Live Session
Room Live - Session LI-WeM1

In-Silico Design of Novel Materials by Quantum Mechanics and Classical Methods Live Session

Moderators: Dr. David Holec, Montanuniversität Leoben, Austria, Dr. Davide G. Sangiovanni, Linköping University, Sweden

10:00am **LI-WeM1-1 Program Chair's Welcome and Introduction of our Special Interest Talk***, Gregorz (Greg) Greczynski (grzegorz.greczynski@liu.se),* Linköping University, Sweden

Welcome to the ICMCTF 2021 Virtual Conference. We hope you will enjoy our Live Session and join us for the post-session discussion and additional Q&A opportunities following the Live Session.

10:15am **LI-WeM1-2 Special Interest Talk: Materials Discoveries at Extreme Conditions: A Path Towards New Advanced Materials***, Igor Abrikosov (igor.abrikosov@liu.se),* Linköping Univ., IFM, Theoretical Physics Div., Sweden **INVITED**

More than 100 years ago Gibbs [1] formulated his theory that still serves as a foundation for understanding of materials stability. Predictive power of the theory is well established for materials in the equilibrium state, the state with the lowest energy called the ground state. However, deep insights into mechanisms leading to the formation of metastable phases with energies above the ground state energy are missing, despite their wide appearance in nature and the broad use in technology. The luck of a consistent theory in this field limits our ability to discover and design novel materials.

In this talk we demonstrate that broadly varying external parameters, pressure, temperature and composition, as well as combining theoretical simulations with experiment, one discovers new materials with properties attractive for applications. Moreover, the studies of the behavior of matter at extreme conditions challenge the accepted concepts within materials science. In particular, the crystal structures two newly discovered high-pressure silica phases, coesite-IV and coesite-V contain SiO_6 octahedra, which, at odds with 3rd Pauling's rule, are connected through common faces [2]. We further illustrate intriguing features of recently discovered transition metal nitrides [3]. Finally, we report the synthesis of metallic, ultraincompressible and very hard rhenium nitride pernitride $Re_2(N_2)(N)_2$. Unlike known transition metals pernitrides, it contains both pernitride $(N_2)^{4-}$ and discrete N^{3-} anions, which explains its exceptional properties. Importantly, $Re_2(N_2)(N)_2$, which was discovered via a reaction between rhenium and nitrogen in a diamond anvil cell at pressures from 40 to 90 GPa has been recovered at ambient conditions, and a route to scale up its synthesis has been developed. Thus, the fundamental understanding of the physical principles behind the formation of the metastable structures generated in our studies is essential for the accelerated knowledge-based design of novel materials.

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11:15am **LI-WeM1-6 Are Protective Coatings Predictable?***, Jochen Michael Schneider (schneider@mch.rwth-aachen.de)*[1]*,* RWTH Aachen University, Germany **INVITED**

Designing the next generation of protective coating materials without utilizing trial and error-based methodologies requires truly predictive computational approaches. Important design criteria for crystalline and amorphous protective coating materials are the mechanical behavior as well as thermal and chemical stability. In this talk an effort is made to describe the good, the bad and the ugly of our predictive capabilities: Which predictions have been validated experimentally, and which experimental data cannot be described theoretically. Implications for future design efforts will be discussed.

11:45am **LI-WeM1-8 Controlling Phase and Microstructure of Ti-Cr-Al-N System Deposited by Arc Ion Plating***, Kenji Yamamoto (Yamamoto.kenji1@kobelco.com),* Kobe Steel Ltd., Japan **INVITED**

Since the discovery of metastable cubic TiAlN [1], which had superior mechanical and chemical property compared to TiN[2,3], experimental effort in searching of composition for improved property has been continued mainly in compositional frame of Ti, Cr and Al such as AlCrN [4-6] and TiCrAlN [7]. Currently, it is well known that each coating system undergoes phase transition from cubic B1 to hexagonal B4 structure once Al composition exceeds certain value depending on the system. Experimental determination of phase boundary between B1 and hexagonal B4 have been reported for each system, TiAlN by Ikeda et al. [8], CrAlN by Sugishima et al. [9] and TiCrAlN by Yamamoto et al [7].

On the theoretical side, Makino predicted, by using band parameter method [10], maximum solubility of AlN into cubic lattice of transition metal nitride while maintaining B1 cubic structure. According to the calculation of Makino, maximum solubility of AlN into cubic TiN and CrN lattice is 65.3at% and 77.2 at% which shows good agreement with above mentioned experimental results.

Phase transition from B1 to B4 dose not only means change in crystal structure, but means change in critical property such as hardness and oxidation resistance. In this presentation, mainly experimental perspective of importance of controlling the phase and micro-structure of multi element nitride systems of TiAlN, CrAlN and TiCrAlN for cutting tool application will be presented.

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12:15pm **LI-WeM1-10 Theoretical Insights into Transition Metal Nitrides for Thermoelectric and Piezoelectric Applications***, Björn Alling (bjorn.alling@liu.se),* Linköping Univ., IFM, Theoretical Physics Div., Sweden **INVITED**

Multicomponent thin films based on transition metal nitrides is a candidate class of materials for thermoelectric applications. In particular, ScN and CrN, being rock-salt structured semiconductors with small bandgaps, have been studied and found to have high power factors and Seebeck coeficients. [1]

In this work I precent our recent theoretical results based on first-principles calculations that are able to explains the anomalous and low thermal conductivity of CrN, which is another crucial parameter for a thermoelectric materials. We have found that there is a non-adiabatic dynamical coupling of disordered magnetic Cr moments in the paramagnetic state with the lattice vibrations that reduces the life time of heat carrying phonons. [2] For ScN, that has a high thermal conductivity, we have studied theoretically which alloying strategies that could reduce it while still keeping suitable electrical properties. Finally, I present the result of our investigations of novel ternary nitrides based on $TM_{0.5}AE_{0.5}N$ (TM=Ti, Zr,Hf; AE=Mg,Ca,Zn) that can combine suitable electrical properties with alloy-scattering of phonons that reduces thermal conductivity.[3] The analogy to our investigations into chemically similar, but structurally different wurtzite nitrides for piezoelectric applications is discussed. [4]

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[1] **2020 Bill Sproul Awardee**

12:45pm **LI-WeM1-12 Closing Remarks & Thank You's***, **Davide Sangiovanni (davide.sangiovanni@liu.se)***, Ruhr University Bochum, Germany

We hope you enjoy the Live Session. Please join us for the post-session discussion and enjoy our On Demand Sessions. We hope to see you tomorrow!

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