American Conference on Neutron Scattering

Structural Materials and Engineering

* Invited Paper

SESSION F02.01: Structural Materials and Engineering I

F02.01.01
Microstructural Evolution during the Fabrication Processes of Metallic Nuclear Fuels
Maria A. Okuniewski[1], Walter J. Williams[1], Alejandro Figueroa[1], Donald W. Brown[2], Sven C. Vogel[2] and Clausen Bjorn[2]; [1]Purdue University, United States; [2]Los Alamos National Laboratory, United States

Metallic nuclear fuels, such as uranium-zirconium (U-Zr) and uranium-molybdenum (U-Mo) fuels, are important for a variety of nuclear reactor types, including fast reactors, as well as research and test reactors. As new fabrication techniques are employed for fuels or the optimization of existing techniques are explored, it is important to consider the microstructural implications, which in turn can affect material properties and in-reactor performance. Both U-Zr and U-Mo fuels are investigated via neutron diffraction techniques, including in situ annealing and tensile testing. U-Zr alloys ranging from 6 to 30 weight percent (wt.%) were investigated using time-of-flight neutron diffraction at ambient conditions to characterize the phases, texture, lattice parameters, and lattice strain. These alloys were characterized following different fabrication stages, including as-cast, rolled, and annealed. Moreover, in situ annealing was performed on the as-cast and rolled foils to capture the phase transformations and kinetics, texture, lattice strain, and linear thermal expansion coefficients. The overall microstructural evolution of the U-Zr alloys will be discussed. U-10wt.%Mo was also investigated to understand the implications of different fabrication parameters selected for a monolithic, plate-based fuel. Time-of-flight neutron diffraction in ambient conditions was performed to characterize the evolution of phases, texture, lattice parameters, lattice strain, and residual stress. The plate fuels were characterized during different stages of fabrication, including the examination of different rolling and annealing schedules. A recent model developed by our group links the initial microstructure of the U-Mo fuel to the in-reactor performance. The microstructural fuel performance model, as well as the critical parameters determined via neutron and X-ray diffraction, will be discussed.

F02.01.03
Neutron Scattering Studies of Rheological and Microstructural Development in Hydrating Cements for Additive Manufacturing of Concrete
Andrew J. Allen[1], Scott Z. Jones[1] and Julie Hipp[2]; [1]National Institute of Standards and Technology, United States; [2]University of Delaware, United States

The advance of the digital age across all industrial sectors is spurring the introduction of additive manufacturing (AM) concepts to an increasingly broad range of engineered products and components. The introduction of AM methods for cement and concrete construction offers significant advantages in exploitation of the world's most used industrial material. However, to realize these opportunities, it is critical to optimize the development of cement properties during the hydration process for their use either as *de facto* 3D printing "inks" or as AM templates. This implies the carefully tuned addition of accelerators (e.g., aluminum sulfate) and retarders (e.g., sucrose) to optimize the hydration process. The hydration reactions between cement clinker and water remain an important topic of research, with many important questions yet to be answered. However, the use of volume- and surface-fractal models applied to small-angle neutron scattering (SANS) has previously provided important insights [1]. To improve the performance of concrete and the

ability to engineer cement for AM concrete applications, the development of the microstructure during hydration must be related to the macroscopic material properties. In this connection, rheology and electrical conductivity are two macroscopic material measurements relevant to concrete construction – rheology providing insight into the flow characteristics and electrical conductivity providing insight into the transport properties of the hardened material. To explore fundamental aspects of cement hydration relevant to AM "ink" applications, results will be presented of simultaneous SANS, small-amplitude oscillatory shear, and electrical conductivity studies of hydrating triclinic and monoclinic tricalcium silicate ("C3S"), the key active raw material in hydrating cement. A sucrose admixture has been added to tune the onset of hydration and demonstrate one mechanism to control the development of the macroscopic properties. The development of the nanoscale calcium-silicate-hydrate (C-S-H), the main strength-giving phase in hydrated cement, has been characterized by *in situ* SANS using fractal models, and the results have been related to the changing rheological and electrical conduction properties of the hydrating paste. The implications will be discussed regarding the different rheological and hydration behaviors observed for the two C3S polymorphs [2]. Extension of this "hard material" rheoSANS approach to realistic Portland cement/limestone blends under development as AM cement inks will also be discussed.

[1] A.J. Allen, J.J. Thomas & H.M. Jennings; "Composition and density of nanoscale calcium-silicate-hydrate in cement," *Nature Mater*., **6**, 311-316 (2007).
[2] S.Z. Jones, J.B. Hipp & A.J. Allen; "Rheology and microstructure development of hydrating tricalcium silicate," *Cem. Concr. Res*., submitted (2020).

F02.01.04
Imaging Hydrogen in Metals Using Neutron Tomography

Hubert E. King[1], Nicole Callen[1], Neeraj Thirumalai[1], Hyun J. Jun[1], Daniel S. Hussey[2], Jacob M. LaManna[2] and David Jacobson[2]; [1]ExxonMobil Research and Engineering, United States; [2]National Institute of Standards and Technology, United States

Imaging of hydrogen in metals and alloys is a well-known challenge due to its small atomic size and fast diffusion in some metals such as steels. As is well known, the presence of hydrogen in metals can cause embrittlement. The dissociated atomic hydrogen at the metal surface dissolves into the matrix and accumulates at defects. In some cases it has been proposed that the accumulated hydrogen can recombine into molecular hydrogen at defect sites, such as in hydrogen induced cracking. However, details of how this process occurs and the intermediate stages still need to be studied. In part, this is due to the difficulties in imaging hydrogen within the metal. Neutron radiography is well suited to this problem, since hydrogen has a large absorption cross section. However, the spatial resolution has been limited, impeding the application of this technique to address the fundamental question about how hydrogen accumulation occurs at defect sites. The new cold neutron imaging beam line at the NCNR on NG6 offers a spatial resolution of <10 μm. We recently utilized this instrument to image a sample of metal which had been exposed to conditions that should lead to hydrogen accumulation. To preserve the hydrogen, this sample was stored cryogenically until starting the neutron experiment. The experiment itself consisted of about 40 hours of beamtime, consisting of a full 360 view of the sample consisting of 720 projections at a resolution of 3 um. In a separate measurement, we have imaged the sample using x-ray microtomography at a resolution of 3 um. Together we anticipate that these imaged volumes should help us detect the location of hydrogen within the sample. We will compare our results with recent electron microscope and modeling results.

F02.01.05
Deep Convolutional Neural Network for Reconstruction of Strain Tensors from Transmission Bragg Edge Measurements

Matthew Connolly, Daniel S. Hussey and Damian Lauria; National Institute of Standards and Technology, United States

The neutron Transmission Bragg Edge (TBE) method has gained interest over the past decade as a technique for providing high-spatial resolution, high-sample penetration, and fast mapping of lattice strain. TBE offers an advantage over traditional strain mapping techniques in increased signal-to-noise compared to diffraction peaks. Lattice strain is, however, a tensor quantity, and because the Bragg edge occurs at the back-scattering condition, only a single component of the full strain tensor can be mapped by TBE. There exists a strong desire to extend the neutron TBE method to provide a full, three-dimensional tomographic reconstruction of each strain component corresponding to the full strain tensor at each sample voxel. However, it has been shown that existing scalar tomographic reconstruction algorithms are, in general, unable to provide a unique solution, as the mathematical problem of inversion of TBE data is ill-posed. Although there has been some success in developing a reconstruction algorithm for some special cases (e.g. axisymmetric strain in the absence of residual

stresses), a general reconstruction algorithm with high-strain resolution through traditional algorithms remains elusive. The nature of the tomography problem lends itself well to machine learning techniques. In particular, the “forward-problem”, in which neutron transmission is calculated from a strain field, is well-known. This allows for the generation of very large data sets, comprised of strain fields and their associated neutron transmission. In this talk, we present a tomographic reconstruction algorithm for TBE data based on Deep Convolutional Neural Networks (DCNN). We present a training strategy and DCNN architecture with success in reconstructing strain fields with overall strain uncertainty on the order of 10^{-5}. We show how the DCNN-based reconstruction algorithm performs on a set of TBE data acquired on the NIST Center for Neutron Research NG-6 beam line on an additively manufactured Ti6Al4 bar which holds residual stresses from the build process.

F02.01.06
Two-Point Spatial Correlation Functions of Paracrystals with Radial Symmetry
Guan-Rong Huang, Yangyang Wang, Changwoo Do and Wei-Ren Chen; Oak Ridge National Laboratory, United States

The precipitates usually originate from the nucleation process in their bulk materials, and their interaction is different from typical particle interactions. However, the widely used hard sphere model for structural analysis of precipitates does not reflect in the physical reality and cannot capture the feature of scattering pattern. Meanwhile, the first-order OZ-equation cannot resolve this problem because of its limitation, such as unknown closure for precipitates and failure in high concentrations. In this work, we develop a phenomenological model to describe the structure by radially symmetric paracrystals whose long-range order are destroyed by propagation of particle fluctuations. General expressions are derived for the spatial correlation functions in one-, two-, and three-dimensional spaces. And the spatial correlation in paracrystals in reciprocal space is further discussed and clarified. The developed method can be used to quantitatively analyze the microstructure of paracrystalline materials in both real and reciprocal spaces via scattering experiments and computer simulations. The research was supported by the Laboratory Directed Research and Development Program at ORNL. G.-R.H. acknowledges the scholarship from the Ministry of Science and Technology in Taiwan (Project No. MOST 108-2917-I-564-103).

F02.01.07
Single Crystal to Polycrystal Neutron Transmission Simulation
Luc L. Dessieux; Oak Ridge National Laboratory, United States

The neutron Bragg-edges transmission (NBET) is developing into an efficient technique to obtain three-dimensional elastic strains maps within the bulk of materials. To date this technique has been applied only to isotropic three-dimensional strains without consideration of texture. Here, a core software for calculation of the neutron beam attenuation by crystalline specimen is presented. The total cross section is calculated as a function of neutron energy, crystal structure, temperature, and crystal orientation. The contribution of Bragg (elastic coherent) scattering to the attenuation is evaluated within secondary extinction theory using both the crystal's mosaic spread value and its orientation with respect to the neutron beam direction as parameters. These routines allow users to consider any distributions of crystal orientations, which enable realistic simulations of structural non-uniformities such as texture and stress/strain. Simulation of neutron transmission curves for single crystal copper benchmarked with experimental data from literature is presented and a procedure of determining the crystal orientation from transmission data is outlined. Further, simulations of neutron energy dispersive patterns on polycrystalline materials are compared with NBET measurements. The effect of addition of the stress state at the single grain level is demonstrated.

SESSION F03.01: Structural Materials and Engineering II

F03.01.01
Using Neutron Diffraction to Safeguard Suspension Bridges against Deterioration and Fire
Adrian Brügger, Jumari Robinson and Raimondo Betti; Columbia University, United States

In order to effectively safeguard critical infrastructure such as suspension bridges from natural and anthropomorphic hazards, maintenance and defense strategies must be informed by meaningful experimental data and realistic simulations. We present results from experiments performed at multiple scales, ranging from the microscale of the steel making up the main cables to multi-ton full scale bridge cable mockups. Conventional techniques

– strength of materials testing, fire testing, and surface analysis – are used to quantify the ASTM A586 high strength steel used in suspension bridge cables both at ambient and high temperature. In-situ nDif experiments are subsequently performed at the Los Alamos and Oak Ridge National Laboratories under various environmental conditions: first, the friction and contact forces between wires in a bundle (strand) are quantified in-situ, as is the interaction of these complex multibody systems with their surrounding wires is critical in quantifying the system's resiliency to local facture and/or creep. Second, we simulate various fire scenarios of single wires, constituent strands, and a full-scale 9200-wire bridge cable to understand the mechanical properties such as creep, plastic flow, annealing/recrystallization of the steel both during and after a fire event. Third, we quantify the thermal conductance of the bridge cables, which turns out to be highly orthotropic due to the packing order of the parallel wires. This broad research effort underwrites the unified goal of informing the stakeholder of the fundamental physics governing the behavior of the structure. The results in turn optimize numerical models that quantify stochastically the internal mechanics of parallel wire bridge cables and assess the resulting collapse risk of suspension bridges under a broad array of hazards.

F03.01.02
Characterizing the Effects of Varying Additive Manufacturing Parameters on Stainless Steel 316L
Chuting Tan[1], Cheng Sun[1], Xinchang Zhang[2], Jeffrey R. Bunn[3], Edward A. Payzant[3], Yuxuan Zhang[3] and Hassina Z. Bilheux[3]; [1]Idaho National Laboratory, United States; [2]Missouri University of Science and Technology, United States; [3]Oak Ridge National Laboratory, United States

Directed energy deposition (DED) is an additive manufacturing (AM) techniques that fabricates components by fusing particles with a high-power heat source, such as a laser, an electron beam, or a plasma arc. It can manufacture components with complex geometries and internal structures, which are difficult to achieve by conventional machining techniques. The various process parameters in the DED technique allow the ability to tailor material properties of the printed parts. Stainless steel 316L (SS316L), thanks to its superior corrosion resistance and mechanical behavior, is widely used in industry and has generated considerable interest in the nuclear energy research community. SS316L fabricated by AM methods has a lot of potential in nuclear energy applications, such as materials for internal structure components. Therefore, it is vital to know the performance of the printed materials as compared to the wrought materials. In this work, SS316L samples were fabricated by DED process with varying hatch spacing and overlap ratio. To investigate the impact of these parameters on microstructure and mechanical properties, this study utilized techniques including neutron diffraction residual stress measurement, tensile testing, neutron tomography, and time of flight neutron Bragg edge imaging. The results of these measurements shed light on the effects of deposition parameters on material performance.

F03.01.03
A Novel Iron Based Superalloy—Using Sans and Apt to Inform Alloy Development
Kenneth C. Littrell, Ying Yang, Jonathan D. Poplawski, German D. Samolyuk and Andrew R. Lupini; Oak Ridge National Laboratory, United States

Structural materials are widely used for almost infinite applications that make modern living possible from transportation, power generation, food delivery, housing, etc. Despite the long history and numerous varieties of steels, metallurgists and materials scientists are always motivated to produce more advanced steels with a combination of superior strength and excellent ductility with the end goal of making infrastructure more efficient and stable. Achieving ultra-high ultimate tensile strength and excellent ductility is of paramount relevance. Using an alloy design strategy informed by modeling in combination with traditional materials testing and microstructural characterization techniques including SANS, APT and electron microscopy, we have developed a novel ultrastrong, ductile, nanostructured, austenitic steel. Unlike other UHSSs, this steel is also strong at high temperature, well into the realm of many age-hardenable Ni-based superalloys. The key to the properties of this novel alloy is the presence of a high volume fraction of L12 nanoprecipitates. The alloy composition was chosen based on modelling predictions that indicated which alloy compositions should form these precipitates and a family of samples of model alloys at different heat treatments was produced. These samples were subjected to mechanical testing, and the microstructure at a few heat treatment conditions was determined using a combination of SANS and APT. The size and volume fractions of the strengthening precipitates as determined from SANS and APT were in good agreement with each other and with modeling predictions Furthermore, the capability of SANS to perform in-situ heat treatment and to separate magnetic and nuclear scattering is valuable for understanding the precipitate nucleation and growth process and the impact of the presence of the precipitates on the phase of the alloy matrix.. In this presentation, we will give an overview of the new alloy characterization process and how SANS has

contributed to it.

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F03.01.06
Residual Stress and Microstructure Evolutions in a Friction Stir Processed on Dual Phase 980 Steel
Koichi Taniguchi[1], Yong Chae Lim[2], Jeffrey R. Bunn[2] and Zhili Feng[2]; [1]JFE Steel Corporation, Japan; [2]Oak Ridge National Laboratory, United States

Friction stir processing or joining is a novel and unique solid-state process to overcome some disadvantages of conventional fusion welding processes for high temperature and high strength materials. In general, a specially designed tool rotates and produces frictional heat, leading to soften a material underneath the tool. The softened material flows around the tool through extensive plastic deformation and finally is consolidated to form a solid-state joint. The complex microstructure evolution e.g., large texture changes and dynamic recrystallization, transiently occurs due to the compressive and shear loading in elevated temperature during the process. In this present work, we employed friction stir processing on advance high strength steel (i.e., dual phase 980) with different welding process conditions. Friction stir processed steel samples were characterized by optical and electron microscopies, microhardness measurement, and residual stress by neutron beam measurement to study quantitative stress state and correlation to microstructure evolutions under various welding conditions.

F03.01.07
Understanding Ethylene Adsorption on Zeolites with Neutron Diffraction
Muyuan Li[1], Raul Lobo[1] and Craig M. Brown[1,2]; [1]University of Delaware, United States; [2]National Institute of Standards and Technology, United States

Effective and energy efficient ethylene separations from other small molecules can reduce significantly energy consumption, as compared to the state-of-the-art cryogenic separation of ethylene. Zeolite materials offer high thermal and chemical stability, low toxicity and moderate cost comparing to other adsorbent materials. ZK-5 (KFI) zeolite (Si/Al = 4) and SSZ-13 (CHA) zeolite (Si/Al = 6) have large concentrations of 6- and 8-rings in the framework, both allowing accessible ion exchange positions for transition metal cations. Paired with metal cations with the appropriate radii (M^{2+} = Zn^{2+}, Mn^{2+}), the 6-rings in zeolite framework could allow for favorable adsorbate-adsorbent interactions with ethylene. Adsorption isotherms of ethylene and ethane show a larger difference in ethylene-ethane adsorption capacity at equilibrium for M^{2+}-ZK-5 than Na-ZK-5, demonstrating a higher ethylene-ethane selectivity at high pressures (> 0.15 atm). Isosteric heat of adsorption data show that adsorption in Mn-ZK-5 yields higher heat of adsorption than Zn-ZK-5 and Na-ZK-5 (at lower coverages). Using Rietveld refinement of neutron (BT-1, NCNR) and synchrotron (APS, ANL) diffraction data, we have been able to locate the metal cations in the zeolite exchange positions (Zn as Zn^{2+} in 6-ring in Zn-SSZ-13 and Mn as Mn^{2+} in Mn-ZK-5). We have also identified potential ethylene adsorption sites with diffraction experiments (over Zn^{2+} in the 6-ring in Zn-SSZ-13 and adjacent to Mn^{2+} in puckered 8-ring in Mn-ZK-5). Such understanding of the interaction between ethylene and metal cations in zeolitic adsorbent materials can guide the future design of ethylene adsorbent and catalysts.

Poster Session: Structural Materials and Engineering

PF.01.02
***In Situ* Neutron Diffraction Study of the Crystallographic Evolution and Thermal Expansion Coefficients in U-Zr Alloys During Annealing**
Walter J. Williams[1,2], Maria A. Okuniewski[1], Sven C. Vogel[3] and Jianzhong Zhang[3]; [1]Purdue University, United States; [2]Idaho National Laboratory, United States; [3]Los Alamos National Laboratory, United States

Low enriched (19.5% U^{235}) uranium-zirconium (U-Zr) foils underwent a novel fabrication process into 180μm foils through hot and cold rolling. Selected U-Zr compositions, consisting of 6, 10, 20, and 30 weight percent (wt.%) Zr, are typical of those observed in irradiated metallic U-Zr fast reactor fuels. Ambient temperature time-of-flight neutron diffraction was performed to investigate the microstructural evolution, texture progression, and

lattice strain of the U-Zr foils throughout casting, rolling, and annealing. In-situ annealing was subsequently performed on the castings and rolled foils in order to probe unirradiated phase transformations, transformation kinetics, texture retention, and phase specific linear thermal expansion coefficients. Samples undergoing an anneal were heated to 900°C for two hours and step cooled at 1°C/hr with data collection continuously occurring in five-minute increments. Rietveld refinement was chosen to qualitatively analyze the diffraction patterns. This work has shown that the β-U+γ''-UZr dual phase region, apparent in most modern U-Zr phase diagrams, is not present at or above U-6wt.%Zr. Rather, only two phase transformations were observed upon cooling from 900°C, corresponding to γ-UZr -> α-U+γ''-UZr -> α-U+δ-UZr_2. Phase specific linear coefficients of thermal expansion were also measured for α-U, δ-UZr2, and γ-UZr. The thermal expansions in U-10wt.%Zr's α-U and δ-UZr_2 phases were shown to have an anisotropic lattice contraction in the 010_b direction (α-U) and in the 001_c direction (δ-UZr_2). Texturing was also measured throughout fabrication and annealing. In U-10wt.%Zr, preferred orientation from rolling was reduced by more than half during heat treatments. This minor texture retention in the U-10wt.%Zr annealed foils may indicate a texture memory of the alloy. Additional results include phase fractions and phase evolution corroborated by scanning electron microscopy and electron dispersive spectroscopy.

PF.01.03
Accelerating Crystallographic Orientations Measurement in Polycrystalline Materials by Utilizing Time-of-Flight Neutron Diffraction
Yan Chen, Alexandru Stoica and Ke An; Oak Ridge National Laboratory, United States

Texture (preferential grain orientation) in a polycrystalline material is a fundamental property in naturally existing minerals and artificially manufactured materials. Texture impacts materials anisotropic properties in their engineering and functional applications, and therefore, understanding the texture formation and evolution is critical in material synthesis, manufacturing and service. Moreover, unaccountable texture may lead to ambiguities in microstructure analysis of a bulk via diffraction approach. Taking advantages of time-of-flight (TOF) neutron diffraction, the full diffraction pattern with multiple Bragg peaks are measured in the stationary detectors, and it thus enables the concurrent measurement of the full pole figures of various crystal planes by rotating the bulk sample along two axes. As demonstrated at Vulcan at the Spallation Neutron Source, the multiple detectors layout with wide coverage reduces the sample rotation angles and further speeds up the measurement (less than 3 hours for a typical steel sample). Moreover, benefiting from the event-base neutron data along with the fine-pixelized detectors, the continuous measurement for the live pole figure is enabled. To convert to the pole figures, the collected peak intensities are processed with normalization, correction with the changes of gauge volume occupancy (for thin samples) and the neutron attenuation in the bulk (for large samples). The development and the practice of texture measurement highlight the utilization of TOF neutron diffraction in the microstructure characterization of realistic polycrystalline materials, and they will also provide guidance on the instrumentation of future material engineering neutron diffractometers.

PF.01.04
Modeling of Local Atomic Structure in Disordered and Nanostructured Materials
Bo Jiang; Oak Ridge National Laboratory, United States

Pair distribution functions (PDF) obtained from total scattering (high energy synchrotron X-ray and Neutron scattering) can reveal both the local and intermediate range structure of crystalline, disordered and nanostructured materials. As we all know that conventional reciprocal space diffraction only probes the average long-range structure of the Bragg planes, and information from EXAFS and XANES is limited to no more than third coordination shell, PDF can reveal both local distortions and measure the *structural coherence* up to several tens of Ångstrøm. With optimized sample environments PDFs can also be collected under *in situ* mechanical and electrical fields. A combination of multiple approaches using *PDFgui* (graphical interface built on the PDFfit2 engine*), RMCProfile* (Reverse Monte Carlo software), *TOPAS v6* (combined reciprocal and real space neutron PDF data) and *DISCUS* (simulate disordered/nano crystal structures) were performed throughout this work. The experimental total scattering PDF activity will be closely supported by density functional theory (DFT) calculations to investigate the electronic structure under simulated electrical and mechanical fields. PDF modeling can give realistic starting models for DFT relaxations of large supercell models. Conversely, DFT relaxations can aid the fitting of experimental PDFs.

PF.01.05
The Interplay of Chemical Pressure and Local Anion Order in Ta Perovskite Oxynitrides
Xin Wang[1], Bo Jiang[2], Yuanpeng Zhang[2], Young-Il Kim[3] and Katharine Page[1]; [1]The University of Tennessee, Knoxville, United States; [2]Oak Ridge National Laboratory, United States; [3]Yeungnam University, Korea (the Republic of)

Partial anion substitution in transition metal oxides provides rich opportunities to control and tune physical and chemical properties, for example, combining the merits of oxides and nitrides. In addition, the possibility of resulting anion sublattice order provides a means to target polar and chiral structures based on a wide array of accessible structural archetypes. Here we investigate the local structures of a family of tantalum oxynitrides - $ATaO_2N$ (A= Ba, Sr, Ca) - using a combination of neutron total scattering, molecular dynamics (MD) simulations, and density functional theory (DFT) electronic structure calculations. Neutron Bragg pattern analysis of long-range structures via the Rietveld method supports the standard settings for these compounds. However, across the A cation size series (from the larger Ba to the smaller Ca), the local structures are increasingly distorted with respect to the long-range average structures. Hereby, through analyzing total scattering patterns, local distortions and anion short-range ordering were explored in detail with both unit-cell based Rietveld-like and supercell based reverse Monte Carlo (RMC) approaches. Overall, structures with *cis*-ordering of the nitrogen anions in each TaO_4N_2 octahedra are favored over those with *trans*-ordering, with Ta off-centering and octahedral tilting playing decreasing and increasing roles with diminishing cation size, respectively. MD simulations and DFT calculations support the observed trends. The influence of these factors on local dipole formation and frustrated dipole ordering are examined.