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14. ABSTRACT This program performed material design for high-performance thermoelectric (TE) cooler with a figure-of-merit $ZT > 3$. The cooler is fabricated from HgCdTe using a low dimensional superlattice structure. The TE coolers can operate at temperatures ranging from 30K to 300K, thereby providing a fundamentally new and disruptive method for achieving cryogenic cooling. In this STIR program we investigated (1) Modeling of HgCdTe Low Dimensional Structures and (2) Thermoelectric Cooler Design and (2) Partnership with Amethyst Research, Inc. and SCD USA to investigate the					
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Report Title

Final Report: STIR: High Performance Thermoelectric Cryo-coolers based on II-VI Low Dimensional Structures

ABSTRACT

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Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
05/26/2015	1.00 Charles W. Myles, Daryoosh Vashaee, Payam Norouzzadeh. Prediction of Giant Thermoelectric Power Factor in Type-VIII Clathrate Si ₄₆ , Scientific Reports, (11 2014): 0. doi: 10.1038/srep07028
05/26/2015	2.00 Payam Norouzzadeh, Jerzy S. Krasinski, Daryoosh Vashaee, Charles W. Myles. Type VIII Si based clathrates: prospects for a giant thermoelectric power factor, Phys. Chem. Chem. Phys., (2015): 0. doi: 10.1039/C5CP00729A
05/26/2015	3.00 Daryoosh Vashaee, Payam Norouzzadeh. The Effect of Multivalley Bandstructure on Thermoelectric Properties of Al _x Ga _{1-x} As, Journal of Electronic Materials, (12 2014): 0. doi: 10.1007/s11664-014-3535-1
TOTAL:	3

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
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Number of Papers published in non peer-reviewed journals:

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Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

<u>Received</u>	<u>Paper</u>
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TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

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Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

<u>Received</u>	<u>Paper</u>
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05/26/2015	4.00	Payam Norouzzadeh, Amin Nozariasbmarz, Jerzy S. Krasinski and Daryoosh Vashae. Thermal conductivity of nanostructured SixGe12x in amorphous limit by molecular dynamics simulation, Journal of Applied Physics (09 2014)
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TOTAL: 1

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

Graduate Students

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	Discipline
Amin Nozariasbmarz	0.00	
	0.00	
FTE Equivalent:	0.00	
Total Number:	1	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Payam Norouzzadeh	0.00
FTE Equivalent:	0.00
Total Number:	1

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Daryoosh Vashaee	0.00	
Jerzy S Krasinski	0.00	
FTE Equivalent:	0.00	
Total Number:	2	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:..... 0.00

Names of Personnel receiving masters degrees

<u>NAME</u>
Total Number:

Names of personnel receiving PHDs

<u>NAME</u>
Total Number:

Names of other research staff

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

This program performed material design for high-performance thermoelectric (TE) cooler with a figure-of-merit $ZT > 3$. The cooler is fabricated from HgCdTe using a low dimensional superlattice structure. The TE coolers can operate at temperatures ranging from 30K to 300K, thereby providing a fundamentally new and disruptive method for achieving cryogenic cooling. In this STIR program we investigated (1) Modeling of HgCdTe Low Dimensional Structures and (2) Thermoelectric Cooler Design and (3) Partnership with Amethysts Research Inc. and SCD.USA to investigate the feasibility of integrating the TEC into their new TEC FPA/Dewar.

Technology Transfer

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Table of Contents

SECTION I – EXECUTIVE SUMMARY	2
SECTION II – WORK CONDUCTED	2
Thermoelectric Cooler Design	2
Partnership with SCD.USA to integrate TEC into new FPA/Dewar assembly	2
Hg _{1-x} Cd _x Te Superlattice Structures (SLS) Modeling	3
Results of the Superlattice Design	3
Thermal Conductivity of the HgCdTe Superlattice	5
Thermal conductivity of HgCdTe superlattice	7
Multi Stage Cryo Cooling	8
TEC Design.....	11
Strategic Partnership with SCD.USA	11
SCD.USA Activities	12
Development of TEC Integrated HOT MWIR detector for Tactical applications.....	12
SECTION III – DISSEMINATION OF RESULTS	13
SECTION IV – REFERENCES	14

SECTION I – EXECUTIVE SUMMARY

This program performed material design for high-performance thermoelectric (TE) cooler with a figure-of-merit $ZT > 3$. The cooler is fabricated from HgCdTe using a low dimensional superlattice structure. The TE coolers can operate at temperatures ranging from 30K to 300K, thereby providing a fundamentally new and disruptive method for achieving cryogenic cooling.

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SECTION II – WORK CONDUCTED

In Phase I the program investigated the following primary tasks.

- Modeling of HgCdTe Low Dimensional Structures
- Thermoelectric Cooler Design
- Partnership with SCD.USA to integrate TEC into their new TEC FPA/Dewar

Thermoelectric Cooler Design

- Thermal conductivity of the HgCdTe SL was calculated versus materials composition and temperature. The model was benchmarked with the existing experimental data and was further extended to predict ZT at cryogenic temperatures for the planned SL structure.
- The optimum parameters for SL well and barrier layer compositions versus doping concentration were calculated and the design rules were drawn. The data will be used for the growth of the SL structures in phase II.
- A three dimensional finite element model of heat transfer, Peltier cooling, and joule heating was developed. The model will be used for design optimization of the TEC modules in phase III.

Partnership with SCD.USA to integrate TEC into new FPA/Dewar assembly

- We worked closely with Amethyst Research Inc. and SCD.USA informing partnership. As part of the SCD.USA support to the Amethyst Research HgCdTe TEC development efforts, SCD.USA will design a new Integrated Dewar-Detector Cooler Assembly (IDDCA). The IDDCA will incorporate the prototype TEC into a typical Long Range thermal Imager dewar package design. After comprehensive performance/reliability analyses, a prototype IDDCA will be fabricated and evaluated. SCD.USA will use High Operating Temperature (HOT) MWIR Focal Plane Arrays (FPA) that have been developed by SCD.LTD (the parent

company of SCD.USA) for use in their low Size/Weight/Power packages. These FPAs will be mounted to ceramic carriers designed for easy integration into the IDDCA. SCD.USA will perform final IDDCA fabrication, integration and test while SCD.USA's contractors will perform piece part fabrications. Amethyst Research will provide the TEC that will be integrated by SCD.USA to the FPA-feedthrough assembly. SCD.USA will then integrate the Cold Shield Assembly, weld the dewar assembly and complete package assembly through bake-out and seal.

Hg_{1-x}Cd_xTe Superlattice Structures (SLS) Modeling

In this section a modified SLS structure based on theoretical model structure calculations for HgCdTe/CdTe system on InSb substrates is presented for TEC applications. During our Phase I program there were concerns as to the thickness of the layers which would require extended growth times of 12 hours. While technically possible, this would drive up TEC production costs. Thus modeling was conducted to design TEC structures with thinner layers. The resulting HgCdTe SL structure thickness is about three times thinner than the initially proposed structure.

Results of the Superlattice Design

The superlattice barrier height and the optimum doping concentration were calculated for HgCdTe superlattice. The material properties of the ternary alloy Hg_{1-x}Cd_xTe are mostly available from the literature or can be approximated by virtual crystal approximation from those of the constituent binary alloys of HgTe and CdTe.

The calculation results for the n-type superlattice barrier height and the optimum doping concentrations are shown in Figure 1 and Figure 2. The SL is assumed to be uniformly doped.

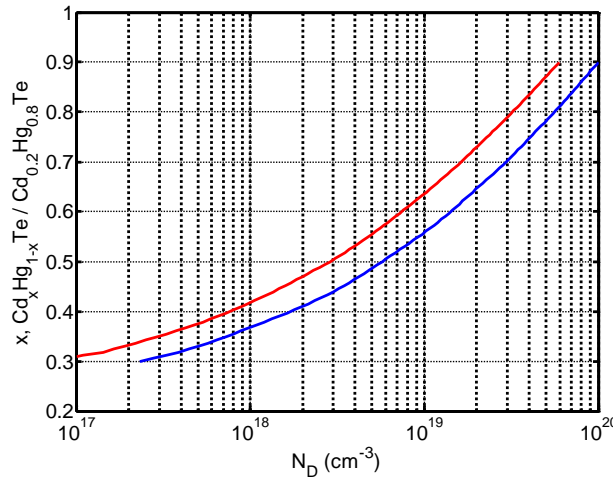


Figure 1: The required amount of Cd composition (x) is calculated for a given doping concentration to achieve the high ZT at 100K (blue) and 300K (red).

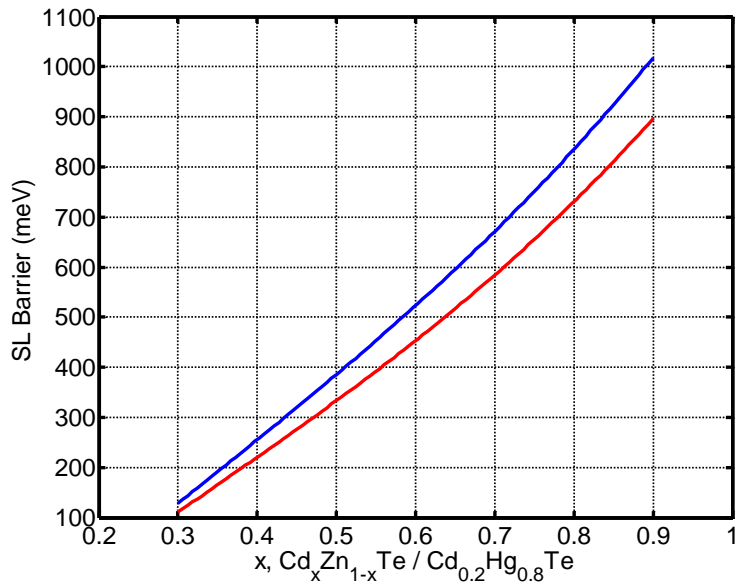


Figure 2: SL barrier height is calculated versus Cd amount at 300K (red) and 100K (blue). This data will be used with the data of the previous figure to find the optimum doping concentration for the HgCdTe superlattice.

A large superlattice barrier height is required to improve the thermoelectric power factor. Since the optimum doping concentration increases with the superlattice barrier height, x is chosen so that the required doping concentration is practically achievable. A tentative superlattice is schematically shown in Figure 3.

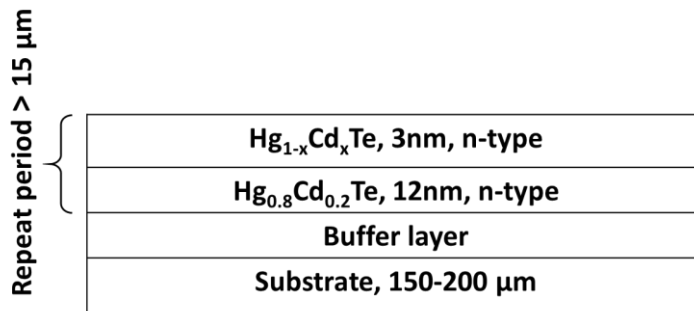


Figure 3: The Schematic of the optimized $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ superlattice structure with uniform doping. These new layer thickness (3/12 nm) will allow us to grow a TEC structure in 6 hours as opposed to 12 hours in previous Phase I design - significantly reducing production costs.

For $x=0.8$, which results in a barrier height of approximately 735meV at 300K and 830meV at 100K, the optimum doping concentration is approximately $3.3 \times 10^{19} \text{ cm}^{-3}$ at 300K and $5.7 \times 10^{19} \text{ cm}^{-3}$ at 100K.

The following tolerances of the superlattice parameters must be maintained:

- Composition: $\pm 10\%$
- Well and barrier widths: $\pm 10\%$

If the target doping concentration turns out to be too large to reach experimentally, we will choose a smaller x value based on the measured value of the highest practically achievable doping concentration. For example, for x=0.6, the optimum doping concentrations are $7.6 \times 10^{18} \text{ cm}^{-3}$ at 300K and $1.5 \times 10^{19} \text{ cm}^{-3}$ at 100K.

Thermal Conductivity of the HgCdTe Superlattice

The lattice thermal conductivity κ_{lattice} can be estimated from the relation: $\kappa_{\text{lattice}} = \frac{1}{3} C_v v_s d$ where C_v is the specific heat at constant volume, v_s is the sound velocity, and d is the mean free path of the phonons. In superlattices, in addition to the phonon-phonon scattering which dominates bulk phonon relaxation time, phonons are also scattered by interfaces. Therefore, the calculation of thermal conductivity is complicated in SLs. To calculate phonon MFPs of an infinite superlattice at various temperatures, the lattice dynamics approach is employed. This first-principles approach relies on the use of harmonic and anharmonic interatomic force constants derived from density-functional perturbation theory (DFPT), which yields accurate interatomic force constants, and a solution of the Boltzmann transport equation to predict the lattice thermal conductivity.¹ This approach leads to excellent agreement between experiments and theory for perfect crystals² as well as alloys.³ Application of this approach to calculate the lattice thermal conductivity of ideal Si/Ge SuperLattices (SLs) with perfect interfaces showed that the thermal conductivity was estimated larger than the experimental values, which is a sign for the need of incorporation of the interfacial roughness effects.⁴ Using perturbation theory or the well-known Fermi Golden rule, one can derive the expression of the relaxation time as a function of the cubic force constants.^{5,6,7} The calculated phonon relaxation times multiplied by the sound velocity gives us the phonon mean free paths. The more detailed version of aforementioned formula can be expressed as:

$$k_\alpha = \frac{h^2}{NVk_B T^2} \sum_{\lambda} c_{\alpha\lambda}^2 \omega_\lambda^2 \bar{n}_\lambda (\bar{n}_\lambda + 1) \tau_\lambda$$

where c , ω , \bar{n} , and τ are the phonon group velocity, frequencies, phonon equilibrium population, and relaxation times, respectively. λ represents the vibrational mode. T , V , and N are temperature, unit cell volume, and size of the k-point mesh used in calculations. The scattering rate, $1/\tau_\lambda$, of a phonon mode λ is taken to be the sum of two terms 1) due to the interfacial roughness and 2) due to anharmonic scattering. These two terms calculated using the following relations respectively:

$$\frac{1}{\tau_{\lambda 1}} = \pi \sum_{\lambda\lambda'} |V_3(-\lambda, \lambda', \lambda'')|^2 \times [2(\bar{n}_\lambda - \bar{n}_{\lambda''}) \delta(\omega(\lambda) + \omega(\lambda') - \omega(\lambda'')) + (1 + \bar{n}_{\lambda'} + \bar{n}_{\lambda''}) \delta(\omega(\lambda) - \omega(\lambda') - \omega(\lambda''))]$$

where $V_3(-\lambda, \lambda', \lambda'')$ is the weighted Fourier transforms of the cubic force constants; and

$$\frac{1}{\tau_{\lambda 2}} = \frac{\pi}{2N} \omega_{\lambda}^2 \sum_{\lambda'} \delta(\omega(\lambda) - \omega(\lambda')) \sum_{\sigma} g(\sigma) |e(\sigma|\lambda') e(\sigma|\lambda)|^2$$

in which σ is the atomic site in the unit cell, g is the magnitude of the mass disorder and e is vibration eigenvector. According to the theory of atomic displacement parameter (ADP) and lattice thermal conductivity,⁸ the mean square displacement amplitude, $\langle u^2 \rangle$, of a quantized harmonic oscillator is given by:

$$U_{iso} = \langle u^2 \rangle = (h/8\pi^2 m\nu) * \coth(h\nu/2k_B T)$$

where m is the reduced mass of the oscillator, h is the Planck's constant, ν is the frequency of the vibration, k_B is the Boltzmann constant, and U_{iso} is the mean isotropic displacement parameter which measures the mean-squared displacement amplitude of the atom averaged over all directions. At high temperatures where $h\nu \leq k_B T$, the preceding equation reduces to $U_{iso} = k_B T / K$ and $K = m(2\pi\nu)^2$ where K is the force constant of the oscillator.

The Debye's temperature, θ_D , is estimated from the slope of the curve drawn between the U_{iso} at various temperatures. Each slope of the curves can be described by the relation:

$$slope = \frac{3h^2}{(mk_B \theta_D^2 4\pi^2)}$$

The slope is estimated from the curve that is extrapolated to the origin. Static disorder that tends to shift these curves upward is ignored. The Debye's temperature, θ_D , is used to determine the average velocity of sound v_s and is given by:

$$v_s = \frac{2\pi\theta_D k_B}{h(6\pi^2 n)^{\frac{1}{3}}}$$

where n is the number of atoms per unit volume.

The vibrational Helmholtz free energy (F_{vib}), vibrational entropy (S_{vib}) and specific heat at constant volume (C_v) can be calculated from vibrational density of states (VDOS).⁹ In the harmonic approximation, the vibrational Helmholtz free energy is given by:

$$F_{vib}(T) = k_B T \int_0^{\infty} \left[\frac{1}{2} \hbar \omega + k_B T \ln(1 - e^{-\frac{\hbar \omega}{k_B T}}) \right] g(\omega) d\omega$$

where k_B is the Boltzmann constant. The VDOS is normalized such that $\int g(\omega)d\omega = 3N$, where N is the number of atoms. The zero point vibrational energy is defined by F_{vib} at $T = 0K$. The specific heat at constant volume is given by: $C_V(T) = -T \left(\frac{\partial^2 F_{vib}}{\partial T^2} \right)_V$.

In this way, all ingredients necessary to compute the thermal conductivity, namely the phonon frequencies, group velocities, populations and lifetimes are derived from first-principles using density functional perturbation theory (DFPT).

Thermal conductivity of HgCdTe superlattice

The total thermal conductivity in TE materials consists of three parts: the transport of heat by (1) phonons (i.e. the lattice thermal conductivity) (2) free electrons and holes (i.e. the electrical thermal conductivity) and (3) electron-hole pair diffusion (i.e. the bipolar diffusion thermal conductivity). The relative strength of a given heat conduction mechanism in a semiconductor material depends on the temperature range, the band structure, and the doping level. At below room temperature, the bipolar part of the thermal conduction is often very small and the electronic and lattice parts become dominant.

The proposed HgCdTe SL cooler is a cross plane device and as such the heat conduction is perpendicular to the SL interfaces. Phonon reflection, confinement, and also diffuse scattering can significantly reduce the cross-plane thermal conductivity. Since the HgCdTe SL is lattice matched, the reflection coefficient dominantly depends on the difference in the unit cell masses in the well and barrier regions. The large deviation of unit cell masses in well and barrier regions of the tall barrier HgCdTe SL (due to large difference in x value) would satisfy the condition for enhanced phonon reflection at SL interfaces.

In Figure 4 we have calculated the thermal conductivity of the prototype $Hg_{0.8}Cd_{0.2}Te / Hg_{0.2}Cd_{0.8}Te$ superlattice in the cross plane as compared with that of $Hg_{0.8}Cd_{0.2}Te$ alloy. Our model calculation agrees with the experimental data of the alloy¹⁰.

To calculate the lattice part of thermal conductivity we used the relaxation time approximation in Boltzmann's equation for phonons based on the Debye model.¹¹ The model calculation takes into account three-phonon scattering, including normal (N) and umklapp (U) processes, electron-phonon scattering, point defect (alloy) scattering, and SL boundary phonon scattering. Defects at interfaces can introduce different types of scattering of phonons depending on the type and size of the defect. MBE grown superlattices usually have better interface morphology than the other types of interfaces. However, even for the best material systems such as MBE grown GaAs/AlAs, the interfaces are not perfect. Interface mixing and regions with monolayer thickness variations exist at the interface. Such imperfections cause diffuse scattering at SL interfaces resulting in further reduction of the thermal conductivity.¹² We may group interface scattering into three different types: (1) regular reflection and refraction scattering when the phonon wavelength (λ) is small compared with the linear dimensions of the SL interface,¹³ (2) diffusive scattering if λ is comparable with defects dimension ℓ ¹⁴ or (3) Rayleigh scattering if $\lambda \gg \ell$.¹⁵ We expect regular reflection and refraction scattering at SL interface be the dominant scattering mechanism. Our model calculations as depicted in Figure 10 predicts a 2-3 fold reduction in thermal conductivity

of the SL structure over the entire range of 100K to 300K, which agrees with the trend of extensive recent experimental data on the thermal conductivity of various superlattices in recent years.^{16,17}

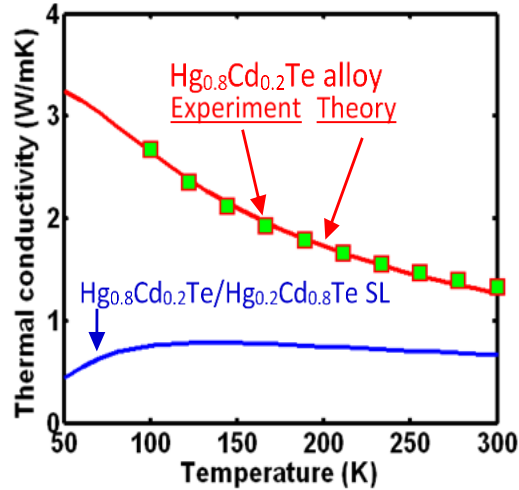


Figure 4: Thermal conductivity of (a) single crystalline $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$ alloy and (b) $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}/\text{Hg}_{0.2}\text{Cd}_{0.8}\text{Te}$ SL. Lines are our model calculations and symbols are experimental data [10]. The SL thermal conductivity is significantly smaller than that of the bulk material especially at low temperature. This would enhance the ZT even further than our previous prediction which was based only on the enhancement of the TE power factor.

Multi Stage Cryo Cooling

The thermoelectric properties of the MCT SL are a function of temperature and doping concentration. For a given working temperature, the SL must be doped to an optimum value to reach the maximum ZT of the material.

Figure 5 shows the calculated ZT of the MCT SL versus temperature for several values of doping concentration. It can be seen that a multi-stage cooler (here five stages) is required to make a solid state cooler that can cool from room temperature down to 30K. With five stages of cooling the ZT remains above one for the entire range of temperature. A doping variation from $3.4 \times 10^{19} \text{ cm}^{-3}$ to $1.82 \times 10^{19} \text{ cm}^{-3}$ changes the peak ZT from 300K to 30K. Therefore, a precise control of the doping concentration is required to tune the location of the peak ZT.

It is possible to reduce the cooling even to lower temperature by further increasing the doping concentration. For example, doping concentration of $3.6 \times 10^{19} \text{ cm}^{-3}$ will result in ZT peak at approximately 10K. For cryogenic application, a five stage cooler can cool from 300K down to under 50K.

It is also seen that as the temperature reduces, the ZT peak becomes narrow indicating that the cooler is efficient over a narrower range of temperature. However, the peak ZT increases as the temperature reduces. $\text{ZT} > 4$ is predicted at $T < 30\text{K}$.

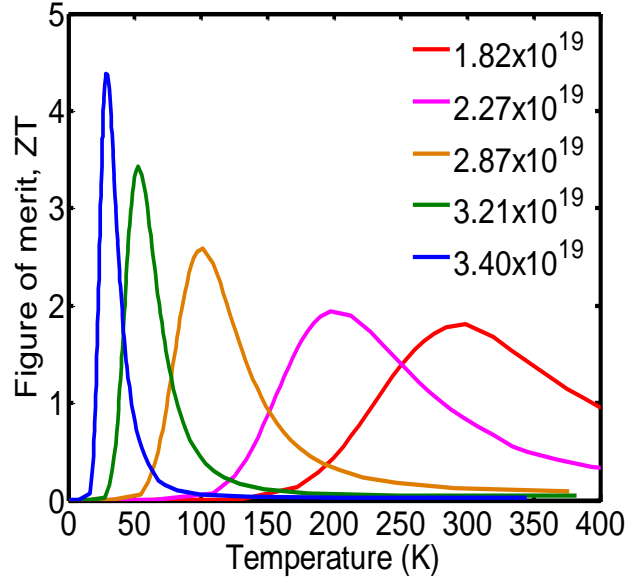


Figure 5: Thermoelectric figure of merit of HgCdTe SL versus temperature for different values of doping concentration. A five stage cooler is required to cool from room temperature down to 30K. A two stage cooler can cool from 90K to 30K (blue and green curves). A five stage cooler can cool from 300K to below 50K.

This value of ZT is obviously a ground-breaking value especially at such a low temperature. The ZT increase at low temperature is the result of narrowing of the carrier distribution that would allow more effective filtering of the high energy carriers by optimizing the location of the Fermi energy with respect to the top of the SL energy barrier [18,19]. At higher temperature, the carriers are broadened around the Fermi energy and the SL potential barrier would reflect a large number of the carriers that would reduce the number of carrier, hence, the electrical conductivity.

The required thickness of the SL structure will be determined by model calculations and comparison with experimental data. In order to determine the feasibility of the required thickness, a three dimensional single leg HgCdTe cryo-cooler was implemented in COMSOL Multiphysics described by coupled heat and Poisson's equations. These equations were extended by the thermoelectric effects and were solved simultaneously to get the solution for independent variables of temperature and voltage. The cooler consisted of one n-type HgCdTe element with cross section are of $50 \times 50 \mu\text{m}^2$ in size. The SL is contacted by two copper electrodes $1 \mu\text{m}$ in thickness. The contact resistance was included at the interface of the SL and the metal contact: therefore a 5-stacked layer of different materials with temperature dependent thermoelectric properties were modeled. Adiabatic boundary conditions were taken on the surrounding surfaces.

Figure 6-(a) shows the calculated temperature distribution along the TE leg. Figure 6-(b) shows the temperature difference at 30K for two SL thickness of $15 \mu\text{m}$ and $50 \mu\text{m}$. A heat load of 1200 W/m^2 was applied at the cold side. The plot shows the optimum working current for both SLs is approximately 0.12 A . It can be seen that while the $15 \mu\text{m}$ SL cools by $\sim 50\text{C}$, the $50 \mu\text{m}$ SL can cool down by $\sim 100\text{C}$. This difference is mainly associated with the effect of joule heating at the metal-SL interface. This effect is demonstrated in Figure 6 -(c) which shows the maximum temperature difference versus the SL thickness for three different values of ohmic contact

resistances (ρ_{oc}). It can be seen that only in the limit of $\rho_{oc}=10^{-8} \text{ cm}^2$ the thickness has small effect on the temperature difference. This value of ohmic contact is often practically too small to reach; however, with a well-designed metal contact, values in the range of $\rho_{oc}=10^{-7}$ are achievable. Although, even with a typical $\rho_{oc}=10^{-6} \text{ cm}^2$ a $15\mu\text{m}$ thick SL can cool for 50 degrees. Our model calculations show similar trend at higher temperature up to the room temperature. Therefore, with 50 degrees cooling across the SL, a three-stage cooler can cool from 300K to 150K.

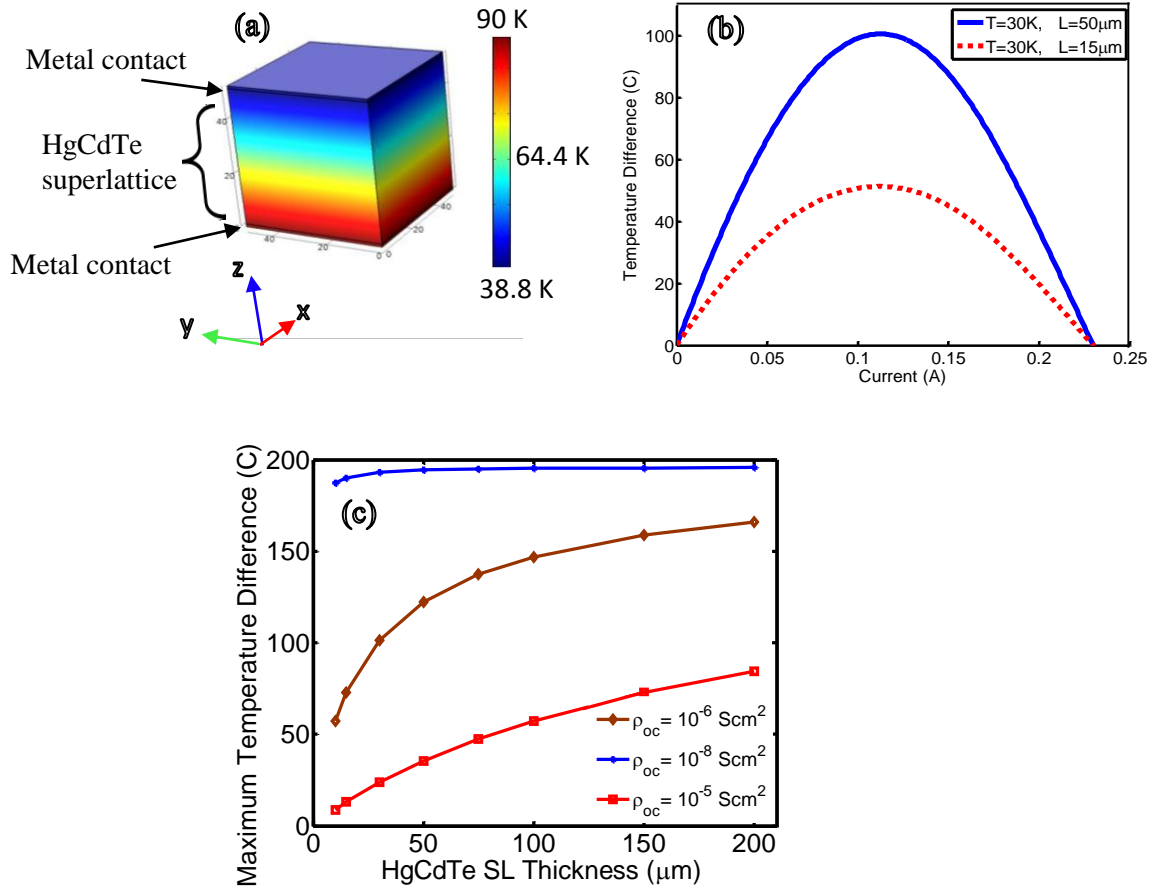


Figure 6: (a) The resultant temperature distribution of an n-type HgCdTe superlattice thermoelectric leg which is contacted by copper electrodes. (b) The temperature difference versus applied current. The optimum current is 0.12A per leg. (c) Maximum temperature difference versus the thickness of the HgCdTe SL for three different values of ohmic contact resistances. A low ohmic contact resistance in the range of $\sim 10^{-7} \Omega\text{cm}^2$ is required to achieve a large ΔT across a $15 \mu\text{m}$ thick HgCdTe SL.

TEC Design

The fabrication of the TEC involves several steps that do not usually exist in fabrication of conventional microelectronic devices. The detailed fabrication steps will be presented in the following phases of the project. However, the new proposed structure is shown in Figure 7, which is a drawing of the final cryo-cooler structure that will be fabricated in Phase II+ of the program. The TEC will consist of multiple stages. A five-stage cooler can cool from 300K to below 50K for the cryogenic application. To cool from 300K to 150K, which is for the FPA applications, a three stage cooler is also required as the ZT peak is broadened at high temperature, which means that each stage can cool over a wider range of temperature. We will collaborate closely with Marlow Industries in the integration of the multi-stage cooler. Marlow is producing multi-stage coolers for above room temperature application. The concept and techniques for multi-staging is similar and their technology can be adapted for our purpose. Marlow with 40 years of business is one of the largest manufacturers of thermoelectric modules in the world. We have signed the NDA with Marlowe and have an ongoing research project on thermoelectric materials with them that can be integrated with the proposed research.

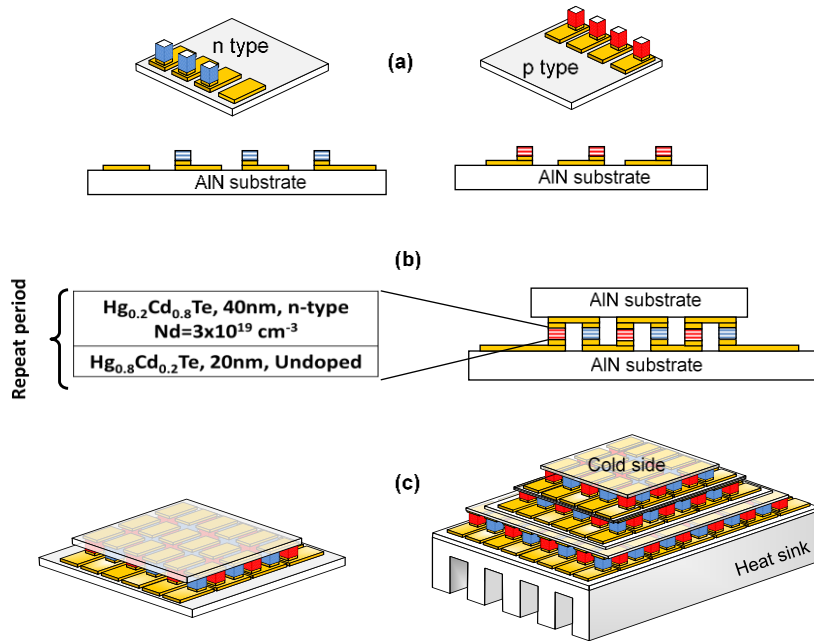


Figure 7: Schematic of the milestones required and final thermoelectric cooler (TEC) planned for the Phase II and Phase II+ program. (a) n and p type doping HgCdTe, (b) TEC fabrication steps and design concept from n and p-type low dimensional HgCdTe superlattice structure. (c) Single (left) and multi-stage (right) TEC device. In order to cool from 90K to operation at 10K a three stage TEC will be required.

Strategic Partnership with SCD.USA

Amethyst has recently entered into a development agreement with SCD.USA to develop these ultra high performance HgCdTe TEC coolers for their IR focal plane arrays. This will generate considerable market pull and a commercial outlet for the proposed structure. This cooler will also be available to other military users.

SCD.USA Activities

Development of TEC Integrated HOT MWIR detector for Tactical applications

Due to strong demand for improved MWIR detector performance, development of cooled technology will bring new capabilities for infrared imaging. Proposed TEC technology is four fold, specifically TEC development, dewer development, ROIC and FPA development, and package development. Ongoing work on development of TEC technologies to raise the efficiency of coolers by raising the ZT factor from 1 to 3 using SL structure is the first step of the proposed work. SCD will design new TEC compatible dewer to minimize the size without compromise to the image quality. SCD also works on existing ROIC/FPA to minimize existing ROIC/FPA power dissipation to reduce active heat load and optimize uncorrected uniformity at highest feasible operating temperature. For further reductions in heat load by replacing traditional wire bonds with low Tc interconnect technology, we need new package development. The improvements in TEC technology will add new features and capabilities to develop highly innovative MWIR products.

Figure 8 shows the schematics of the dewar design concept for the two-stage cooler. In future work with SCD we are proposing two stage cooler integrated into the MWIR detector. These two-stage coolers will provide significant improvement in the high temperature differentials hence allows operating the device at lower temperatures than conventional single-stage modules.

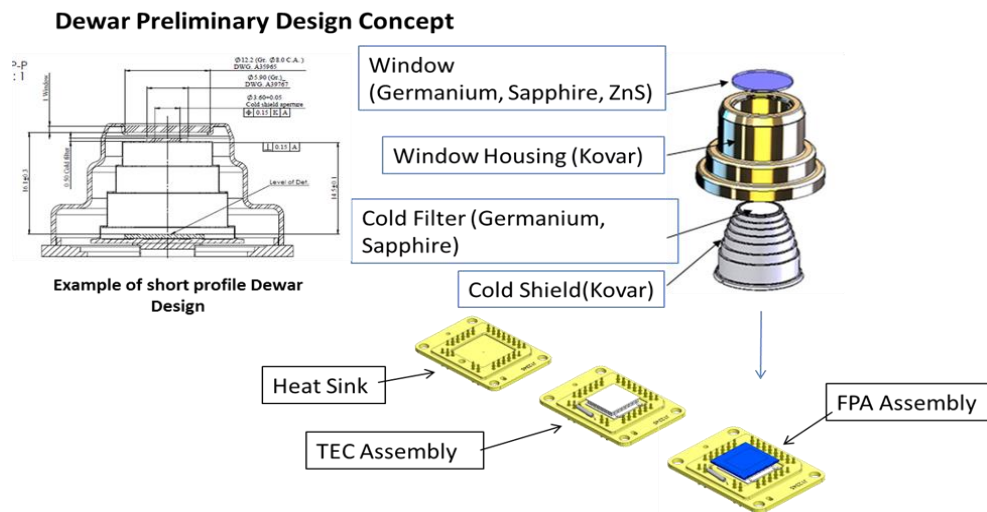


Figure 8: Schematic of the SCD.USA dewar design for the proposed two-stage cooler for a new generation of TEC FPA's.

These are preferable option where operating temperature is around 210-250K and where the requirement of noise reduction and improving the signal resolution is crucial, such as in case of infrared detectors.

As part of the SCD.USA support, they will design a new Integrated Dewar-Detector Cooler Assembly (IDDCA). The IDDCA will incorporate the prototype TEC into a typical Long Range

thermal Imager dewar package design. After comprehensive performance/reliability analyses, a prototype IDDCA will be fabricated and evaluated. SCD.USA will use High Operating Temperature (HOT) MWIR Focal Plane Arrays (FPA) that have been developed by SCD.LTD (the parent company of SCD.USA) for use in their low Size/Weight/Power packages. These FPAs will be mounted to ceramic carriers designed for easy integration into the IDDCA. SCD.USA will perform final IDDCA fabrication, integration and test while SCD.USA's contractors will perform piece part fabrications. Amethyst Research will provide the TEC that will be integrated by SCD.USA to the FPA-Feedthrough assembly. SCD.USA will then integrate the Cold Shield Assembly, weld the dewar assembly and complete package assembly through bake-out and seal. After Proxy electronics integration, SCD.USA will then perform Radiometric Characterization of the FPAs at the temperatures achieved with the integrated prototype TEC. Finally we will integrate the prototype IDDCA with appropriate optics and electronics to provide a camera system that can be used to demonstrate the capabilities of the technology. The camera system will include an opto-mechanical mounting platform (i.e. optical bench), lens mount, lens, interface electronics, computer based video data storage and image quality evaluation software. SCD.USA has provided similar detector evaluation & test systems to customers over the past few years. Figure 19 shows the expected steps in the detector development and test. SCD.USA can also utilize its in-house environmental test capability to evaluate IDDCA reliability.

SECTION III – DISSEMINATION OF RESULTS

Four journal articles were published based on the multi-scale computational tools developed through the course of this program. Publications are listed below:

1. Norouzzadeh, Payam, Charles W. Myles, and Daryoosh Vashae, *Scientific reports* 4 (2014).
2. Norouzzadeh, Payam, Jerzy S. Krasinski, Charles W. Myles, and Daryoosh Vashae. , *Physical Chemistry Chemical Physics* 17.14 (2015): 8850-8859.
3. Norouzzadeh, Payam, and Daryoosh Vashae, *Journal of Electronic Materials* 44.2 (2015): 636-644.
4. Payam Norouzzadeh, Amin Nozariasbmarz, Jerzy S. Krasinski, and Daryoosh Vashae, *Journal of Applied Physics* 117 (2015) in-Press

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- ¹⁸ Daryoosh Vashaee, Ali Shakouri, HgCdTe superlattices for solid-state cryogenic refrigeration, *Appl. Phys. Lett.* 88, 132110 (2006)
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