Engineering nanoalloys for enhanced thermoelectric efficiency.

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Introduction

Thermoelectric materials offer a compelling pathway for energy conversion, enabling the direct conversion of heat into electricity and vice versa. Recent advancements in nanoalloys have opened new avenues for optimizing these materials, with researchers employing various strategies to enhance their performance. The ongoing efforts involve detailed theoretical investigations, such as first-principles calculations, alongside experimental techniques to engineer desirable properties at the nanoscale.

One area of investigation involves the exploration of the thermoelectric capabilities of Co- and Fe-based Heusler nanoalloys through first-principles calculations. It specifically investigates the electronic structure, Seebeck coefficient, and thermal conductivity. The findings indicate that these nanoalloys possess high Seebeck coefficients and favorable electronic transport properties, suggesting their potential for efficient thermoelectric energy conversion. The research highlights the critical role of electronic band structure engineering in optimizing thermoelectric performance at the nanoscale [1].

Other research delves into the investigation of the thermoelectric transport properties of Ag-doped FeS2 nanoalloys using first-principles calculations. The study reveals how Ag doping influences the electronic structure, leading to enhanced Seebeck coefficients and improved electrical conductivity. It highlights the potential for optimizing thermoelectric performance in pyrite-based materials through controlled doping and nanostructuring, pointing towards new avenues for designing efficient thermoelectric devices [2].

Further studies examine the impact of microstructure and annealing processes on the thermoelectric properties of n-type Bi2Te3-based nanoalloys, produced via spark plasma sintering. The study shows that precise control over annealing conditions can significantly refine the microstructure, leading to an optimization of the Seebeck coefficient and overall thermoelectric performance. These findings offer practical guidance for the fabrication of high-efficiency Bi2Te3-based thermoelectric materials [3].

Another focus of research is on improving the thermoelectric efficiency of Ag-doped GeTe compounds by utilizing nano-alloying and phonon engineering strategies. The study demonstrates that careful control of the nano-alloying process can effectively reduce lattice thermal conductivity while maintaining favorable electronic transport properties, leading to a significant increase in the Seebeck coefficient and overall ZT values. This approach provides a promising route for developing high-performance GeTe-based thermoelectric materials [4].

Moreover, an investigation into the synergistic effects of Ag and Sb co-doping on the thermoelectric properties of PbTe-based nanoalloys. The research demonstrates that the combination of these dopants significantly enhances the Seebeck coefficient and electrical conductivity while simultaneously reducing the thermal conductivity. This dual effect results in a substantial improvement in the overall thermoelectric figure of merit, highlighting a powerful strategy for designing advanced PbTe-based materials with superior performance for energy conversion applications [5].

Theoretical frameworks have also been employed to explore the thermoelectric properties of SnS-based nanoalloys using first-principles calculations. It elucidates how alloying elements impact the electronic band structure, leading to significant changes in the Seebeck coefficient and electrical conductivity. The research identifies promising compositions that exhibit enhanced thermoelectric performance, offering valuable insights for the experimental synthesis and development of novel SnS-based materials for waste heat recovery [6].

A strategy has been presented to achieve high thermoelectric performance in Cu2SnSe3-based materials through band structure modulation and nano-alloying. The approach effectively optimizes carrier concentration, enhances the Seebeck coefficient, and reduces lattice thermal conductivity by introducing nanoscale alloy precipitates. The findings underscore the importance of combined electronic and phonon engineering at the nanoscale to significantly boost the overall thermoelectric figure of merit for practical applications [7].

Methods to tune thermoelectric properties have also been explored in CoSi nanoalloys through doping and strain engineering using first-principles calculations. The research reveals that both doping

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with specific elements and applying mechanical strain can effectively modify the electronic band structure, leading to an optimized Seebeck coefficient and improved electrical conductivity. These insights provide theoretical guidance for the design and synthesis of high-performance CoSi-based thermoelectric nanoalloys for energy harvesting [8].

A first-principles approach has investigated the electronic and thermoelectric properties of Ag-doped SnSe nanoalloys. The findings demonstrate that Ag doping effectively optimizes the carrier concentration and significantly enhances the Seebeck coefficient, while also improving the electrical conductivity. The research provides a fundamental understanding of the role of doping in modulating the electronic structure and transport properties, offering a viable strategy for developing advanced SnSe-based thermoelectric materials with enhanced performance [9].

Efforts have also concentrated on improving the thermoelectric performance of n-type Mg3Sb2-based nanoalloys through synergistic engineering approaches. The study shows that a combination of doping and nanostructuring can simultaneously optimize the electronic transport properties, leading to a higher Seebeck coefficient and electrical conductivity, while effectively scattering phonons to reduce thermal conductivity. These integrated strategies significantly boost the overall thermoelectric figure of merit, demonstrating a promising pathway for next-generation energy conversion devices [10].

Conclusion

Recent research in thermoelectric materials, particularly nanoalloys, focuses on enhancing energy conversion efficiency through diverse engineering strategies. Investigations into Co- and Fe-based Heusler nanoalloys, for example, reveal high Seebeck coefficients and favorable electronic transport, underscoring the importance of electronic band structure engineering [1]. Similarly, Ag-doped FeS2 nanoalloys demonstrate improved Seebeck coefficients and electrical conductivity, highlighting the potential of controlled doping and nanostructuring in pyrite-based materials [2].

Other studies explore the impact of microstructure and annealing on n-type Bi2Te3-based nanoalloys, showing that precise control can optimize Seebeck coefficients and overall performance [3]. For Ag-doped GeTe compounds, nano-alloying combined with phonon engineering effectively reduces lattice thermal conductivity while maintaining electronic transport, boosting Seebeck coefficients and ZT values [4]. The synergistic effects of Ag and Sb co-doping in PbTe-based nanoalloys further illustrate how combined dopants can enhance Seebeck coefficients and electrical conductivity while simultaneously reducing thermal conductivity, leading to significant improvements in the thermoelectric figure of merit [5].

Theoretical studies on SnS-based nanoalloys delineate the influence of alloying elements on electronic band structure, identifying compositions with enhanced performance for waste heat recovery [6]. Cu2SnSe3-based materials benefit from band structure modulation and nano-alloying, which optimize carrier concentration, enhance Seebeck coefficients, and reduce lattice thermal conductivity [7]. Doping and strain engineering are also effective in tuning CoSi nanoalloys, modifying their electronic band structure for optimized Seebeck coefficients and improved electrical conductivity [8]. Ag doping in SnSe nanoalloys likewise enhances Seebeck coefficients and electrical conductivity by modulating electronic structure [9]. Finally, synergistic engineering approaches involving doping and nanostructuring significantly improve the thermoelectric properties of n-type Mg3Sb2-based nanoalloys by optimizing electronic transport and scattering phonons to reduce thermal conductivity, demonstrating a promising pathway for next-generation energy conversion devices [10].

References

1. Md Tanvir I, Zeeshan K, Mohammed RH D. Thermoelectric Properties of Co- and Fe-Based *Heusler Nanoalloys. Appl Nanosci.* 2022;12:2673-2680.

2. Shijie Y, Guosheng D, Ruiyuan Z. Thermoelectric transport in Ag-doped FeS2 nanoalloys: A first-principles study. *J Alloys Compd.* 2023;958:170503.

3. Yuyang M, Yanmei Z, Jie M. Role of microstructure and annealing on the thermoelectric properties of n-type Bi2Te3-based nanoalloys fabricated by spark plasma sintering. *J Phys Chem Solids.* 2022;160:110363.

4. Guoying S, Mengjiao W, Qingxue L. Thermoelectric performance enhancement of Ag-doped GeTe compounds through nano-alloying and phonon engineering. *J Mater Sci Technol.* 2023;154:109-119.

5. Qiang L, Meng-Yuan L, Yong-Li Y. Synergistic Effects of Ag and Sb Doping on the Thermoelectric Properties of PbTe-Based *Nanoalloys. ACS Appl Mater Interfaces.* 2021;13(48):57375-57383.

6. Zhipeng Z, Guangchao Y, Jiawei Y. Thermoelectric properties of SnS-based nanoalloys via theoretical calculations. *J Materiomics.* 2021;7(6):1184-1192.

7. Yan L, Xiaoyue Y, Jiawei Z. High-Performance Thermoelectric Cu2SnSe3-Based Materials with Modulated Band Structure and Nano-Alloying. *ACS Appl Mater Interfaces.* 2021;13(27):31825-31832.

8. Hao L, Min H, *Li S. Tuning the thermoelectric properties of CoSi nanoalloys by doping and strain engineering. J Mater Sci Mater Electron.* 2020;31(21):18636-18644.

Citation: *Martinez D. Engineering nanoalloys for enhanced thermoelectric efficiency. Mater Sci Nanotechnol. 2025;09(03):200.*

9. Yan L, Lei W, Qianqian L. Electronic and thermoelectric properties of Ag-doped SnSe nanoalloys: A first-principles study. *Phys Chem Chem Phys*. 2020;22(36):20689-20697.

10. Yuheng Z, Zhicheng L, Junjie C. Enhanced thermoelectric properties of n-type Mg3Sb2-based nanoalloys via synergistic engineering. *Mater Today Phys*. 2022;27:100787.

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