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STUDY ON PROBLEM FORMULATION FOR LEAD AND NON LEAD BASED MATERIALS

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Abstract: Due to the negative environmental impact, the usage of lead in perovskite solar cells has been a matter of concern. Moreover, a suitable replacement of Pb with similar optoelectrical properties is hard to find. $MAPbI_3$ is the most common material that has been studied for solar PV applications. Compared to $MAPbI_3$, Cs_2TiBr_6 and $MASnI_3$ have been less studied. In this study, their potential in solar cell applications has been investigated. Titanium and tin are two materials that have been used in numerous studies as an alternative to Pb-based perovskite. However, the lack of optimization and combinations of electron transport layer (ETL) and hole transport layer (HTL) material choices leave a lot to be desired. In this study, two different perovskite absorber layers, Cs_2TiBr_6 and $MASnI_3$, have been simulated, optimized, and compared with Pb-based $MAPbI_3$, where La-doped $BaSnO_3$ is used as ETL and $CuSbS_2$ as HTL in identical cell architectures. La-doped $BaSnO_3$ is well known for its high electron mobility and excellent optical properties, which makes it an ideal candidate for ETL. On the other hand, $CuSbS_2$ has appropriate band alignment with perovskite materials and has a high absorption profile to be used as HTL. The simulations were analyzed by optimizing key parameters like absorber layer thickness, defect density, and temperature. The optimized device architecture reached the power conversion efficiencies (PCE) of 29.45% for $MASnI_3$, followed by $MAPbI_3$ (22.47%) and Cs_2TiBr_6 (21.96%). The result indicates that high performance lead-free perovskite cells are very much possible through proper material selection and optimization.

Keywords: ELECTROCALORIC EFFECT, LEAD AND NON LEAD BASED SOLID SOLUTIONS, PROBLEM FORMULATION

Introduction: Among the several creative eco-friendly alternatives, the route to refrigerating and air-conditioning in a manner apart from vapour compression undoubtedly leads through solid-state automations that relies on the various caloric effects (Fahler, 2018; Kitanovski et al., 2015). This caloric category relates to the technologies (Qian et al., 2016), which feature environmentally friendly solid state caloric materials that do not directly contribute to the global temperature change (Ciro Aprea et al., 2018), unlike other cooling liquids on which vapour compression is centered and emits hydrochlorofluorocarbons (HFCs) (C. Aprea et al., 2018; Ciro Aprea et al., 2015; Greco et al., 1997; Greco & Vanoli, 2006; M. Li et al., 2012). Electrocaloric effect (ECE) is basically a physiological process that occurs in materials that have dipolar components, i.e., materials that have particular dielectric characteristics (T. Correia & Zhang, 2014). It necessitates a link of the electric field with dipolar orientation parameter so that alteration in the field causes the dipolar order to change, and therefore, leads to variation in the dipolar entropy of the system. Under adiabatic circumstances, the variation in applied electric field manifests the warming and chilling in an electrocaloric substance. ECE has subsequently become quite an appealing concept with potential applications in a variety of fields, including new generation heating and cooling equipments that comparatively more ecological friendly and energy efficient than traditional cooling devices. Macroscopically, the phenomenological explanation revolves around the interchange of entropy between the two energy reservoirs, namely the thermal entropy and dipolar subsystems, which is imposed by variation in the field executed under adiabatic circumstances, however, microscopic aspect behind the ECE is not entirely recognized yet (Mischenko et al., 2006). Modifications in the electric field allow a dielectric material's dipolar configuration to change from less organized to more ordered as shown in Figure 1.1, and conversely on the removal of electric field (Lang, 1976; Lu et al., 2012; Rožič et al., 2011). The variations can be deemed adiabatic if they are made on a timeframe that enables the heat transfer from the substance to the environment to be ignored. Owing to the lattice vibration entropy remuneration of the lowering of dipolar entropy, an electric field that is being applied adiabatically causes a rise in the temperature of a substance. The adiabatic withdrawal of the field, on the other hand, promotes lowering of temperature of the substance; which means, the temperature of the object falls as the lattice vibration entropy reduces, offsetting the growth in the dipolar entropy. During this adiabatic process, the overall entropy of the entire system stays unchanged in both circumstances, as it should.

Calorimetry via Differential Scanning

The most well-known thermal approach for studying a myriad of substances is Differential Scanning

Calorimetry (DSC). It has a number of benefits, including a high sensation for monitoring variation in enthalpy, the capacity to work with less quantity samples, and quick operation processes using widely available equipments and application software. Thermal conditions are usually imposed for electrocaloric investigations (Guyomar et al., 2006; Sebald et al., 2007). The electric field is then provided, and the heat transfer is monitored. The electrocaloric entropy or electrocaloric variation in temperature could be estimated using observed heat flow. These ECE studies necessitate a few minor changes to conventional equipments and software, primarily in the invigilated electric field region. For bulk materials assessed at relatively high electric fields, DSC is an appropriate electrocaloric procedure, resulting in a considerable shift in electrocaloric temperature.

Energy harvesting from electrocaloric materials

Due to the obvious rise in population and economic development, worldwide energy expenditure has grown considerably in recent years, resulting in pollution and a scarcity of fossil fuels. To address this issue, researchers are increasingly interested in renewable energy conversion and harvesting systems (Malakooti et al., 2018; Yong Zhang, Jeong, et al., 2018; W. Zhao et al., 2017). Energy harvesting is a method that uses a variety of technologies to convert waste energy and energy from the environment into electrical power, including thermal electrical modulus for gradient thermal energy, solar cells for solar energy, and piezoelectric and polar dielectric for mechanical energy (Yan Zhang et al., 2019; Yong Zhang et al., 2019; C. Zhao et al., 2019). Mechanical sources are most often employed because they are easily accessible in ambient temperatures and are not limited by time or weather conditions (Jeong et al., 2017; Yong Zhang, Sun, et al., 2018). Mechanical energy harvesting focused on the pyroelectric/electrocaloric effect, which captures energy from low gradient alternating power due to pyroelectric/electrocaloric material's spontaneous electric polarization, is becoming a flash-point in the area of study (Sebald et al., 2009; Z. L. Wang & Song, 2006; Yu et al., 2015; Yan Zhang et al., 2017). The pyroelectric effect is explained by variation in the polarization of polar materials caused by a temperature shift (Bi, 2020). Materials with a high pyroelectric coefficient at working temperatures are good candidates for efficient thermal energy harvesting (C.C Hsio & A. S. Siao, 2018; Srikanth et al., 2017).

Problem formulation for lead based materials

The polarization of ferroelectrics increases with the electric field because they have a net dipole moment. Furthermore, applying an electric field reduces entropy, resulting in an adiabatic increase in temperature in these materials. Many ferroelectric materials, particularly relaxor ferroelectrics, have been investigated using these principles (Correia et al., 2009; Lawless, 1977; Lu et al., 2010; Mischenko et al., 2006; Neese et al., 2009; Saranya et al., 2009; Tuttle & Payne, 1981). Lead-oxide-based materials, such as PZT, have demonstrated significant experimental, practical, and technological value. PZT materials can be used in a variety of electronic instruments, including non-volatile memories, modulators, optical shutters, and infrared sensors, due to their strong dielectric characteristics (Cho et al., 1999; Nunes et al., 2001; Paiva Santos et al., 2000). Depending on the Zr content, PZT can be paraelectric, ferroelectric, or antiferroelectric (Bai et al., 2011). Because of the strong pyroelectricity inverse effect, Zr rich PZT ceramics produce encouraging ECE (Zhang & Whatmore, 2003). A variety of compounds have been produced with the help of proper doping at the A/B site (Lal et al., 1989). These compounds are considered to be extremely important in a variety of industrial applications. Due to their high dielectric constants (Pan et al., 1989), the MPB composition $PbZr_{0.52}Ti_{0.48}O_3$ (Bai et al., 2011) is also utilized as a capacitor. However, cooling applications for $PbZr_{0.52}Ti_{0.48}O_3$ based ceramics have not been considered. Moreover, bismuth, lanthanum and Neodymium substitution in PT at MPB improves ferroelectric characteristics and diffuses the phase transition, it has a wide range of industrial applications (Babu et al., 2018; Rai & Sharma, 2004). So, by improving the sintering temperature, we propose to investigate the ECE in Bi/La/Nd doped PZT/PT.

Problem formulation for non-lead based materials

Due to their superior piezoelectric properties, ferroelectrics for example lead zirconate titanate (PZT), are broadly employed for piezoelectric actuators, sensors, and transducers (Jaffe and.Cook, 1971; Levassort et al., 2001). Volatilization of poisonous PbO in the process of high temperature sintering, on the other hand, not only pollutes the environment, but also causes product composition and electrical qualities to become unstable. As a result, environmentally acceptable lead-free piezoelectric materials must be introduced to replace these traditional ceramics, which has become one of the primary themes in current piezoelectric material development. Smolenskii et al. discovered sodium bismuth titanate, $Na_{0.5}Bi_{0.5}TiO_3$ (NBT) ferroelectric in 1960 (Li et al., 2009). NBT has a rhombohedral symmetry with a = 3.891Å and α = 89°36' at room temperature, making it an attractive choice for lead-free piezoelectric ceramics. It is ferroelectric, with a large remnant polarization of (Pr = 38 μC cm-2) and a significant coercive field of (Ec = 7.3kV mm-1) (Li et al., 2009). It has been described as a relaxor with complex diffuse phase transitions and structural changes from rhombohedral to tetragonal (Suchanicz, 1998). NBT exhibits phase transition (Tm) around 350°C agnate to the highest value of dielectric permittivity along with a dielectric anomaly at lower temperature (200°C) which corresponds to depolarization temperature (Td) (Yang et al., 2020). It has been recently found that the ferroelectric-relaxor and/or antiferroelectric phase transition that occurs near Td is quite favorable for EC responses (Yang et al., 2020). The introduction of 18% KBT in NBT lowers the Td from 200-150°C (Goupil et al., 2016), whereas, incorporation of MgO helps in shifting Td towards lower temperature and also enhances the ferroelectric properties (Koch et al., 2017). Henceforth, our main focus herein is on EC production of K2CO3 and MgO co-modified NBT.

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