FINAL SCIENTIFC/TECHNICAL REPORT

Report Title: An Integrated Study on a Novel High Temperature High Entropy Alloy

Type of Report: Final Scientific and Technical

Reporting Period Start Date: 10/1/2013

Reporting Period End Date: 9/30/2016

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Date Report was Issued: December 2016

DOE Award Number: DE-FE-0011550

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DISCLAIMER:

ABSTRACT

This report summarizes our recent works of theoretical modeling, simulation, and experimental validation of the simulation results on the new refractory high entropy alloy (HEA) design and oxide doped refractory HEA research. The simulation of the stability and thermal dynamics simulation on potential thermal stable candidates were performed and related HEA with oxide doped samples were synthesized and characterized. The HEA *ab initio* density functional theory and molecular dynamics physical property simulation methods and experimental texture validation techniques development, achievements already reached, course work development, students and postdoc training, and future improvement research directions are briefly introduced.

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EXECUTIVE SUMMARY

In modeling and simulation part, we studied the mechanical and optical properties of HfNbTaTiZr high entropy alloy (HEA) based on the maximum entropy model. The results match well with available similar HEAs' experiment data. From *ab initio* density functional theory (DFT) method simulation, we optimized the geometry cell structures of body centered cubic (BCC) MoNbTaVW, BCC HfNbTaTiZr, and face centered cubic (FCC) CoCrFeMnNi HEAs, and mechanical and electronic structure properties are studied and details are introduced in the next section. This confirmed method using the simplest *ab initio* models to predict physical properties, when applied to large scale materials screening, will save materials developing time since the calculation is reduced to minimum, as we have known that the accurate *ab initio* DFT based simulation cost is in an exponential relation to the cell size and atom numbers when solving Schrödinger equation of the studied material model. We have studied the interface structure of MoNbTaVW/Y_2O_3, structure optimization, bonding energy simulation, and molecular dynamics (MD) stability simulation. In the brittleness mechanism study, the dislocation dynamics (DD) model simulation of S doped Nickel (Ni) metal systems verified our compress and decompress texture experiment results very well. The

In collaboration with NETL and starting from *ab initio* DFT calculation combined with CALculation of PHAse Diagrams (CALPHAD) technique, we have discovered two refractory senary HEAs MoNbTaTiVW and HfNbTaTiVZr. The two HEAs were then synthesized and characterized in our Louisiana State University (LSU) labs. By further tuning up, the application required properties can be reached, here for sure more studies are needed. Our dislocation dynamics (DD) model simulation on high pressure S doped Ni metal model systems shows that the pressure-induced S doped Ni metal ductility can be well explained by strain - stress changes and dislocation density changes. This study contradicts traditional Ni metal embrittlement mechanism and sheds light on the improvement of ductility study of FCC metals and doped complex systems. The pressure induced ductility study can be extended to other materials study such as metal/oxide or ceramic in material science and earth science study.

In the experimental validation part, we collaborated with LSU, synthesized the optimized senary HEAs MoNbTaTiVW and HfNbTaTiVZr, and MoNbTaVW/Y_2O_3 model system samples. The samples were characterized by x-ray diffraction (XRD), scanning electron microscope (SEM), and thermogravimetric analysis (TGA). The dislocation dynamics texture experiment was conducted at Lawrence Berkeley National Lab (LBNL) beamline 12-2-2.

Ten students and two postdocs were trained to setup the needed ab initio DFT and MD simulation models, perform high performance computing (HPC) simulations, process and analyze the simulation data sets, write analysis reports, and present the results and conclusions through participating group meeting, workshop, international conferences etc. They were also trained in sample preparation, XRD, TGA, and synchrotron XRD materials characterization techniques such as the full width at half maximum (FWHM) synchrotron XRD data processing radial texture measurement and data interpretation. All the recent advances were included into the Advanced Topics in Computational Science course. One postdoc, Dr. Starovoytov, was hired recently as a new tenure track full time faculty in the department, with starting funds from IBM and NSF CIMM project seed support. Supported by this project, five peer reviewed papers and three conference papers were published. They are given in the Bibliography. Through this DOE project, the collaboration with IBM Company, LBNL, HPSTAR institute, and NETL is enhanced.

REPORT DETAILS

Simulation Methods

In this project, the materials design package (MedeA) is used for all the models setup. All of our MD simulation is based on the DFT method. All the HPC MD simulations were performed on Louisiana Optical Network Initiative (LONI) machines qb2 and eric. In the ab initio DFT and MD simulation, we first studied the mechanical and optical properties of HfNbTaTiZr high entropy alloy (HEA) based on the maximum entropy model shown in Fig. 1.

(a) (b)

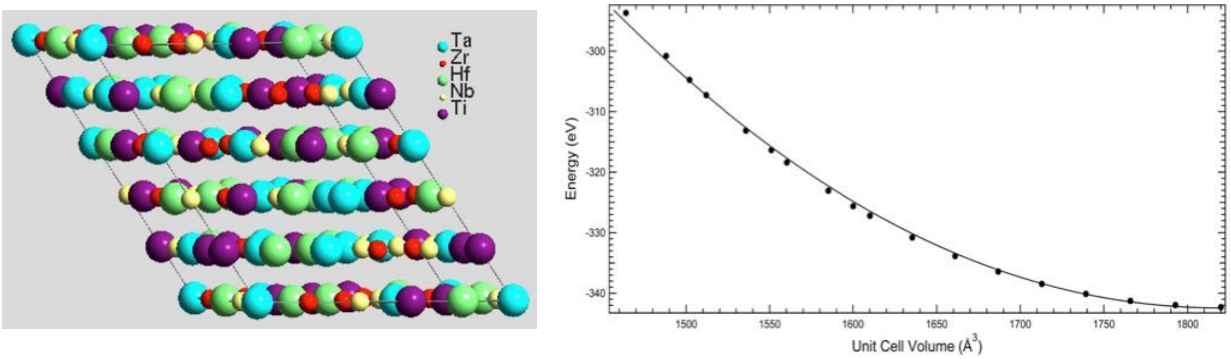

Fig. 1. (a) The model used in simulation for HfNbTaTiZr. (b). The black dot represents compression data. According to the best fit solid line of the Birch–Murnaghan equation, the bulk modulus is calculated to be 198 GPa.

Although the above method, models, and simulation results are successful, the expensive computing expense is relative high since they have 100 plus atoms in the simulation systems and current ab initio simulation methods expense is exponentially increasing when the system size and atom number increase. To save computing time and keep the same accuracy, we recently studied three HEA model systems: BCC MoNbTaVW, BCC HfNbTaTiZr, and FCC CoCrFeMnNi. The simulation BCC models are shown in Fig. 2 and the FCC CoCrFeMnNi models are shown in Fig. 3. Since both BCC and FCC structures studied now are simplest the computing expense is minimized and the screening application is accelerated when applying this method to a large scale. The physical properties is a weighted summation over the available individual model simulations, based on symmetry analysis. The successful confirmation of the three model HEA systems gives us a solid base for further materials design and validation.

(a) (b)

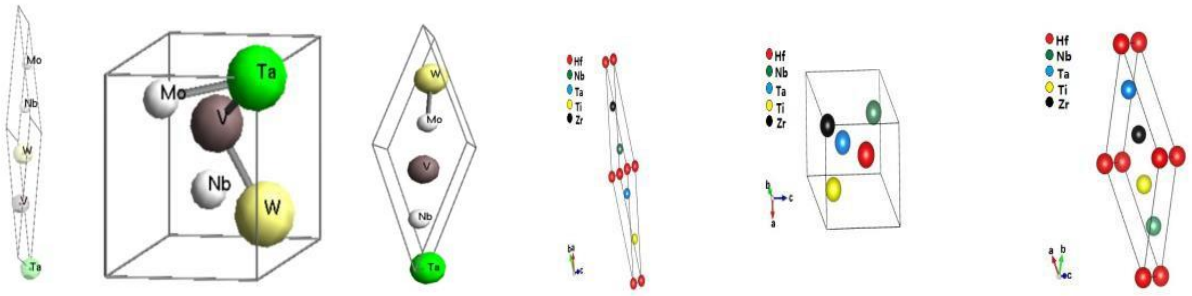

Fig. 2. Three ordered (a) MoNbTaVW and (b) HfNbTaTiZr structures were built and

optimized for efficient mechanical electronic structure, and thermal dynamics properties screening and prediction.

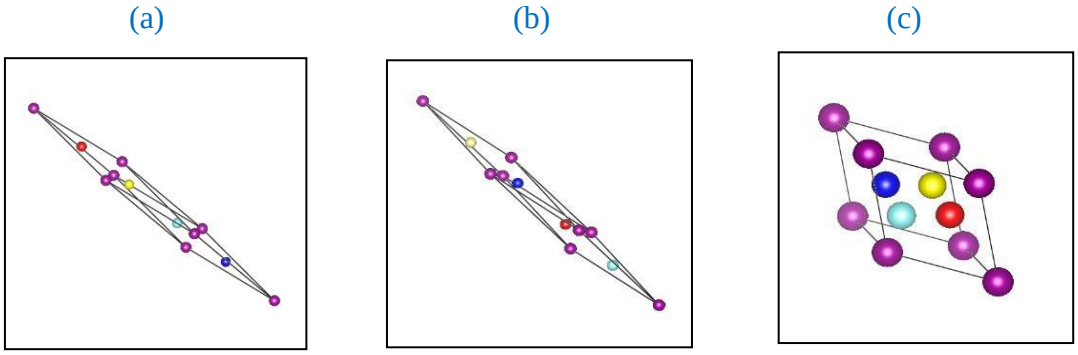

Fig. 3. Models of the three optimized five atom FCC CoCrFeMnNi HEA structures used for modeling and calculations.

Thermodynamically, the surface energy can be expressed as:

$$\delta G = \delta \int \gamma \, dAss \quad (1)$$

where G is the total interface energy of the system, γ is the solid−solid interface energies, and A_{SS} is the solid−solid interface area. From the above equation, the interface energy can be calculated by comparing the energy differences between bulk states and interfaced states. The lower the interface energies, the more stable the interface structure. We studied the MoNbTaVW/Y_2O_3 sandwich models, and based on the thermal dynamics data and stability analysis at different temperatures, the samples with different nano Y_2O_3 concentrations were synthesized and structures and oxidation resistance properties characterized.

The effects of dislocation development on a model system Ni-S, S as a dopant, were evaluated using the ParaDiS software package. The ParaDiS package is based on non-singular continuum theory of dislocations that allows accurate numerical calculations of dislocations in terms of multiple dislocation nodes. Since ParaDiS is typically used for micro scale dislocation dynamics simulations, we set up isotropic models occupying $1 \times 1 \times 1$ μm^3 space and implemented FCC_0 mobility law for static pressure simulation. As a model system studied, different Ni/S ratios were indirectly implemented by changing corresponding shear moduli and Poisson's ratios obtained from our ab initio simulations. We have tested DD ParaDiS on this model system and the simulation results explain the experiment data very well. The method can be extended to DD study and evaluation in novel HEA and doped HEAs development.

Experimental Methods

We used mechanical alloying (MA) plus arc melting method to synthesize HEAs and HEA/oxide samples for further characterization. The metal and oxide were ball-milled at room temperature and then pressed into a cylinder pellet. After clean, the sample was characterized by powder XRD analysis.

Small samples were put directly in TGA for oxidation analysis. The synthesized specimens were examined from the cross-section images using scanning electron microscopy (SEM: JEOL JEM 2010 200kV). Crystallographic characteristics observations of specimens were conducted by using XRD with Cu Kα radiation. Thermal analyses of the oxidized specimens were conducted using TGA (model: STA 449 C Jupiter, Netzsch). The TGA experiments were carried out from

room temperature up to ~ 1500 K with a controlled heating/cooling rate. The dislocation dynamics texture study was conducted at LBNL by adding radial shear stress to the DAC loaded sample. The Fit2D and MAUD software were used to process the texture data.

Results and Discussions

We have calculated mechanical and electronic structure properties of MoNbTaVW, HfNbTaTiZr, and CoCrFeMnNi HEAs. The results of CoCrFeMnNi HEA simulations are shown in the following Fig. 4 and 5.

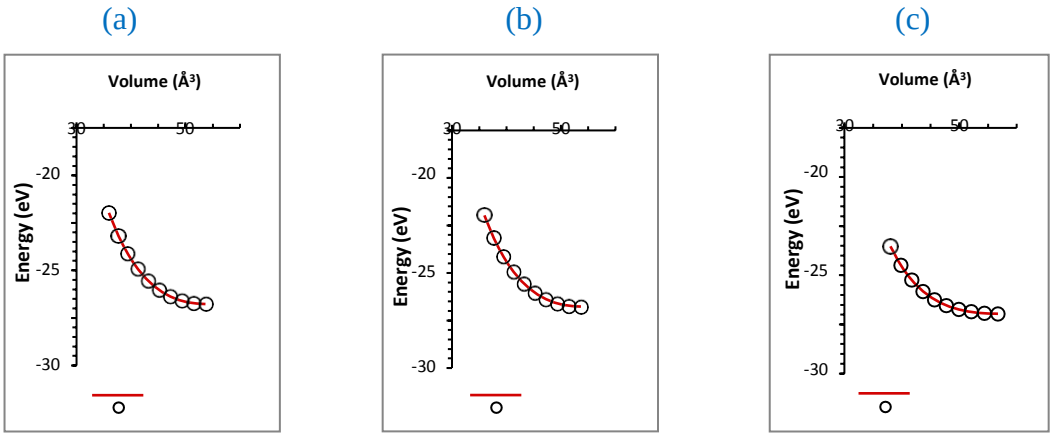

Fig. 4. Plots of energy vs. volume for corresponding structures a, b, and c seen in Fig. 3. The line of best fit shown in each plot is the Birch-Murnaghan equation of states, with the fit being done by least squares analysis solving for the bulk modulus of the respective structure. The plots individually gave bulk modulus values of 264, 256, and 117 GPa, with weights of 0.2, 0.2, and for a, b, and c respectively.

The bulk modulus was originally calculated using PAW local density approximation (LDA) pseudopotentials, but this gave a value of over 300 GPa, which was vastly different compared to literature values. However, upon switching to PAW generalized gradient approximation (GGA) pseudopotentials as reported above, the resulting bulk modulus was much closer to experimental values seem to fluctuate around approximately 140 GPa. Further, it appears to be well within the range obtained by other computational methods, which were between approximately 160 and 190 GPa. This is reasonable since for light weight metal alloy, PAW GGA normally gives better physical properties, lattice constants, mechanical

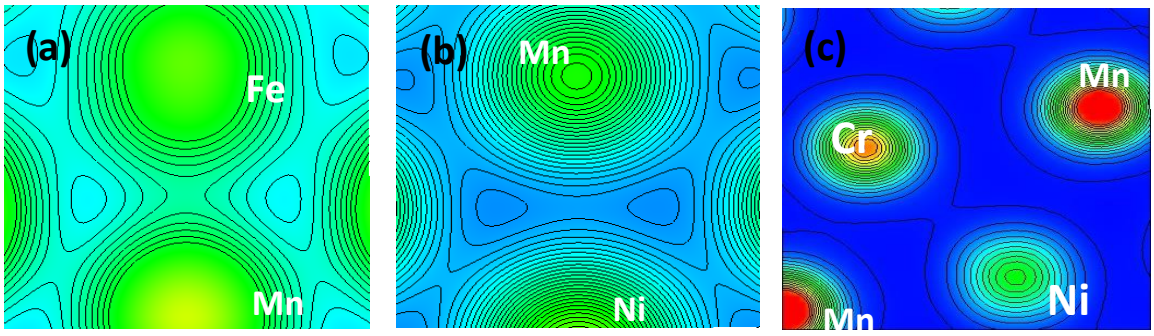

Fig. 5. Plots of electron charge density surrounding certain atoms within each structure shown in Fig. 3 correspondingly. Images generated using VESTA software application.

properties etc., predictions compared with relative experiment results. Also, each CoCrFeMnNi small structure was treated as paramagnetic. As such, future studies of spin polarized effects need to be investigate the influence of treating it as ferromagnetic and non-magnetic, since it seems that such differences can lead to significantly different results in theoretical models if spin polarization plays an important role in real application. Also, the electron density in the charge density contour plots shown in Fig. 5 (c) appear to be slightly enhanced between pairs of atoms rather than being equally shared amongst all surrounding metals, as one would expect of normal FCC metals. This seems to imply a partial covalent nature in the bonding between some of the atoms, but has only really observed in this one five atom structure. So far no literature images could be found to compare thus this is a specifically useful tool to analyze the chemical bonding in HEAs.

Similarly, no published Bader charge values were found for this HEA either. The results can be understood by considering the components' respective electronegativity values.

To sum up the CoCrFeMnNi HEA study, it seems that the results for the bulk modulus calculations were reasonably accurate, and thus indicate this method could be used to approximate the bulk modulus and other bulk mechanical properties of other HEA materials as well. Also, it seems the charge density data obtained appeared to indicate some potential for unexpected covalent nature in some of the bonds between the metal atoms, this is ahown in the Fig. 6 as well, which will need further investigation to quantifiably verify. These will provide important data for developing a system of accurately designed other HEA composition when spin polarization is needed to be considered.

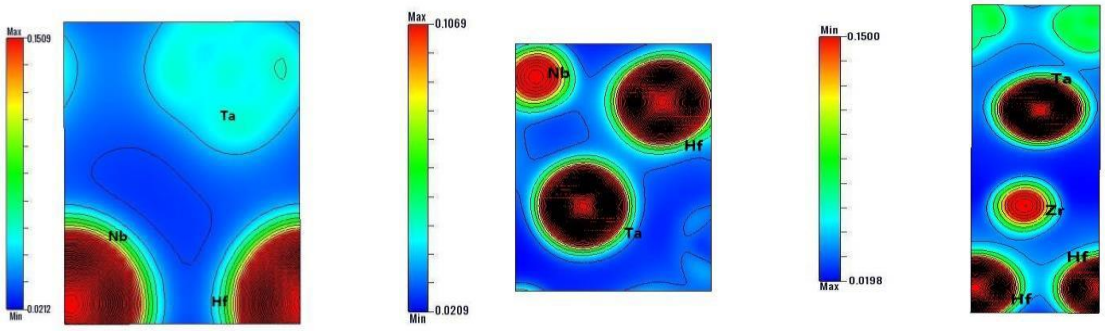

Fig. 6. Plots of electron charge density surrounding certain atoms within each HfNbTaTiZr Alloy structure shown in Fig. 2 (b) correspondingly.

The interface MoNbTaVW/Y_2O_3 sandwich model consists of 90 (16x5) transition metal atoms, 14 Y and 21 O atoms. This model represents the atomic physical interactions well while simplified the simulation expense especially for MD simulation. We analyzed the interatomic bonding and performed cluster analysis. Three samples of MoNbTaVW/Y_2O_3 with 0, 3, and 15 wt% Y_2O_3 dopants were synthesized through mechanic alloy plus arc melting. Then the SEM, XRD, and TGA analysis were performed to study the structure changes and oxidation resistance at high temperature. The SEM results are shown in Fig. 7, XRD in Fig. 8, and TGA in Fig. 9. It is observed that 0 wt% BCC MoNbTaVW is easy to form uniform bulk crystal while oxide doped

ones need extra force to reach the similar bulk. The SEM images in Fig. 7 show that there are pores inside the bulk samples and empty spaces between the crystal boundaries. Thus to make the HEA denser enough for device application, hot press or spark plasma sintering synthesis method may be applied. This is a potential research project in the near future.

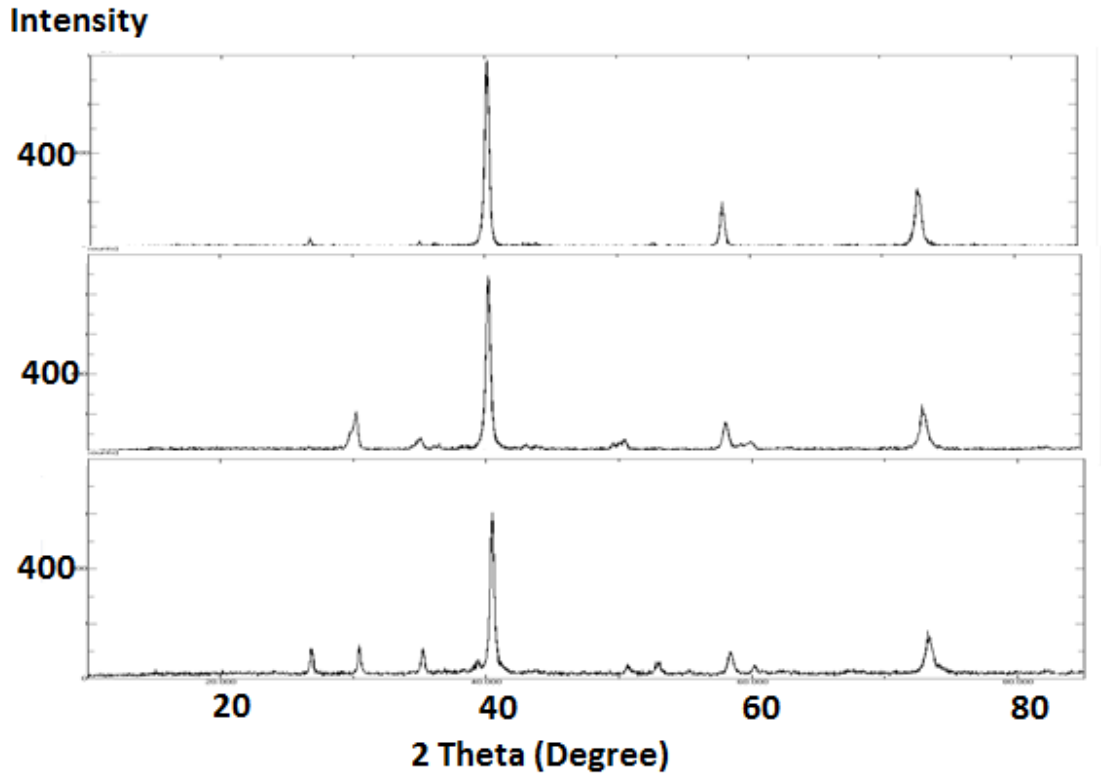

Fig. 7. SEM image of (a) 3 wt% and 15 wt% MoNbTaVW/Y_2O_3.

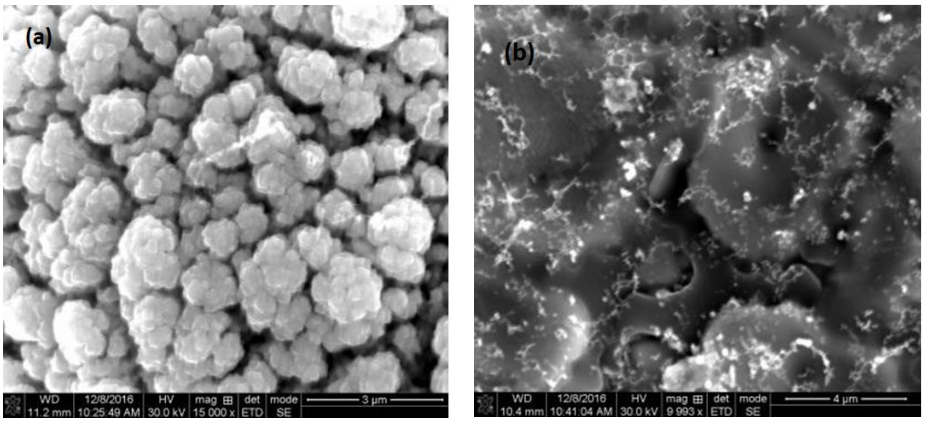

Fig. 8. XRD results of (a). top graph with 0 wt%, (b). 3 wt%, and (c). 15 wt% Y_2O_3 dopant.

The Fig. 8 shows the XRD of three dopant concentrations samples. The major BCC highest peak shifted slightly to the right indicating that Y most probably entered the bulk MoNbTaVW crystal. In the meantime, the existence of pure Y_2O_3 shows that the Y_2O_3 still exists which most probably stays at the grain HEA boundaries. Since O is hard to move in the HEA bulk, the Y atom doping

thus distorts the original HEA cell and causes the peak shift. The TGA graph of 3 wt% $MoNbTaVW/Y_2O_3$ shown in Fig. 9 is obtained from oxidation experiment. It shows that in room temperature ~ 400 °C, no oxidation is observed, at 400 °C ~ 450 °C, fast oxidation is shown,

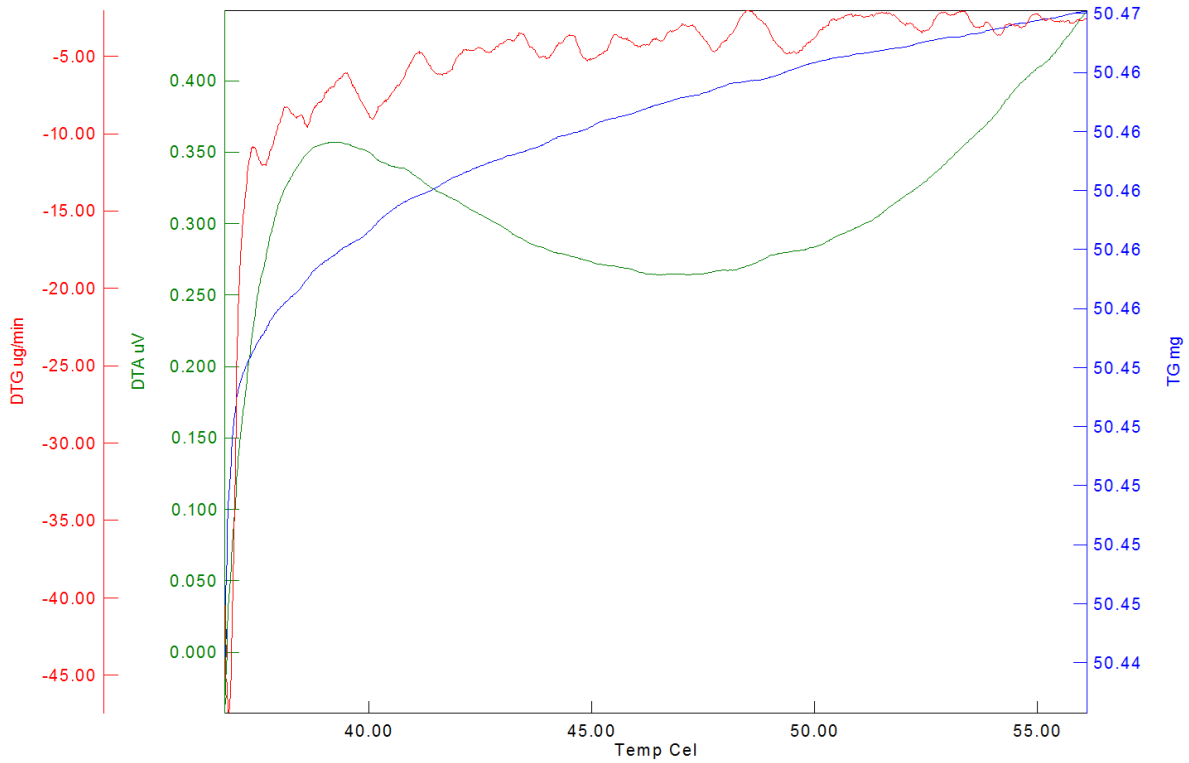

Fig. 9. TGA analysis of 3 wt% Y_2O_3 doped $MoNbTaVW/Y_2O_3$.

while at 450 °C ~ 1100 °C, a linear oxidation relation is displayed. Since there are large spaces between the grain boundaries, the Y_2O_3 and doped HEA cannot form close contact and thus the pure Nb metal or pure MoNbTaVW HEA like oxidation behavior is very nature and can be eliminated using the two HEA synthesis methods mentioned earlier.

Conclusions

From *ab initio* DFT method simulation, we optimized the geometry cell structures of body centered cubic (BCC) MoNbTaVW, BCC HfNbTaTiZr, and face centered cubic (FCC) CoCrFeMnNi HEAs, and mechanical and electronic structure properties are studied and the results are in good agreement with experiment data and large cell simulation results. This confirmed method using the simplest ab initio models from symmetry analysis to predict physical properties, when applied to a large scale materials screening, will save tremendous materials developing time since the calculation is reduced to minimum. The combination research of DFT based bulk and interface modeling, HPC MD simulation, DD simulation, and experiment validation study on oxide doped HEA was conducted. This integrated method as has been shown from this HPC materials design group's other research can accelerate novel high temperature materials design and save tremendous expenses and developing time. The simulation and experiment both show that the dopant oxide can

stay at the bulk HEA boundary while the oxide transition metal entered the bulk HEA.

Our simulation and experiment works on Ni-S system DD study explains our dislocation texture data well. This DD method can be applied to predict HEA and doped HEA dislocation behavior and be used as a checking and component screening tool in new materials development. The synchrotron XRD shear stress texture study is an effective technique to understand in-situ dislocation density and mobility changes. Future research includes dislocation dynamics study at room and high temperature, HEA XANES simulation, new oxide dopant screening, hot press and SPS synthesis comparison, and large scale high performance HEA screening.

Acknowledgement

We'd like to thank DOE NETL for funding support and program management team: J. Mullen, S. Markovich, and Bethan Young for their support during this project implementation period. Besides, are gratitude for the following list graduate students: B. Zhang, Y. Zhang, L. Chilla, Y. Yang, J. Lei, C. Guo, and D. Hart; undergraduate students: M. Jackson, M. Jones, and Y. Liu;

postdocs: Drs. L. Tan and O. Starovoytov; Drs. S. Guo, Y. Dong, D. Cao at LSU; prof. P. Liew at UTK; Dr. E. Khosravi at SU; Dr. J. Yan at LBNL; Dr. B. Chen at HPSTAR; LONI Institute and LSU CCT for supercomputer time and internal support; NASA/LaSPACE RAP-12; NSF-LASiGMA LINK Travel fund; NSF-CIMM; NIH-INBRE funding support; SU CS Department & IBM.

GRAPHICAL MATERIALS LIST

Fig. 1. (a) The model used in simulation for HfNbTaTiZr. (b). The black dot represents compression data. According to the best fit solid line of the Birch–Murnaghan equation, the bulk modulus is calculated to be 198 GPa.

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Fig. 9. TGA analysis of 3 wt% Y_2O_3 doped MoNbTaVW/Y_2O_3.

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LIST OF ACRONYMS AND ABBREVIATIONS

BCC	body centered cubic
DD	dislocation dynamics
DFT	density functional theory
FCC	face centered cubic
FWHM	full width at half maximum
GGA	generalized gradient approximation
HEA	high entropy alloy
HPC	high performance computing
LDA	local density approximation
MD	molecular dynamics
MedeA	Materials Design software
ParaDiS	parallel dislocation simulator
SEM	scanning electron microscope
TGA	thermogravimetric analysis
XRD	x-ray diffraction

APPENDIX A: How the Projected Successfully Completed the Goals, Objectives, and Tasks Defined in the Statement of Project Objectives

A. Objectives

The goal of this project is to effectively screen out the optimal oxide dispersion strengthened (ODS) high entropy alloy (HEA) for the advanced gas turbines through an integrated method combining computational materials simulation and experimental validation in material sciences to simulate the elastic constants, interface bonding, dislocation creep, high temperature microstructures at high pressure. The students will be trained in materials design, high performance computing (HPC) simulation, and the state-of-the-art materials characterization research.

It is proposed that the following investigations be carried out within a two-year period: (1). Perform interface energy and molecular dynamics/Monte Carlo HPC simulation on the HEA models to screen out the potential low temperature ductile and high temperature and high pressure oxidation resistant HEA candidates. (2). Perform experiments on the high temperature and high pressure property of the most promising HEA systems from the simulation. (3). Train students especially HBCU graduate students and integrate the materials design and HPC simulation into course work. The primary theoretical method of investigation is the *ab initio* molecular dynamics method based on the density functional theory (DFT).

Successful Achievement of Objectives

Two single BCC phase HEAs were predicted and experiment verified. They are HfNbTaTiVZr and MoNbTaTiVW. The MoNbTaVW/Y_2O_3 system was simulated and experiment verification showed reasonable oxidation trends. There were seven graduate and three undergraduate students were supported and trained in computer simulation, materials modeling, high performance computing, sample synthesis, sample characterization with XRD, synchrotron XRD, TGA, etc.

B. Scope of Project

This proposed research work will be on developing high temperature ODS HEAs and on the experimental evaluation of high temperature ODS HEA performance. This project will develop an understanding of the processes at the atomic level which control high temperature high pressure oxidation and low temperature ductility performance of ODS HEAs. In the theoretical/simulation part, Dr. Yang (PI) group will start from the potential high temperature HEA candidates: NbMoTaW and TaNbHfZrTi. First, the molecular dynamics and adaptive kinetic Monte Carlo (aKMC) HPC simulation on the potential HEA candidates will be performed. The NVT ensemble will be chosen to simulate the elastic constants at high temperature and high pressure and the NPT ensemble will be chosen to get the possible stable disordered or/and ordered structures. Then reasonable interface models of the ODS HEAs will be built and optimized through *ab initio* DFT method. The limit size effect can be mostly eliminated by the sandwich like periodic unit cell. After that, the interface energies and bonding of different transition metal oxides (such as La_2O_3,

CeO_2 etc. at both oxides) will be compared and optimized to get the most stable structure. The cell sizes will be gradually increased till the interface energy convergence is reached. After that, The HPC high temperature molecular dynamics simulation will be performed on Louisiana Optical Network Initiative (LONI) and XSEDE supercomputers.

In the experimental validation part, the high temperature and high pressure property of the theoretical optimized ODS HEA alloys will be studied using a unique high temperature materials test rig and along with related materials characterization in the Department of Mechanical Engineering at LSU. The high pressure dislocation texture and related embrittlement of the ODS HEAs will be studied at Lawrence Berkeley National Laboratory (LBNL) using the state-of-the-art radial synchrotron radiation XRD texture technique at Beamline 12-2-2. The students and postdoc will be trained to perform the state-of-the-art materials modeling, simulation, synthesis, and testing.

Successful Adherence to Project Scope

An integrated modeling, computer simulation, data analysis, and experiment verification method was implemented on a novel HEA design. Several high performance HEAs were predicted first and then verified by experiment synthesis and characterization. Our simulation successfully predicted two single BCC phase HEAs: MoNbTaTiVW and HfNbTaTiVZr. The MoNbTaVW/Y_2O_3 was simulated and experiment thermal evaluation is performed by TGA measurement. High pressure compress/decompress synchrotron XRD experiment confirmed the prediction of the ductileness of HEA MoNbTaVW compared with pure W.

C. Tasks to Be Performed

Task 1: Project Management and Planning

The recipient shall update the Project Management Plan (PMP) submitted with the Application. The updated PMP should be designed to achieve the project objectives covering the entire project period and address the following elements: Executive Summary; Risk Management; Milestone Log; Funding and Costing Profile; Project Timeline; Success Criteria and Decision Points; and the Statement of Project Objectives. Specifically the PMP shall include a task structure and supporting narrative that concisely addresses the overall project, organizational structure, technical objectives and approach, an assessment of risk and risk management strategies, and include a detailed plan for reporting on the key activities and/or tasks that is consistent with the Federal Assistance Reporting Checklist. The PMP shall also provide detailed schedules and planned expenditures for each Task, major milestones, and decision points, including the development of the criteria upon which GO/NO decisions are based.

The PMP shall be updated and submitted to the U.S. Department of Energy (DOE) Federal Project Manager (FPM) within 30 days of execution of the Cooperative Agreement. Specifically, quarterly management progress report shall use the scope, schedule, and cost included in the PMP as the baseline, and either verification that the PMP is still valid or suggested PMP revisions deemed desirable for optimum achievement of program objectives. The recipient will submit reports in

accordance with Attachment 4 -- Federal Assistance Reporting Checklist.

Successful Achievement of Task 1: Project Management and Planning

This project team has reported quarterly through email submission the required quarterly report and attended annual report meetings. The progress, schedule, and related budget adjustment were reported to our program manager on time. Both research and students training were within the planned/adjusted schedule.

Task 2: Computer Simulation on Novel HEAs

The MD and MC HPC simulation on the high temperature and high pressure properties of the potential HEA candidates will be performed and the reasonable interface models and will be built and optimized through *ab initio* DFT method. The NPT ensemble will be chosen to study the structure changes under ambient and high pressure. The NVT ensemble will be chosen to simulate the high temperature elastic constants and diffusion properties. The interface energies and bonding of different dopant elements and concentrations will be compared and optimized to get the most stable ODS HEA structures. The HPC high temperature molecular dynamics simulation will be performed on Louisiana Optical Network Initiative (LONI) and XSEDE supercomputers, which can be directly accessed from SUBR campus. Both graduate and undergraduate students will be trained and the materials modeling, HPC simulation and related materials design techniques will be integrated into course work.

Successful Achievement of Task 2: Computer Simulation on Novel HEAs

In this task, the project ab initio DFT method was applied to screen out the stable components of potential HEAs. Based on current available HEAs such as MoNbTaVW, HfNbTaTiZr etc., the major stable components were calculated first, e.g. in MoNbTaTiVW, the MoTa, Mo_2TiW, $MoTi_2$, Nb, TaV_2, TiW_3 stable components were simulated while in HfNbTaVZr, those components are Hf, $HfZr_2$, Nb, Ta, TaV_2. The interface models such as $MoNbTaVW/Y_2O_3$ are setup and the possible stable interface structures were optimized. MD/MC simulations were performed on these HEAs and doped HEAs to confirm the properties and structure stability. Figs. 1-6 show our simulation models and electronic structure property results. The research results were published in references Publication 3, 4, 5, 6, and 7.

Collaborated with NETL, we successfully predicted the possible single BCC phase MoNbTaTiVW and HfNbTaTiVZr using ab initial simulation and CALPHAD. This was verified by synthesis, SEM, and XRD characterization. These were published in Publication 6 and 7. To verify the brittle/ductile model system, the DD simulation was successfully performed on sulfur doped Ni metal system. This is published in references Publication 1 (AIP Advances).

The simulation methods and results of this doped HEA project was adopted and used in our current CIMM project, a combined NSF and LA BoR supported five year state wide big alloy manufacturing project. Several other funding agencies, such as DoD & NASA,

are also interested in this data based simulation/experiment combined materials design frame work.

Task 3: Experimental Validation

Experimental work will be started immediately after the first promising candidate can be found in task 2. The candidate samples such as La_2O_3 doped TaNbHfZrTiMo will be prepared most at Southern University (SU) through mechanical ball milling. The arc melt for samples will be performed at Turbine Innovation and Research Center (TIER) of LSU Mechanical Engineering Department. Small samples can also be put directly in thermogravimetric analysis (TGA)/differential scanning calorimetry (DSC) for thermal and oxidation analysis in the center. The high pressure dislocation related ductility experiments will be performed at LBNL. The texture related embrittle-ductile under high pressure tests will be performed with a state-of-the-art radial synchrotron X-ray diffraction (XRD) technique through which the dislocation information can be obtained. Students and postdoc will be trained in materials characterization and design validation tests.

Successful Achievement of Task 3: Experimental Validation

The experiments were performed in three sites: Southern campus, LSU Tier Center, and LBNL. Most regular synthesis and characterization works were done at LSU. The compress/decompress (DD verification) experiments were performed at LBNL beamline 12.2.2. The Figs. 7, 8, and 9 shown are HEA/ODS SEM, XRD, and TGA results respectively. The experiment results are published in references Publication 1, 6, and 7. The references Publication 2 and 8 are extended research on graphene resistance changes with respect to light frequencies and platinum grain boundary rotation detection at nanometer level through dislocation analysis respectively. These two publications are partially supported by and are not directly linked to SOPO but an extension of this HEA design project.

The SEM and XRD results of MoNbTaVW/Y_2O_3 show that doping oxide needs extra force to reach a solid bulk with less pore. Thus to make the HEA denser enough for device application, hot press or spark plasma sintering synthesis method may be applied.

The XRD results in Fig. 8 shows that the major BCC highest peak shifted slightly to the right indicating that Y most probably entered the bulk MoNbTaVW crystal while in the meantime, the existence of pure Y_2O_3 shows that the Y_2O_3 still exists which most probably stays at the grain HEA boundaries. The TGA graph in Fig. 9 of 3 wt% MoNbTaVW/Y_2O_3 shows that in room temperature ~ 400 °C, no oxidation is observed, at 400 °C ~ 450 °C, fast oxidation is shown, while at 450 °C ~ 1100 °C, a linear oxidation relation is displayed. Thus the above mentioned two HEA synthesis methods are necessary to synthesize high quality oxide doped HEAs.

In sum, the predicted doped HEAs are synthesized and characterized by SEM, XRD, synchrotron XRD, and TGA. The MoNbTaVW and MoNbTaTiVW both have good high temperature mechanical properties. The oxide Y_2O_3 was doped into the HEA bulk and

boundary and may be a potential better high performance high temperature alloy through hot press and spark plasma sintering methods.

D. Deliverables

The Recipient shall provide reports in accordance with the enclosed Federal Assistance Reporting Checklist and the instructions accompanying the Checklist. A Technical/Scientific Topical Report shall be provided on an annual basis no later than 30 days after each 12-month period. This annual Topical Report is to document the technical work and progress achieved during the preceding 12 months.

Successful Achievement of Deliverables

The quarterly/annual reports were provided to our manager promptly for reviewing and guidance. This final report summarize our achievements reached in both research and students training and potential future development and research areas.

E. Briefings

The Recipient shall attend the annual HBCU-OMI / UCR Review Meeting throughout the duration of the project, and provide a presentation detailing the project work that has been completed up to that point. The Recipient and FPM shall also hold a project kick-off meeting within 30 days of the start of the award, and shall hold a project closeout meeting within 30 days after the final technical report is approved.

Successful Achievement of Briefings

We attended the annual HBCU-OMI/UCR Review Meeting throughout the duration of this project. The detailed project work and implementation progress completed were reported. The publications and students training progress are reported in each quarter's report and project final report. The project kick-off and closeout meetings were hold on time.