MRS JOURNAL HIGHLIGHTS

mrs.org/publications-news

Double perovskite ($Sr_2B'B''O_6$) oxides for high-temperature thermoelectric power generation—A review

Tanmoy Maiti, Mandvi Saxena, Pinku Roy

Double perovskite-based oxide materials are proposed for thermoelectric (TE) applications due to better environmental and high-temperature stability, and lower processing cost. Decoupling of phonon-glass and electron-crystal behavior is possible by reducing thermal conductivity, a consequence of induced dipolar glassy state in a relaxor ferroelectric. Metal-like electrical conductivity (~105 S/m) in materials that are inherently insulating in nature, and temperature-driven *p*–*n* type conduction switching assisted colossal change in thermopower in some oxides, hitherto, obtained only in chalcogenides.
https://doi.org/10.1557/jmr.2018.376

Deformation behavior of nanocrystalline and ultrafine-grained CoCrCuFeNi high-entropy alloys

Seungjin Nam, Jun Yeon Hwang, Jonggyu Jeon, Jihye Park, Donghyun Bae, Moon J. Kim, Jae-Hun Kim, Hyunjoo Choi

Authors report the structure and deformation of nanocrystalline (NC) and ultrafine-grained (UFG) CoCrCuFeNi high-entropy alloy (HEA) with grain sizes ranging between 59 and 386 nm. The as-sintered HEA exhibited two face-centered-cubic (FCC) phases (CoCrFeNi-rich and Cu-rich phases) and a 59 nm grain size, but an FCC CoCuFeNi-rich phase of 386 nm was observed heating at 1000°C. The yield strength decreased from 1930 to 883 MPa, and plastic strain to failure increased by 8–32%. Grain boundary strengthening coupled with lattice distortion was the dominant strengthening mechanism for NC HEAs, possibly because of significant lattice distortion. https://doi.org/10.1557/jmr.2018.477

Thin water films covering oxide nanomaterials: Stability issues and influences on materials processing

Gilles R. Bourret, Oliver Diwald

Ambient water condenses readily on metal oxides which can lead to water-mediated reactions at the oxide surface. Water films of <10 molecular layers thickness can modify the oxide surface chemical reactivity and stability. However, due to the confinement of mass transport at the oxide surface, these processes do not proceed the same as in bulk water. The authors illustrate these interactions for MgO and TiO_2 nanostructures and show that condensed water films can induce significant dissolution/precipitation, morphological changes, crystallization, and self-assembly in the nanocrystalline solid state.
https://doi.org/10.1557/jmr.2018.429

Neural network analysis of dynamic fracture in a layered material

Pankaj Rajak, Rajiv K. Kalia, Aiichiro Nakano, Priya Vashishta

The authors demonstrate using a neural network to examine fracture in $MoWSe_2$ using molecular dynamics. Through addressing the relative importance of the model parameters, and noting how different phases/defects are identified in the network the model performance is improved both in simulation time as well as accuracy.
https://doi.org/10.1557/adv.2018.673

Number density descriptor on extended-connectivity fingerprints combined with machine learning approaches for predicting polymer properties

Takuya Minami, Yoshishige Okuno

The authors use machine learning to successfully predict the refractive index, bandgap, and dielectric constant of linear polymers by adapting ECFPs. However, the materials' mechanical properties, which are more strongly influenced by larger scale structure, were not captured accurately with this methodology, demonstrating the capabilities and limitations of this ML approach for these materials.
https://doi.org/10.1557/adv.2018.454

Silver chlorobromide nanocubes: A class of reactive templates for synthesizing nanoplates and nanocages of silver thiolates

Sasitha C. Abeyweera, Yugang Sun

Creating colloidal nanoparticles with uniform chemistry and size distribution presents significant challenges. The authors demonstrate an experimental approach of creating silver metal–organic complexes that constrain the precursor ion to control the kinetics of particle formation. The resulting materials have predictable optical properties, and the process may be applicable to other applications such as catalysis.
https://doi.org/10.1557/adv.2019.219

MRS MATERIALS RESEARCH SOCIETY®
CAMBRIDGE UNIVERSITY PRESS