Optimization of electrophoretic deposition technique to control doping and densification of protective spinel coatings for SOC interconnects

11:20 AM

(PACRIM-328-2021) Optimization of electrophoretic deposition technique to control doping and densification of protective spinel coatings for SOC interconnects

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Manganese cobaltite spinel coatings have been reported to limit oxidation and Cr-evaporation from ferritic stainless steel interconnects in solid oxide cell stacks; however, the implementation of the functional properties of the base Mn–Co spinel coating and compatibility with the substrate can be pursued through the optimisation of the coating composition, as well as the deposition method and sintering profile. Electrophoretic deposition (EPD) allows to deposit homogeneous layers in few seconds on complexly shaped steel components; it also offers the possibility to produce in-situ doped coatings, avoiding time and energy consuming multi-step processes. In this work, various EPD suspensions are optimised to achieve a single step co-deposition of CuO, Fe_2O_3 and $Mn_{1,5}Co_{1,5}O_4$ on Crofer 22 APU. Different Fe-Cu doped Mn–Co spinel are successfully obtained by controlling the precursors amount in the EPD suspension and subsequent reactive sintering, as proved by detailed SEM and TEM analyses. Improved functional properties of produced coatings are evaluated in terms of oxidation kinetics and area specific resistance. Both the iron and copper amount in the coating and the sintering process significantly influence the coating densification, with benefits to the protective properties and thermomechanical compatibility with the interconnect.

PACRIM Symposium 25: Direct Thermal to Electrical Energy Conversion Materials, Applications, and Thermal Energy Harnessing Challenges

Tellurides

Room: Oxford

Session Chairs: Matt Beekman, California Polytechnic State University; Emmanuel Guilmeau, CNRS CRISMAT

8:30 AM

(PACRIM-329-2021) Thermoelectric Properties of Various Barium Copper Chalcogenides (Invited)

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Binary copper chalcogenides as well as several ternary and quaternary variants have been investigated because of their low thermal conductivity values, high earth abundancy constituents, and tunable electrical properties. In particular, materials such as $Cu_{2-x}S$ and $Cu_{2-x}Se$ have low thermal conductivity values (< 1 W $m^{-1}K^{-1}$) due to their 'liquid like' structures. Unfortunately, these materials often lack stability due to the migration of Cu ions, and therefore efforts have been undertaken to hinder the Cu ion movement, enhancing the stability. Several Ba containing copper chalcogenides such as $BaCu_2Te_2$, $Ba_3Cu_{14-x}Te_{12}$, $BaCu_{6-x}S_{1-y}Te_{6+y}$ and $BaCu_{6-x}Se_{1-y}Te_{6+y}$, $Ba_3Cu_{16-x}S_{11-y}Te_y$ and $Ba_3Cu_{16-x}Se_{11-y}Te_y$ have been characterized in the last decade or so. These materials exhibit typical copper chalcogenide attributes, such as $Cu(S,Se,Te)_4$ tetrahedral frameworks and p-type semiconductivity within a moderate temperature range, in part with peak zT values of the order or even in excess of 1. In this presentation, these materials will be compared to each other, and their properties presented, as well as efforts to stabilize them despite noticeable Cu ion conductivity.

9:00 AM

(PACRIM-330-2021) Defect engineering to enhance thermoelectric performance of GeTe

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There is a vital need to develop technologies for energy saving and also dynamically harvest energy from surroundings to power IoT applications. Thermoelectrics is a good candidate, and nanostructuring yield some powerful material enhancement principles. Initially trying to achieve a magnetic enhancement effect, Cr doping was tried in GeTe, and had the serendipitous effect to lower the formation energy of Ge defects. This led to creation of homogenously distributed Ge precipitations and Ge vacancies, coupled with typical band convergence doping to lead to ZT~2. A high entropy approach of AgInTe2 alloying into GeTe, stabilized the cubic phase, thereby enabling enhanced doping of Bi, leading to the first stable n-type conduction in GeTe. The hidden role of rhombohedral distortion degree on the Ge-vacancy formation energy was revealed and utilized leading to high power factor and excellent average ZT. Acknowledgments: Members of JST Mirai Large-Scale Program (JPMJMI19A1) are thanked.

9:20 AM

(PACRIM-331-2021) First principles calculations of electronic and thermoelectric transport properties of $Pb_2Bi_2Te_5$ with different atoms sequences

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Chalcogenide compounds such as PbTe, $PbBi_2Te_4$, $PbB_{i4}Te_7$ and Bi_2Te_3, belong to the homologous series of ternary phases n(PbTe) m(Bi_2Te_3), exhibit both excellent topological insulators and promising thermoelectric properties. For 2(PbTe)(Bi_2Te_3) also read as $Pb_2Bi_2Te_5$, two different possible atoms sequences have been reported: -Te-Pb-Te-Bi-Te-Bi-Te-Pb-Te- (S1) and -Te-Bi-Te-Pb-Te-Pb-Te-Bi-Te- (S2). In this paper, we performed a series of first principles calculations using density functional theory (DFT) to determine electronic and thermoelectric properties of $Pb_2Bi_2Te_5$ with these 2 different atoms sequences. The related compounds PbTe and Bi_2Te_3 were investigated for comparison. Different exchange-correlation functionals (LDA, PBE, EV, TB-mBJ potentials, and rev-vdW-DF2) were tested, w/o spin-orbit coupling, which has been found to have important effects. The calculated electronic bands indicate that both of the 2 sequences lead to indirect band gap semiconductors. We also calculated elastic moduli, dielectric constants, Born effective charges, and phonon dispersion within the quasi-harmonic approximation. Based on the above-mentioned calculations results, thermal conductivity has been obtained by solving the Boltzmann transport equation. The most interesting compound for thermoelectric applications was found to be $Pb_2Bi_2Te_5$ with the S2 sequence.