Electronic and Thermoelectric Properties of NiTiSi

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Abstract

The electronic and thermoelectric properties of half-heusler compound NiTiSi has been studied using density functional theory and Boltzmann transport theory within the constant relaxation time approximation. NiTiSi is found to be an indirect band gap semiconductor with a band gap of 0.747 eV. Seebeck coefficient greater than 200 μV/K at 1000 K is observed. The calculations suggests that p-type doping can significantly improve the thermoelectric properties of the compound with a maximum value of 0.13 at 1000 K.

Keywords: Half-heuslers, Thermoelectrics, BoltzTraP

Introduction

- Thermoelectrics can be used to generate electricity from waste heat.

- The efficiency of thermoelectric (TE) materials is measured by dimensionless figure of merit, ZT

$$ZT = \frac{S^2 \sigma T}{\kappa} \qquad (1)$$

where, S is Seebeck coefficient, σ is electrical conductivity, T is the temperature and κ is the total thermal conductivity of material

- A good TE material has ZT value greater than 1.

- State of the art TE materials: PbTe, $\mathrm{Sb_2Te_3}$, $\mathrm{Bi_2Te_3}$

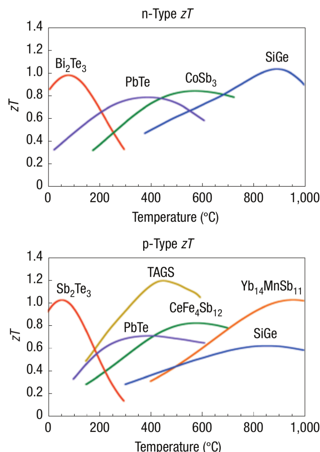

Figure: ZT values of some state of the art TE materials at different temperatures (G. J. Snyder and E. S. Toberer, Nat. Mat. **7**, 105 (2008))

Introduction:Half Heusler

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- TE materials have applications: power generation for space probes, temperature sensor etc.,
- Skuterrudites, chalcogenides, Heusler alloys, Clathrates commonly used TE materials.
- Half-heusler materials:
  - Are mostly narrow band gap
  - High temperature sustainable
  - Generally non-toxic

Computational Details

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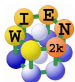
- Density functional theory calculations were performed using Full-potential linearized augmented plane wave + local orbital method as implemented in WIEN2k code.



- mBJ exchange potential was used as it gives better estimate of band gap for semiconductors.

- BoltzTraP code was used to study transport properties and constant relaxation time approximation (CRTA) was used.

- Quantum Espresso package was used to calculate phonon dispersion.

Structure Optimization

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Space group F$\bar{4}$3m (216)

- $a = 5.584$ Å, $\alpha = 90°$

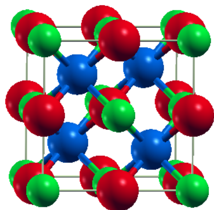

Figure: Conventional Unit cell of NiTiSi. Blue balls are Ni, red are Ti and green balls are Si.

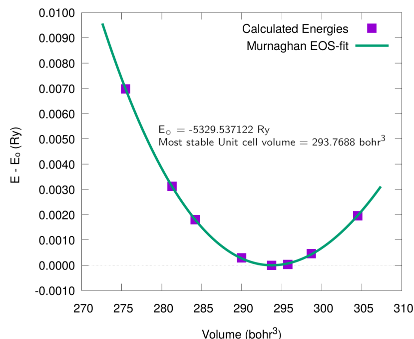

Figure: Volume optimization of NiTiSi. The displayed volumes are for primitive unit cell. E_O is the energy for the most stable unit cell volume.

- The frequencies are real throughout the Brillouin zone.
- Thus, the crystal structure of NiTiSi is stable.

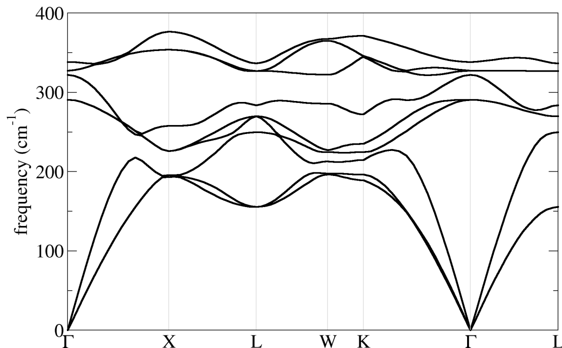

Figure: Phonon dispersion curves for NiTiSi

- Band gap of 0.759 eV under GGA
- Band gap reduced slightly to 0.747 eV under mBJ.

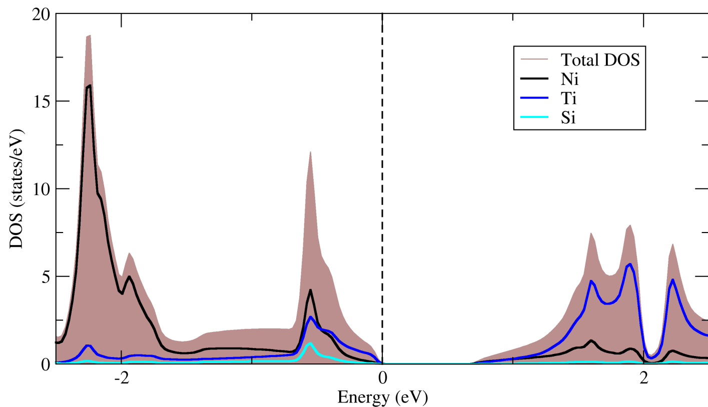

Figure: Total Density states for NiTiSi.

- Conduction region is dominated by Ti 3*d* orbitals.
- Valence region is dominated by Ti-3*d* and Ni-3*d* orbitals.
- Hybridization of Ti-3*d*, Ni-3*d* and Si-3*p* states at $\sim$ -0.5 eV.

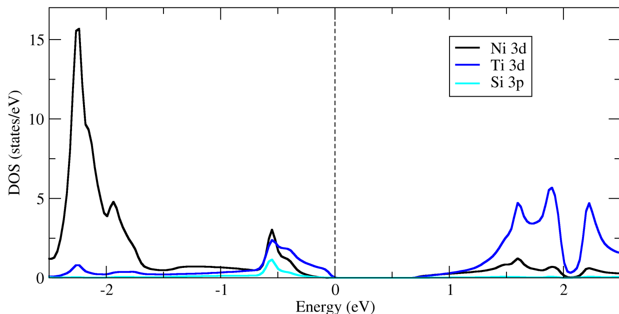

Figure: Partial Density of states Ni-3*d*, Ti-3*d* and Si-3*p* orbitals. This figure shows the contributions from orbitals with major contribution to DOS near Fermi level.

Results and Discussion

Band Structure

- NiTiSi is an indirect gap semiconductor
- Band gap = 0.747 eV
- Valence band seems to be heavier than the conduction band.

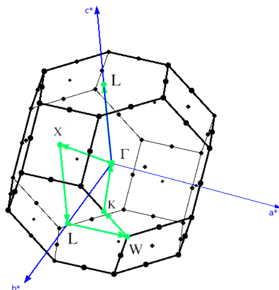

Figure: Selected K- path for band structure

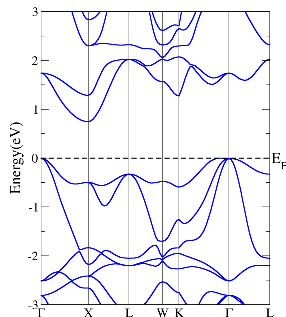

Figure: Band structure along high-symmetry point.

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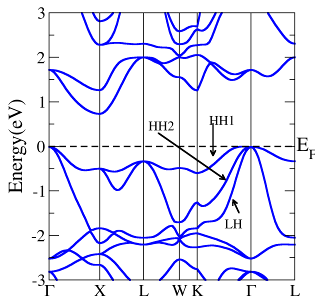
- In order to check the shift of Fermi level with temperature, effective mass of charge carriers were calculated.
- At 300 K the Fermi level is shifted by about 1.835 eV towards conduction band.

High-symmetry point	Effective mass (m^*/m_e)
Valence Band (Γ-KΓ)[†]	
HH1	– 8.71
HH2	– 1.48
LH	– 0.45
Conduction band (X-ΓX)	
Electron	3.38
Conduction band (X-XL)	
Electron	0.91

[†] The notation $\Gamma - K\Gamma$ denotes that the effective mass is calculated at Γ point along $K\Gamma$ direction in primitive reciprocal lattice space and similarly for others too.



- At all temperatures Seebeck coefficient has positive values. So NiTiSi is expected to be a p-type semiconductor.

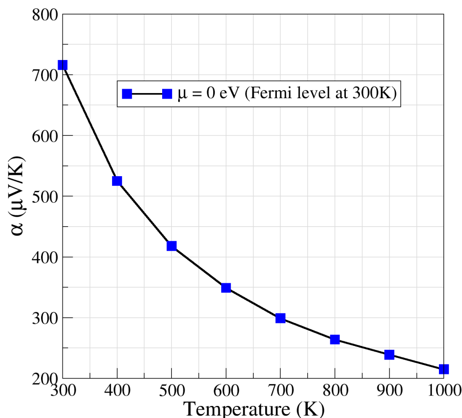


Figure: Seebeck coefficient vs Temperature plot for NiTiSi.

- Power factor (PF) $= S^2\sigma$, where S is Seebeck coefficient and σ is the electrical conductivity.
- Power factor increases with temperature for both p-type and n-type doping.
- Larger values of maxima for negative μ implies that *p*-type doping will be more stable for enhancing the TE properties of NiTiSi.
- Using a constant relaxation time for charge carriers , $\tau = 2 \times 10^{-15}$ s, the maximum value of ZT attainable by *p*-type doping is 0.01 at 300 K and rises upto 0.13 at 1000 K.

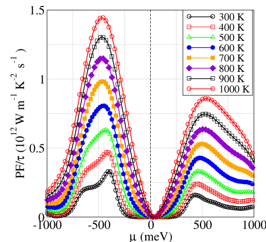


Figure: Power factor vs chemical potential plot for NiTiSi. Power factor is coupled with the relaxation time τ

Conclusions

- Electronic and TE properties of NiTiSi were studied using density functional theory.
- Band gap of NiTiSi was found to be 0.747 eV.
- Large value of Seebeck coefficient greater than 200 μV/K observed even at 1000 K signifies suitability of NiTiSi for high temperature TE applications.
- p-type doping is more favorable to enhance the ZT value of NiTiSi.
- ZT value can be increased upto 0.13 at 1000 K.

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Thank you !