## Nano and 2D Materials

## Room Naupaka Salon 5 - Session NM1-ThM

### Nanomaterials - Properties and Applications I

**Moderator: Santosh KC**, San Diego State University

8:40am **NM1-ThM-3 Different Directions In Layered Materials*, Joshua Goldberger,*** The Ohio State University **INVITED**

Layered and 2D materials are currently one of the most well-studied classes of solid- state compounds, due to the plethora of unique physical phenomena found in these anisotropic materials. Here we will describe our recent work in the synthesis, properties, and applications of layered materials that exhibit either n-type or p-type conduction behavior depending on the crystallographic direction, a phenomenon we refer to as "goniopolarity". We will establish the origin of this exotic behavior and the band structure design principles for identifying new goniopolar materials.[1] This has led to a significant expansion in the number of compounds that we have experimentally demonstrated to exhibit this effect, such as $NaSn_2As_2$, NaSnAs, $WSi_2$ and $PdSe_2$.[2-5] Finally, considering that most modern electronic devices require the integration of p-type and n-type regions for functionality, we will show how the unique charge separation in goniopolarmaterials have the potential to create new efficient energy-harvesting and electronics technologies.

[1] Y. Wang; K. G. Koster; A. M. Ochs; M. R. Scudder; J. P. Heremans; W. Windl; J. E. Goldberger, *J. Am. Chem. Soc.* **142**, 2812-2822 (2020).

[2] B. He; Y. Wang; M. Q. Arguilla; N. D. Cultrara; M. R. Scudder; J. E. Goldberger; W. Windl; J. P. Heremans, *Nat. Mater.* **18**, 568-572 (2019).

[3] K. G. Koster; Z. Deng; C. E. Moore; J. P. Heremans; W. Windl; J. E. Goldberger, *Chemistry of Materials* **35**, 4228-4234 (2023).

[4] R. A. Nelson; Z. Deng; A. M. Ochs; K. G. Koster; C. T. Irvine; J. P. Heremans; W. Windl; J. E. Goldberger, *Mater. Horiz.* **10**, 3740-3748 (2023).

[5] A. M. Ochs; P. Gorai; Y. Wang; M. R. Scudder; K. Koster; C. E. Moore; V. Stevanovic; J. P. Heremans; W. Windl; E. S. Toberer; J. E. Goldberger, *Chem. Mater.* **33**, 946-951(2021).

9:20am **NM1-ThM-5 Evaluation of Vapor Pressure of $MoO_2Cl_2$ and Its Initial Chemical Reaction on a $SiO_2$ Surface by Ab Initio Thermodynamics*, Hyun-Kyu Kim, Na-Young Lee, Yeong-Cheol Kim,*** Korea University of Technology and Education, Republic of Korea

The vapor pressure of $MoO_2Cl_2$ and its initial chemical reaction on a $SiO_2$ surface were evaluated and analyzed using *ab initio* thermodynamics. The vapor pressure of $MoO_2Cl_2$ was calculated using the Gibbs free energy, while considering the zero-point energy, temperature-dependent enthalpy change, and entropy. The initial surface reaction was also studied as a function of temperature and partial pressure. The calculated sublimation temperature of $MoO_2Cl_2$ was 410 K, and its vapor pressure at 350 K was 8.2 torr. The partial pressure calculated for $MoO_2Cl_2$ agreed reasonably well with the experimentally measured value. The surface reaction energy barrier between $MoO_2Cl_2$ and $SiO_2$ was 0.8 eV.

9:40am **NM1-ThM-6 Development of TiAl Alloys: A Future Light-Weight Material for Extreme Condition*, Seong-Woong Kim,*** Korea Institute of Materials Science, Republic of Korea

Research on developing new TiAl alloys for high temperature (> 900°C) applications is introduced. TiAl alloys have been gained interest for automobile and aerospace applications due to their low density, good oxidation resistance and high temperature strength. However, lack of room temperature ductility and the limitation of operating temperature hindered the practical applications of TiAl alloys. At KIMS, we have developed new TiAl alloys which have excellent room temperature and high temperature properties. Expecially, the alloy #16 showed excellent oxidation resistance in the temperature range from 900 to 1000°C by forming stable $Al_2O_3$ oxidation layer. Moreover, alloy #16 exhibit room temperature ductility up to 0.78% solely by casting.

In addition, we introduced some in-situ transmission electron microscopy experiments in order to understand an underlying mechanism on room temperature ductility of TiAl alloys. Also, molecular dynamics simulation was conducted to calculate the stacking fault energy of TiAl alloys and to show which deformation mode is dominant. The difference in deformation mode was explained by stacking fault energy of the TiAl alloys which was calculated by molecular dynamics. Furthermore, the role of lamellar orientation of tensile direction on deformation behavior was examined using Schmid factor of each orientation. Finally, we proposed the important microstructural factors to have room temperature ductility of TiAl alloys.

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