UTBORN-PT

Unconventional Thermoelectrics Based on Self-Organized Binary Nanocrystal Superlatices

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TEAM

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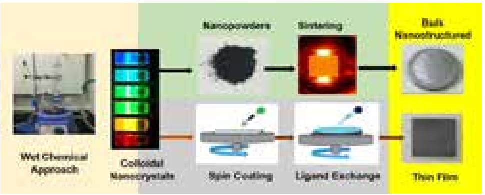
NANOTECHNOLOGIES

Background

Self-organized binary nanocrystal superlattices (BNSLs) based on semiconducting colloidal nanocrystals is of great significance in thermoelectrics, both from a fundamental and applications perspective. In recent years, the prevailing need for facile fabrication which is solution-process able, and transport property optimization for high thermoelectric figure-of-merit, has driven the development of colloidal quantum dots (QDs) in which electrical and thermal transport can be readily modulated by dimensional constraints via quantum confinement and coupling between the nanocrystals. The chalcogenides monodisperse nanocrystals proposed in this project enable a unique combination of transport properties with proximal interaction, ligand engineering and nanostructuring in nanocrystal ensembles. This will lead to a decoupling of phonon and electron transport parameter and unprecedented enhancement in TE figure-of-merit for practical applicability in thin film thermoelectrics.



Approach/Methodology

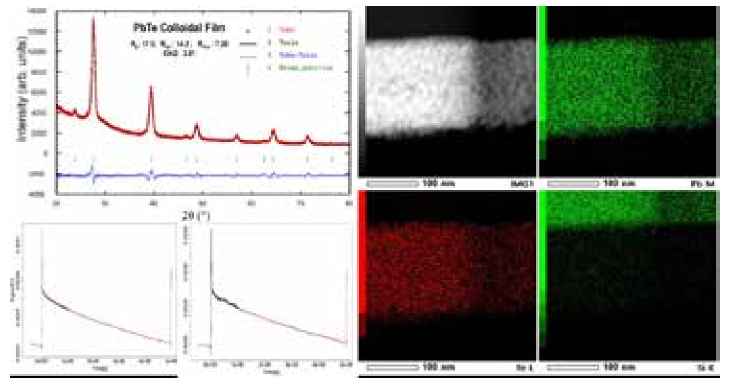
Synthesis and characterization of high quality chalcogenides based colloidal nanocrystals:
Facile and up-scalable thermo-chemical alloying route for high purity Bi2Te3, Bi2Se3, Cu2Se Bi0.5Sb1.5Te3, Bi2Te2.7Se0.3, PbTe and Ag based colloidal nanocrystals which had been corroborated by XRD and electron microscopy (SEM, TEM) based structural characterization.
Assembly, theoretical analysis and characterization of NPs as superlattices:
The implication of ligand exchange, deposition condition and thermal sintering on NPs assembly were examined and theoretically validated for optimal thermal and electrical transport.
Investigation and optimization of electrical & thermal transport properties in NPs ensembles:
The thermal and electrical transport property characterization and their correlation studies to optimize ZT. Advance approaches including defect engineering, carrier filtering, strain and mass fluctuation, Spinodal decomposition were demonstrated. Efficacy of wet chemical approaches for attaining high ZT and scalable production is presented.
High ZT thermoelectric via. Bottom-up assembly of nanocrystals:
This was realized in bulk nanostructured Bi2Te3 based p-type and n-type material for low temperature TE application.

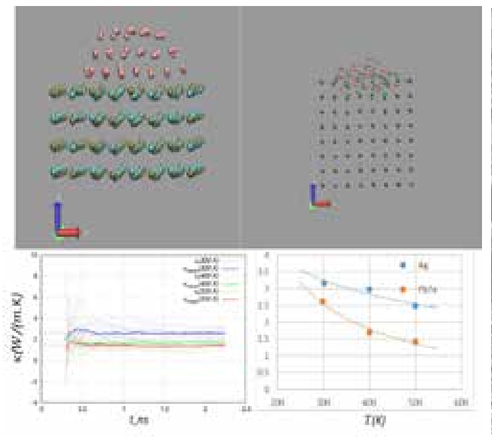
Implementation Challenges

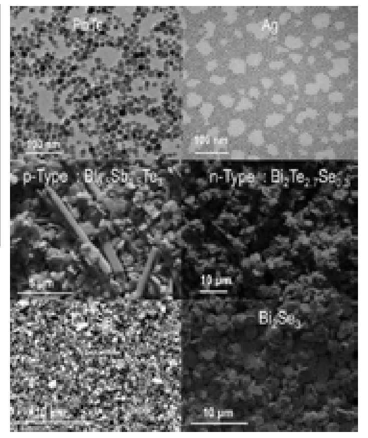
- Monodispersed growth of colloidal semiconductor nanocrystals.
- Optimal deposition and sintering conditions for film and bulk samples of nanocrystals ensembles.
- Accuracy and precision of thin film thermal and electrical transport properties measurement.
- Ubiquitous thin-film interfacial problems resulting in transport properties deterioration.
- Modelling heterogeneous interfaces of binary superlattices, such as the PbTe-Ag junction or the surface of PbTe nanoparticle, passivated with protective ligands, proved to be unreliable with currently published interaction-potentials
- Attaining lower resistivity in ligand stripped binary nanocrystal superlattices of films with thickness > 100 nm.

Main Findings

- Large-scale colloidal synthesis of Bi2Te2.7Se0.3 plate-like particles give access to high-performing n-type thermoelectric material for low temperature application
- High Performance p-type Bi-Sb-Te nanocomposite for low temperature power generation by spark plasma sintering
- Ligand engineered phase-pure 150 nm thick films of oleate-capped PbTe NCs with reduced thermal conductivity.







Expected Impact

Thermoelectric generators (TEGs) interconverts heat and electrical energy, and are energy recovery and conversion devices with enormous potential to harvest the dissipated heat from power plants, automotive engines, housing heating systems, and even electronic devices for micro-power generation applications. The synthesized BNSLs based thermoelectric materials have led to the development of next generation of thermoelectrics and concurrently will provide fundamental breakthrough for simple, scalable and low-cost processing of high performance TEGs. The significant improvement of the heat to electricity conversion factor ZT is expected to result from the proposed program, which will substantially improve the conversion efficiency.
The attained ZT values for both p-type and n-type materials at near room temperature regime corresponds to approx. 5 - 8% conversion efficiency and represent a "factor of 2" improvement in the currently operational TE modules. This will provide a long-term solution for utilizing the huge amount of available low grade waste energy and practical usability for newly emerging applications like wearable electronics, chilling of electronic micro-devices, medical body implants, remote sensing etc. Additionally, discovered difficulties with modelling of heterogeneous interfaces pinpoint particular direction for future development in the filed of interaction potentials.

Project Highlights

- Scalable thermochemical alloying route for synthesizing chalcogenides nanocrystals.
- Cumulative temperature dependence approach for estimation of realistic thermoelectric performance.
- Bulk nanostructured n-type alloys with ZTavg≈0.7 with estimated thermoelectric conversion efficiency of approx. 5-6%
- Bulk p-type nanocomposite with ZTavg≈1.2 for low temperature thermoelectric application.
- Ligand engineered phase-pure 150 nm thick films of oleate-capped PbTe NCs with reduced thermal conductivity.

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