundaries at high temperatures and reduces the dislocation motion. This leads to a highly unusual tensile creep behavior, including the absence of any apprec
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Date Submitted: 10/8/20 12:00AM Date Published: 1/1/21 5:00AM
Publication Location:
Article Title: Stress-driven grain refinement in a microstructurally stable nanocrystalline binary alloy
Authors: K.A. Darling, S. Srinivasan, R.K. Koju, B.C. Hornbuckle, J. Smeltzer, Y. Mishin, K.N. Solanki
Keywords: Nanocrystalline material Grain refinement Thermally stable Recrystallization
Abstract: Deformation-induced grain-growth in nanocrystalline materials is a widely-reported phenomenon that has been attributed to grain boundary (GB) processes. In this paper, we report on the opposite phe- nomenon, wherein a stable nanocrystalline (NC) Cu-Ta alloy undergoes a further refinement of the nano- grains during severe plastic deformation (SPD). SPD up to 250% results in a significant grain-size re- duction despite the 350°C increase in temperature caused by the deformation process. Experiments and atomistic-simulations show that this unexpected grain-refinement is a direct result of well-dispersed Ta- nanoclusters throughout grain centers and along GBs acting as kinetic-pinning agents and suppressing GB processes that occur during recrystallization.
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Intellectual Property Type: Patent Date Received: **31-Aug-2020**
Patent Title: Extreme Creep Resistant Nano-Crystalline Metallic Materials
Patent Abstract:
Patent Number: 10,766,071
Patent Country: USA
Application Date: 02-Dec-2019 Application Status: 3
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Patent Title: Extreme Creep Resistant Nano-Crystalline Metallic Materials
Patent Abstract:
Patent Number: 10,766,071
Patent Country: USA
Application Date: 02-Dec-2019 Application Status: 3
Date Issued: 08-Sep-2020

Partners

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RPPR Final Report
as of 03-Jan-2023

I certify that the information in the report is complete and accurate:
Signature: Yuri Mishin
Signature Date: 1/3/23 12:51PM

Stabilization and strengthening of nanocrystalline materials by alloying

Principal Investigator: Y. Mishin

Department of Physics and Astronomy, MSN 3F3, George Mason University, Fairfax, VA 22030

AWARD FROM THE U.S. ARMY RESEARCH OFFICE

Agreement Number: W911NF-18-1-0110

December 28, 2022

Final Report

Reporting period: March 12, 2018 to September 11, 2022

Major Goals

The goal of the project was to advance the fundamental understanding of the thermodynamic and kinetic mechanisms of grain stabilization in nano-materials. The model systems chosen for this project are Cu-Ta alloys stabilized by Zener pinning of grain boundaries (GBs) (kinetic mechanism), and Cu-Bi alloys stabilized by reduction of the GB free energy (thermodynamic mechanism). A wide range of atomistic computer simulation methods were applied to investigate the thermodynamics and kinetics of GBs in the chosen alloys and the effect of GB segregation on their mechanical behavior. This required the development of a new interatomic potentials and computationally efficient algorithms for GB free energy calculations in the high-throughput mode. The simulations were performed on both polycrystalline samples, representing collective behavior of multiple GBs, and on individual, crystallographically characterized boundaries. In the latter case, the goal was to establish a link between GB structure, bicrystallography, and thermodynamic and kinetic factors of thermal stability. This project contributed to the fundamental knowledge base needed for the optimization of synthesis and processing routes and discovery of new thermally stable nanocrystalline alloys. This research was synergistic with experimental work on stabilized nanocrystalline alloys conducted at the Army Research Laboratory.

Accomplishments during the reporting period

Tensile creep deformation of Cu-Ta alloys

Several research directions were pursued in this project. One of them was the modeling of tensile creep deformation of Cu-Ta alloys. Previous work of the ARL and ASU collaborators [K. A. Darling et al, Nature 537, 378-381 (2016)] has revealed highly unusual creep behavior of Cu-Ta alloys. In pure metals, the creep rate increases as the grain size decreases. For grain sizes in the nanometer range, the creep rates become high due to the contribution of the large grain

boundary area by the Coble creep mechanism. By contrast, it was discovered that nano-crystalline Cu-Ta alloys exhibit extremely low creep rates in comparison with pure Cu with the same grain size under the same (temperature, stress) test conditions.

In the previous work mentioned above, the creep tests were conducted in the compression mode. It was hypothesized that the role of Ta alloying was to block the grain boundary processes such as grain boundary diffusion, grain boundary sliding and grain rotation. However, no direct evidence to support this supposition was presented at the time. Furthermore, the ARL and ASU collaborators are currently performing similar creep tests in the tension mode. The difference in the creep rates between the Cu-Ta alloys and pure Cu is even more impressive than in the compression case.

To support the experimental observations and help understand the underlying fundamental mechanism, systematic atomistic computer simulations have been launched. Some of the results are reported below.

The nanocrystalline material tested had the grain size of about 30 nm with random grain orientations. Ta was introduced into the system by semi-grand canonical Monte Carlo simulations. It was found that Ta formed nanometer-scale clusters with preferred locations at grain boundaries, although many clusters formed inside the grains as well. The average cluster size and the size distribution were very close to those found in experiments. Variations in the Ta content in the alloy only changed the number of clusters with little effect on their size, which was also consistent with experiment. Several Ta compositions were tested in addition to pure Cu.

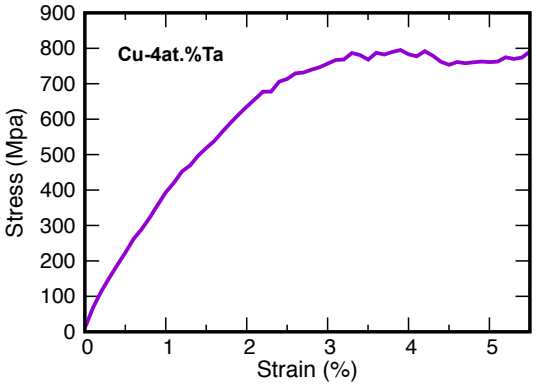

Figure 1: Stress-strain curve for the Cu-4at.%Ta alloy at the temperature of 1100 K showing the yield stress of 500 MPa and flow stress of 800 MPa.

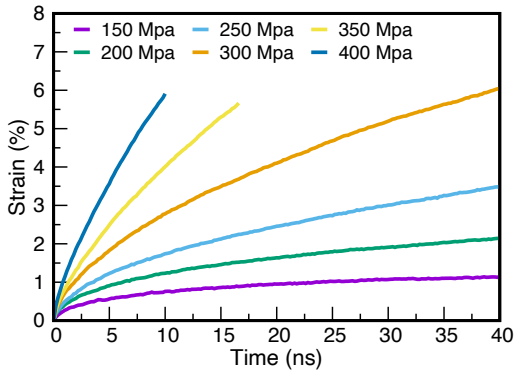

Figure 2: Strain versus time during creep tests of the Cu-4at.%Ta alloy at the temperature of 1100 K. The creep stresses are indicated in the legend.

The samples were first tested for uniaxial tension by ramping the strain to determine the yield stress. An example is shown in Fig.1 for the Cu-4at.%Ta alloy at the temperature of 1100 K. The creep stresses were chosen in the 150 to 400 MPa range, which is less than half of the flow stress. The creep tests were performed by applying a sustained tensile load of a chosen magnitude in the *x* direction while maintaining zero-stress conditions in the perpendicular (*y* and *z*) directions. After the initial fast deformation period corresponding to the primary creep stage, the creep rate $\dot{\varepsilon}$ became nearly constant, signifying the onset of steady-state creep. Examples of creep deformation curves are shown in Fig.2 for the particular case of the 1100 K tests. The steady-sate creep rate rapidly increases with the level of stress. Similar results were obtain for

other alloy compositions. An important observation was that the creep rate in Cu-Ta alloys was much smaller than the creep rate in pure Cu with the same grain size. Furthermore, the creep rate significantly decreased when more Ta was added to to the alloys, as illustrated in Fig.3. This observation is in agreement with the experimental results.

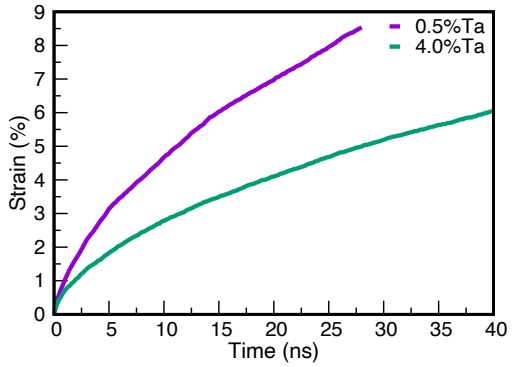

Figure 3: Stress-strain curve for two compositions of Cu-Ta alloys at the temperature of 1100 K. Note the suppression of the creep rate by adding more Ta.

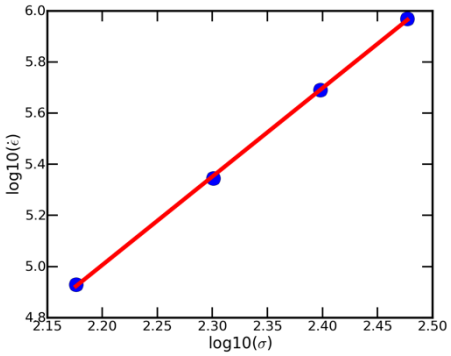

Figure 4: Log-log plot of the strain rate versus stress from tensile creep simulations of the Cu-4at.%Ta alloy at the temperature of 1100 K. The slope of the plot gives the stress exponent of about 3.5.

The simulation results allowed us to find the stress exponent *n* appearing with the creep law $\dot{\varepsilon} \propto \sigma^n$ (Fig.4). The latter was found to be about 3.5, which corresponds to the dislocation climb mechanism. The formation of an enhanced dislocation density was indeed found by visualizing the slip traces near grain boundaries and triple junctions.

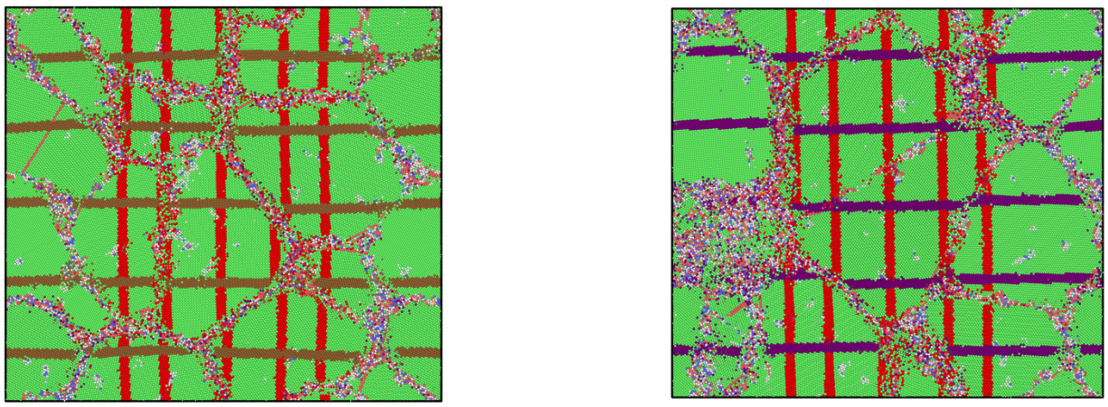

Figure 5: Typical projection of Cu-4at.%Ta alloy after a creep test at the temperature of 1100 K. The compression direction is normal to the page (left) or horizontal (right). The horizontal (purple) and vertical (blue) stripes represent two sets of artificial marker lines. The discontinuities and rotations of the marker lines are indicators of grain boundary sliding and grain rotation. The smearing of the marker lines when they cross grain boundaries was caused by grain boundary diffusion.

The marker line method was applied to identify the dominant creep mechanisms (Fig.5). The analysis indicates extensive grain boundary diffusion consistent with the Coble creep mechanism. The amount of grain boundary sliding and grain rotation is much smaller than in pure, which again is consistent with the experimental studies showing that the strain-rate sensitivity of the Cu-Ta alloys is small.

Thermal stability and mechanical properties of Cu-Ta alloys

In the previous work within this project, the creep tests of Cu-Ta were conducted in the compression mode. Our ARL and ASU collaborators have also performed similar creep tests in the tension mode. The results show that retardation of the creep rates in Cu-Ta alloys in comparison with pure Cu is even more impressive than in the compression case. To support the experimental observations and help understand the underlying fundamental mechanism, systematic atomistic computer simulations have been performed.

It was confirmed that Ta formed nanometer-scale clusters with preferred locations at GBs, although many clusters formed inside the grains as well. The average cluster size and the size distribution were very close to those found in experiments. While several alloy compositions were tested, the work was focused on the Cu-4at.%Ta alloys. A pure Cu sample with the same grains was studied for comparison. The creep tests were performed by applying a sustained stress and measuring the resulting strain as a function of time. The simulations were performed at 7 temperature and 5 different values of the stress σ (Fig.6).

The creep rate was found to follow the power law $\dot{\varepsilon} \propto \sigma^n$ at all temperatures studied. The stress exponent *n* obtained was found to be in good agreement with the experimental data. Figure 7 shows a $\log \dot{\varepsilon}$ versus $\log \sigma$ plot used for the calculation of the stress exponent *n*. Furthermore, from the temperature dependence of the strain rate at a fixed stress we have been able to evaluate the activation energy of the secondary creep process. Figure 8 shows an example of an Arrhenius plot from which the activation energy of 1.48 was extracted. This value is close to the activation energy of Ta GB diffusion, confirming that the creep process fall into the Cobble creep category and that the deformation is controlled by GB processes.

To demonstrate improvement in the creep resistance by the addition of Ta to nanocrystalline Cu, creep simulations were performed for pure nanocrystalline Cu as well as Cu-Ta alloys with chemical compositions 0.5%Ta, 1at.%Ta, 2at.%Ta and 4at.%Ta at 1100 K under the applied stress σ = 300 MPa. The nanocrystalline pure Cu and Cu-Ta alloys with compositions up to 2at. %Ta displayed grain growth accompanied by grain rotation, twinning, dislocation emission and propagation. Figure 9 shows rapid grain growth in pure Cu during the deformation process. However, the Cu-4at.%Ta alloy easily survives the creep simulations, demonstrating significant elongation along the tensile direction with simultaneous compression in the lateral directions (Fig.10).

The results obtained are in excellent agreement with the experiments conducted at ARL and ASU, demonstrating that the addition of a few at.% of Ta drastically increases the structural stability and creep resistance of nanocrystalline Cu. They also reveal the underlying mechanisms of the creep deformation process, showing that the latter is controlled by GB processes such as GB diffusion, GB sliding and micro-rotation of the grains. The simulation results also produce process parameters that are difficult or impossible to obtain by experiment, such as the GB diffusivities, the stress exponent as a function of temperature, the activation energies of the primary and secondary creep processes, and many others.

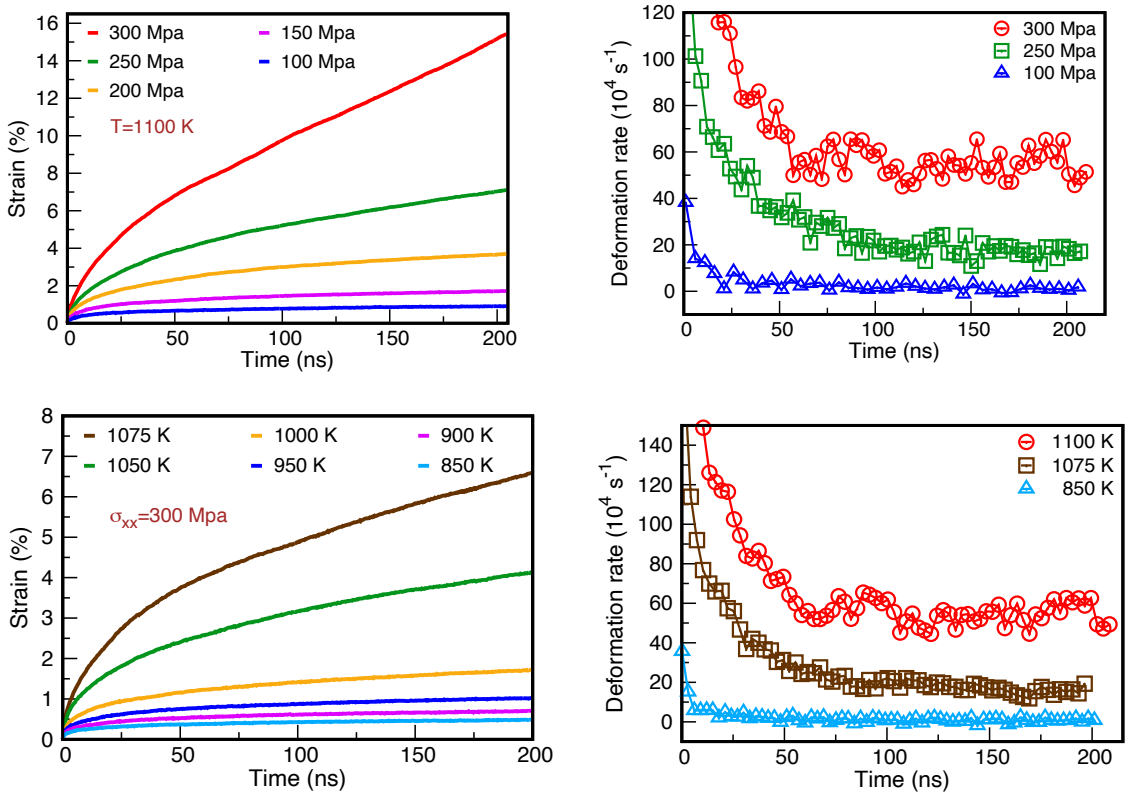

Figure 6: Creep deformation of the Cu-4at.%Ta alloy at different temperatures and applied stresses. The strain rate curves identify the primary and secondary creep regimes. Note that the steady-state creep rate increases with temperature and stress.

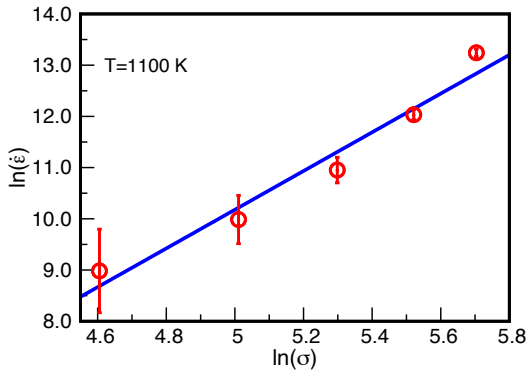

Figure 7: Strain rate as a function of stress for tensile creep in the Cu-4at. %Ta alloy at the temperature of 1100 K.

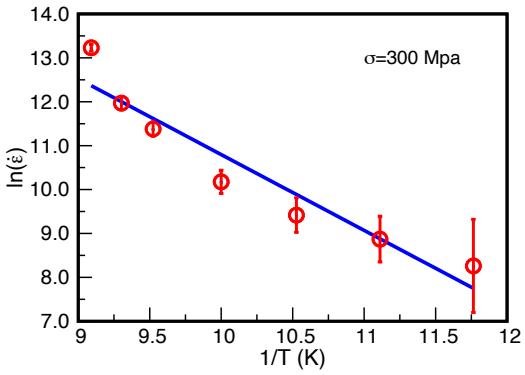

Figure 8: Arrhenius plot of the strain rate in the Cu-4at.%Ta alloy at the stress of 300 MPa.

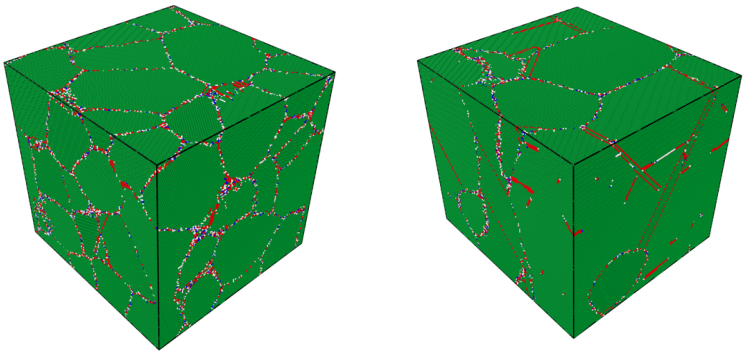

Figure 9: The initial (left) and final (right) structures of nanocrystalline Cu during the creep test under the stress of 300 MPa at the temperature of 1000 K. Note the significant grain growth.

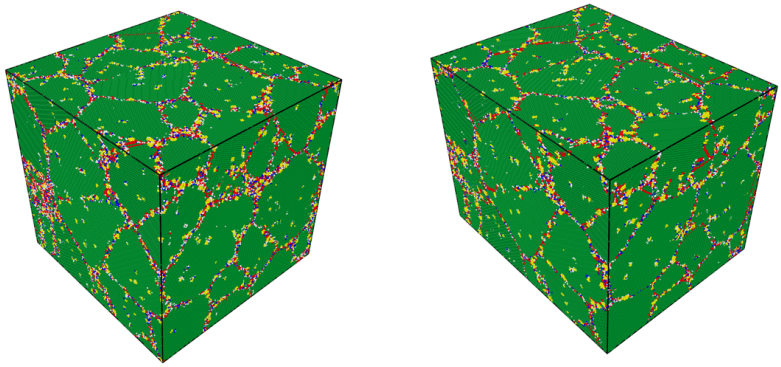

Figure 10: The initial (left) and final (right) structures of nanocrystalline Cu-4at. % Ta alloy during the creep test under the stress of 300 MPa at 1000 K. The grain growth is negligibly small, demonstrating high structural stability.

Microstructure stability of Cu-Ta alloys under severe plastic deformation

One of the weaknesses of nanocrystalline materials is the lack structural stability resulting in grain growth at elevated temperatures (in some cases, even at room temperature). The grain growth is especially extensive if the material is plastically deformed in addition to exposure to high temperatures; and it is even more extensive under severe plastic deformation. Stress-temperature induced grain growth in nanocrystalline materials has been widely reported in the literature for many metals and alloy systems.

Meanwhile, our previous collaborative work with ARL and ASU researchers, sponsored by this award, has shown that nanocrystalline Cu-Ta alloys exhibit excellent thermal stability up to very high temperatures. The microstructure of these alloys is strongly stabilized by a distribution of Ta nanoclusters inside the grains and especially at grin boundaries.

During the reporting time period, we addressed the question of whether these alloys are also stable under severe plastic deformation occurring, for example, during machining or friction stir processing. Specifically, our goal was to determine if severe plastic deformation causes grain growth and other microstructure changes that typically occur in other nanomaterials.

To answer this question, experiments were performed in which a nanocrystalline Cu-Ta material was subject to severe plastic deformation by machining. Advanced electron microscopy was applied to characterize and compare the microstructures before and after the deformation. These experiments were integrated with atomistic computer simulations capable of providing insight into the microscopic mechanisms responsible for the observed grain boundary processes. An unusual phenomenon was discovered wherein the nanocrystalline alloys undergoes a significant **refinement** of the nanograins under severe plastic deformation at an elevated temperatures.

This highly unusual behavior is contrary to the commonly observed grain growth and results in enhanced wear and fatigue resistance. Both experiments and atomistic simulations have shown that the Ta nanoclusters prevent the grain growth by pinning the grain boundaries and arresting lattice dislocations. These pinning processes strongly stabilize the nanostructure and block the grain growth mechanisms that normally operate in other nanocrystalline materials under severe deformation conditions, such as the shear-coupled grain boundary migration, grain boundary sliding, and grain rotation. Furthermore, by arresting the dislocations inside the grains, the Ta clusters create a high dislocation density that drives processes such as grain fragmentation and dynamic recrystallization, while simultaneously restraining the growth of new grains. As a result, a 250% plastic deformation of the nanocrystalline Cu-Ta alloy by machining causes a significant **reduction** in the grain size, despite the increase in temperature due to the heat released during the deformation. The inherent immiscibility of these Cu-Ta alloys puts them among the most resilient alloys known today. Some of the computer simulations preformed by our team are highlighted below.

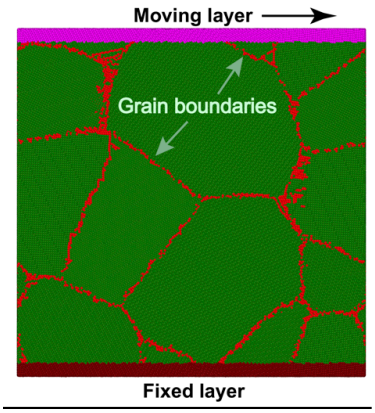

Figure 11: Cross-section of the simulation block used for the modeling of severe plastic deformation of nanocrystalline Cu-Ta alloy. The material is attached to two parallel layers with fixed atomic positions. The lower layer is fixed while the upper layer moves to the right producing shear deformation. The grain boundaries are shown in red.

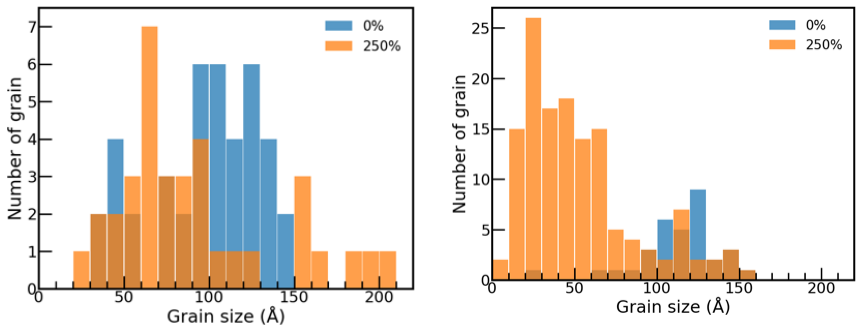

Figure 12: Grain size distribution in (left) pure Cu and (right) nanocrystalline Cu-3Ta alloy before and after severe shear deformation by 250%. The results were obtained by MD simulations at a temperature of 673 K. Not the formation of large (200 nm) grain upon deformation of nanocrystalline, by contrast to massive grain refinement observed in the Cu-Ta alloy.

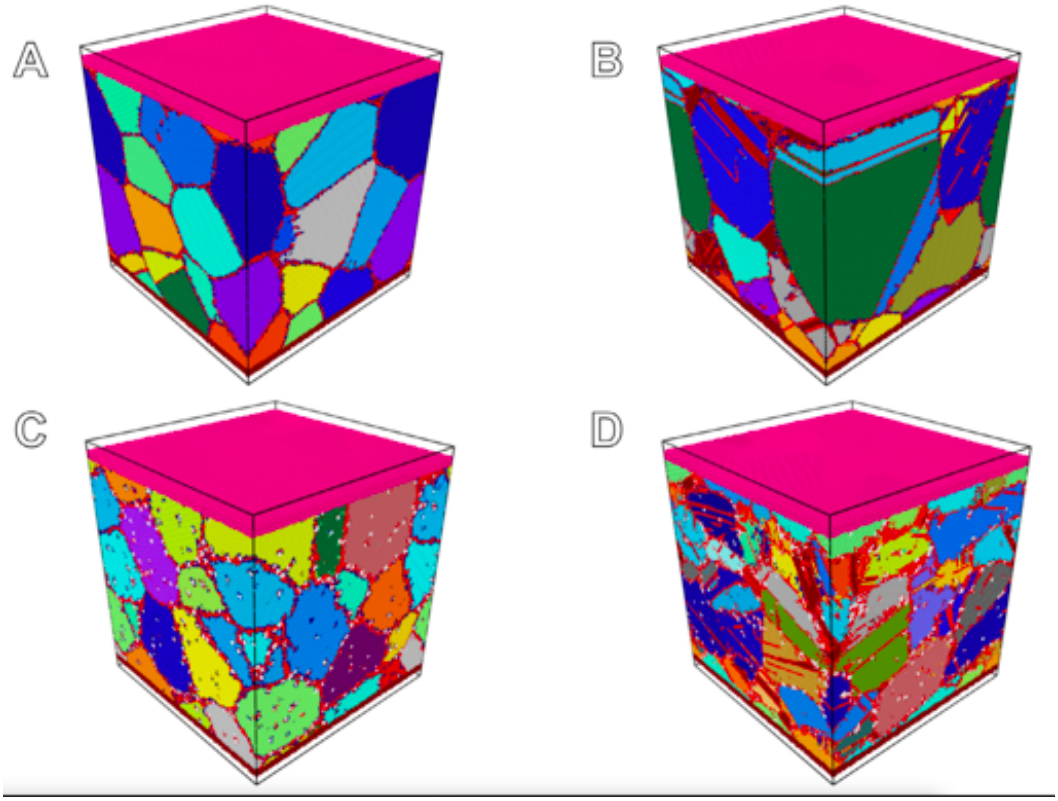

Figure 13: Comparison of grain structures of (A,B) pure nanocrystalline Cu and (C,D) nanocrystalline Cu-3Ta alloy before (A,C) and after (B,D) severe shear deformation to 250% strain at the temperature of 673 K. The grains are colored according to lattice orientation. The grain boundary, HCP, and other structural atoms are colored in red. Ta clusters are colored in white.

Training Opportunities

The postdoc and PhD student supported by this grant have been trained in a large spectrum of atomistic simulation methods, ranging from the construction of classical interatomic potentials to the implementation of large-scale MD and Monte Carlo simulations of structural evolution, diffusion and mechanical behavior of alloys. They further expanded their knowledge of the field by attending a number of workshops and conferences and giving presentations.

In particular, they attended the TMS-2018 Conference. The student has also attended the LAMMPS Workshop at Sandia National Labs (2019).

Results Dissemination

The results obtained in this project have been presented in the following journal publications:

R. K. Koju, K. A. Darling, K. N. Solanki and Y. Mishin: Atomistic modeling of capillary-driven grain boundary motion in Cu-Ta alloys, *Acta Materialia*, **148**, 311-39119 (2018).

Y. Mishin: Solute drag and dynamic phase transformations in moving grain boundaries, *Acta Materialia* **179**, 383-395 (2019).

M. Rajagopalan, K.A. Darling, C. Kale, S.A. Turnage, R.K. Koju, B.C. Hornbuckle, Y. Mishin, K.N. Solanki: Nanotechnology enabled design of a structural material with extreme strength as well as thermal and electrical properties, *Materials Today* **31**, 10-20 (2019).

C. Kale, S. Srinivasan, B.C. Hornbuckle, R.K. Koju, K. Darling, Y. Mishin, K.N. Solanki: An experimental and modeling investigation of tensile creep resistance of a stable nanocrystalline alloy, *Acta Materialia* **199**, 141-154 (2020).

K. Darling, S. Srinivasan, R.K. Koju, B.C. Hornbuckle, J. Smeltzer, Y. Mishin, K.N. Solanki: Stress-driven grain refinement in a microstructurally stable nanocrystalline binary alloy, *Scripta Materialia* **191**, 185-190 (2021).

Honors and Awards

Y. Mishin was elected Fellow of the American Physical Society (2020).

Technology Transfer

Work on this project was conducted in close collaboration wth ARL. Atomistic simulations performed at GMU guide the experimental studies at ARL and at two other experimental groups (UNT and ASU). At the same time, the modeling and simulation work at GMU was driven by the goal of explaining and better understanding the experimental observations. The collaboration with the experimental groups also allowed us to focus on models and situations that were most relevant to experimental conditions and technological applications. Most of our publications were co-authored with ARL collaborators, some with UNT and ASU collaborators. The collaboration with ARL kept our work aligned with the Army missions.

The following patent application has been approved:

“Extreme Creep Resistant Nano-Crystalline Metallic Materials”, Inventors: L. J. Kecskes, K. A. Darling, R. S. Mishra, Y. Mishin, K. N. Solanki, and M. Rajagopalan. U.S. Patent 10,766,071.