High-temperature Transport Behavior and Thermoelectric Properties of Rare-earth Barium Copper Oxide Compounds

Anucha Watcharapasorn[1,5], Atsuko Kosuga[2], Poom Prayoonphokkharat[3], Paitoon Boonsong[4], Pimpilai Wannasut[1], Sireetone Yawirach[1], Pornsawan Sikam[5,6], Pairot Moontragoon[7], Kattaliya Chaipisan[1], Ampika Rachakom[8], Penphitcha Amonpattaratkit[9], Panupong Jaiban[10], Nittaya Keawprak[11]

[1]Department of Physics and Materials Science, Faculty of Science, Chiang Mai University, Thailand
[2]Department of Physical Science, Graduate School of Science, Osaka Metropolitan University, Japan
[3]Department of Science, Takpittayakhom School, Thailand
[4]Regional Medical Sciences Center 1 Chiang Mai, Department of Medical Sciences, Ministry of Public Health, Thailand
[5]Research Center for Quantum Technology, Faculty of Science, Chiang Mai University, Thailand
[6]Office of Research Administration, Chiang Mai University, Thailand
[7]Department of Physics, Faculty of Science, Khon Kaen University, Thailand
[8]Faculty of Science and Agricultural Technology, Rajamangala University of Technology Lanna, Thailand
[9]Synchrotron Light Research Institute (Public Organization), Nakhon Ratchasima, Thailand
[10]Faculty of Science, Energy and Environment, King Mongkut's University of Technology North Bangkok, Thailand
[11]Thailand Institute of Scientific and Technological Research, Thailand

Our work investigates the transport behavior and thermoelectric properties of RE-$Ba_2Cu_3O_{7-x}$ compounds (where RE = rare-earth elements) at intermediate and high temperatures. Nearly all RE-BCO compounds with stoichiometric compositions are well-known as high-Tc superconductors and they therefore possess very high electrical conductivity but very low Seebeck coefficient. To make these materials useful for thermoelectric applications, these electrical properties need to be tuned and optimized. Some inherent factors that are of concerns include oxygen vacancies and valence fluctuation that may also affect the crystal and electronic band structures. Starting with $YBa_2Cu_3O_{7-x}$ (YBCO) ceramics where typical solid-state reaction and sintering methods under normal air atmosphere were employed, the compounds showed metallic conduction up to as high temperature as 800 K. Substituting Y with other rare-earth elements such as Nd, Sm, Eu and Dy still showed similar metallic conduction behavior. Exception being Pr whose electrical conductivity shows semiconducting behavior. This suggests that the valence variation inside the material plays an important role. By doping some elements or compounds in YBCO, some apparent changes in electrical and thermal transport properties can also be observed. To obtain some insight knowledge regarding these changes, the theoretical study was performed within density functional theory (DFT) via Vienna Ab initio Simulation Package (VASP) code. Supercells as large as nine times of the primitive YBCO are designed as the pristine YBCO. After that, atomic substitution and extraction of oxygen with the different doping concentration are carried out. The theoretical and experimental results are then compared to see if these methods can be used for optimizing the design of thermoelectric materials based on these RE-BCO type compositions.

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