IOP PUBLISHING JOURNAL OF PHYSICS D: APPLIED PHYSICS

J. Phys. D: Appl. Phys. **42** (2009) 125109 (4pp) doi:10.1088/0022-3727/42/12/125109

# A numerical design of opto-thermionic refrigeration with perovskite oxide heterostructures

**Li-li Zhang, Peng Han, Kui-juan Jin[1], Leng Liao, Chun-lian Hu and Hui-bin Lu**

Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, People's Republic of China

E-mail: kjjin@aphy.iphy.ac.cn

Received 25 March 2009, in final form 7 May 2009
Published 5 June 2009
Online at stacks.iop.org/JPhysD/42/125109

**Abstract**

Opto-thermionic refrigeration is an environment-friendly method. To improve the opto-thermionic refrigeration efficiency, a system with a perovskite oxide multilayer of p-$BaTiO_3$/$BaTiO_3$/$SrTiO_3$/$BaTiO_3$/n-$BaTiO_3$ is proposed based on the model of opto-thermionic refrigeration. Because the Auger coefficient of $SrTiO_3$ is two orders smaller than that of GaAs, the calculated refrigeration power of the p-$BaTiO_3$/$BaTiO_3$/$SrTiO_3$/$BaTiO_3$/n-$BaTiO_3$ system is much higher than that of the p-AlGaAs/AlGaAs/GaAs/AlGaAs/n-AlGaAs system. A refrigeration power of as high as 39 W cm$^{-2}$ is obtained numerically in the p-$BaTiO_3$/$BaTiO_3$/$SrTiO_3$/$BaTiO_3$/n-$BaTiO_3$ system, which suggests a potential application of the oxide structures in opto-thermionic refrigeration.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

In 2001, opto-thermionic refrigeration, which combines laser refrigeration with thermionic refrigeration, was proposed [1]. This refrigeration creates no pollution and is noiseless. This refrigeration method is environment-friendly. A theoretical study of a traditional semiconductor p-AlGaAs/AlGaAs/GaAs/AlGaAs/n-AlGaAs opto-thermionic refrigeration system shows that the predicted refrigeration power is about several W cm$^{-2}$ at 300 K [1]. Moreover, it has been found that a small Auger coefficient leads to a high opto-thermionic refrigeration efficiency [1, 2]. The Auger coefficients of traditional semiconductors are usually larger than $10^{-31}$ cm$^6$ s$^{-1}$ [3]. For example, the Auger coefficient of GaAs is about $(7 \pm 4) \times 10^{-30}$ cm$^6$ s$^{-1}$ [4]. Such large Auger coefficients quite limit the opto-thermionic refrigeration efficiency of conventional semiconductor structures. For perovskite oxide strontium titanate ($SrTiO_3$), it has been found that the Auger coefficient is about $(1.3 \pm 0.4) \times 10^{-32}$ cm$^6$ s$^{-1}$ [5]. This value is two orders of magnitude smaller than that of GaAs. Therefore, the opto-thermionic system, which consists of perovskite oxide $SrTiO_3$, should have a much higher refrigeration efficiency. In addition, perovskite oxide heterostructures can be fabricated by laser molecular-beam epitaxy with atomically smooth interfaces [6–11]. Therefore, it is possible to study opto-thermionic refrigeration systems based on perovskite oxide heterostructures.

## 2. Model

In this paper, perovskite oxide heterostructures are first introduced to the field of opto-thermionic refrigeration. We propose a system which consists of a p-doped $BaTiO_3$ (BTO), an undoped BTO spacer, an undoped $SrTiO_3$ (STO) well, an undoped BTO spacer and an n-doped BTO connected in series. The widths of p/n doped regions $L_{p/n}$, spacers $L_{spacer}$ and the width of the well $L_{well}$ are 200 nm, 20 nm and 40 nm, respectively.

The opto-thermionic refrigeration process is simply explained as follows. When the voltage is applied to the whole system, hot electrons and holes are emitted into the well by the

[1] Author to whom any correspondence should be addressed.

 © 2009 IOP Publishing Ltd Printed in the UK

**Table 1.** The material parameters used in the calculation.

| Material | Radiative coefficient ($cm^3\ s^{-1}$) | Auger coefficient ($cm^6\ s^{-1}$) | References |
|---|---|---|---|
| GaAs | $1.9 \times 10^{-10}$ | $3.0 \times 10^{-30}$ | [4] |
| $SrTiO_3$ | $1.0 \times 10^{-11}$ | $1.7 \times 10^{-32}$ | [5, 15] |

thermionic emission process. They can recombine radiatively to emit photons, which are the media to extract the heat $Q_{\text{rad}}$ from the system. The dissipate heat $Q_{\text{dissipate}}$ is generated by the radiative recombination and the Auger recombination processes. If $Q_{\text{rad}}$ is more than $Q_{\text{dissipate}}$, the refrigeration is realized.

In order to obtain the refrigeration power of the system, the drift-diffusion model [2, 12, 13] is used to perform a self-consistent calculation. The Richardson current boundary condition [12] is applied to the interfaces between STO and BTO.

Under steady state, the fundamental equations used in the calculation are as follows:

$$\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2} = \frac{q}{\varepsilon}[n(x) - p(x) + N_{\text{acceptor}} - N_{\text{donor}}], \tag{1}$$

$$D_n\frac{\mathrm{d}^2n(x)}{\mathrm{d}x^2} - \mu_n\frac{\mathrm{d}n(x)}{\mathrm{d}x}\frac{\mathrm{d}\phi(x)}{\mathrm{d}x} - \mu_n n(x)\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2} - R(x) = 0, \tag{2}$$

$$D_p\frac{\mathrm{d}^2p(x)}{\mathrm{d}x^2} + \mu_p\frac{\mathrm{d}p(x)}{\mathrm{d}x}\frac{\mathrm{d}\phi(x)}{\mathrm{d}x} + \mu_p p(x)\frac{\mathrm{d}^2\phi(x)}{\mathrm{d}x^2} - R(x) = 0, \tag{3}$$

where $\phi(x)$ is the electrostatic potential, $n(x)$ and $p(x)$ are the electron and hole densities, $N_{\text{acceptor}}$ and $N_{\text{donor}}$ are the acceptor and donor densities, $q$ is the electron charge, $\varepsilon$ is the dielectric permittivity, $D_n$ and $D_p$ are the electron and hole diffusion coefficients, $\mu_n$ and $\mu_p$ are the electron and hole mobilities and $R(x)$ is the recombination rate, respectively. The three equations are solved by the finite difference discrete method.

In the doped and undoped BTO regions of the p-BTO/BTO/STO/BTO/n-BTO system, the main recombination mechanism is the Shockley–Read–Hall recombination [12]. In the well region, the main recombination mechanisms are radiative recombination and nonradiative Auger recombination. The radiative recombination rate is [14]

$$R_{\text{rad}}(x) = B(n(x)p(x) - n_{\text{i}}^2), \tag{4}$$

where $B$ is the radiative recombination coefficient and $n_{\text{i}}$ is the intrinsic carrier density in the well.

And the nonradiative Auger recombination rate is [3]

$$R_{\text{Aug}}(x) = C(p(x) + n(x))(p(x)n(x) - n_{\text{i}}^2), \tag{5}$$

where $C$ denotes the Auger coefficient. These two parameters are listed in table 1 for STO and GaAs. When voltage $V_{\text{bias}}$ is applied to the system, the dissipated heat is

$$Q_{\text{dissipate}} = JV_{\text{bias}} = V_{\text{bias}}\int_{L_{\text{well}}}(R_{\text{rad}}(x) + R_{\text{Aug}}(x))\,\mathrm{d}x \tag{6}$$

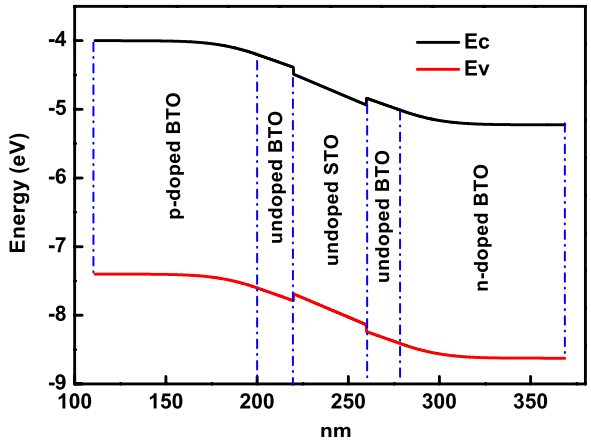


**Figure 1.** The calculated band structure of the p-BTO/BTO/STO/BTO/n-BTO system with $V_{\text{bias}} = 2.0$ V and $N_{\text{donor}} = N_{\text{acceptor}} = 5.0 \times 10^{18}\ \text{cm}^{-3}$.

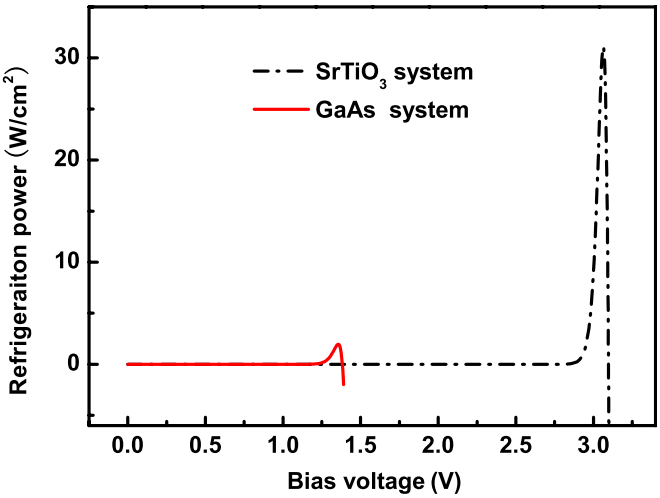


**Figure 2.** Refrigeration power versus bias voltage for the p-BTO/BTO/STO/BTO/n-BTO opto-thermionic system (black dashed–dotted line) and the p-AlGaAs/AlGaAs/GaAs/AlGaAs/n-AlGaAs opto-thermionic system (red solid line) with $N_{\text{donor}} = N_{\text{acceptor}} = 5.0 \times 10^{18}\ \text{cm}^{-3}$.

and the heat extracted by photons is

$$Q_{\text{rad}} = E_{\text{g-well}}\int_{L_{\text{well}}}R_{\text{rad}}(x)\,\mathrm{d}x \tag{7}$$

where $E_{\text{g-well}}$ is the band gap of STO. And the refrigeration power is written as

$$Q_{\text{refrig}} = Q_{\text{rad}} - Q_{\text{dissipate}}. \tag{8}$$

## 3. Results and discussion

The calculated band structure of p-BTO/BTO/STO/BTO/n-BTO system with $V_{\text{bias}} = 2.0$ V and $N_{\text{donor}} = N_{\text{acceptor}} = 5.0 \times 10^{18}\ \text{cm}^{-3}$ is plotted in figure 1.

The refrigeration power $Q_{\text{refrig}}$ versus $V_{\text{bias}}$ is plotted in figure 2 for the p-BTO/BTO/STO/BTO/n-BTO system and the p-AlGaAs/AlGaAs/GaAs/AlGaAs/n-AlGaAs system with $N_{\text{donor}} = N_{\text{acceptor}} = 5.0 \times 10^{18}\ \text{cm}^{-3}$, respectively. It is

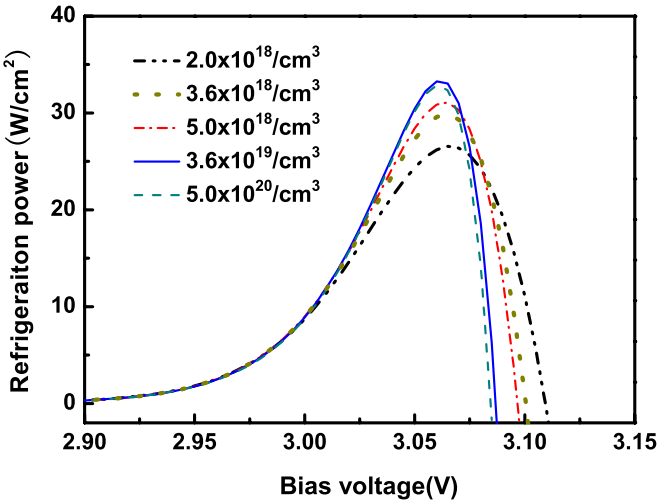


**Figure 3.** Refrigeration power versus bias voltage for different doping densities when $N_{\text{donor}} = N_{\text{acceptor}}$.

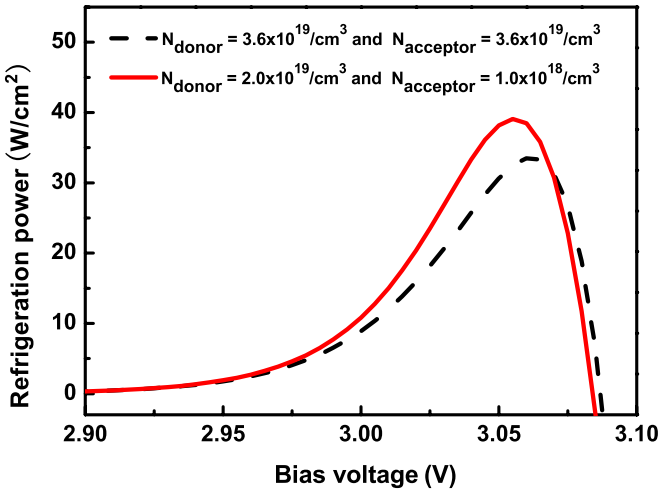


**Figure 4.** Refrigeration power versus bias voltage with the optimal doping density (red solid line) and with $N_{\text{donor}} = N_{\text{acceptor}} = 3.6 \times 10^{19}\,\text{cm}^{-3}$ (black dashed line).

shown that for both systems, $Q_{\text{refrig}}$ increases with $V_{\text{bias}}$ and then reaches a maximum value. With further increase in $V_{\text{bias}}$, $Q_{\text{refrig}}$ decreases and then becomes negative when $Q_{\text{dissipate}}$ exceeds $Q_{\text{rad}}$. The maximum refrigeration power $Q_{\text{refrig}}$ is $2\,\text{W cm}^{-2}$ for the p-AlGaAs/AlGaAs/GaAs/AlGaAs/n-AlGaAs system at $V_{\text{bias}} = 1.36\,\text{V}$ and $31\,\text{W cm}^{-2}$ for the p-BTO/BTO/STO/BTO/n-BTO system at $V_{\text{bias}} = 3.06\,\text{V}$ with the same doping density of $N_{\text{donor}} = N_{\text{acceptor}} = 5.0 \times 10^{18}\,\text{cm}^{-3}$. It is clearly seen that under the same conditions, refrigeration power of the p-BTO/BTO/STO/BTO/n-BTO system is much higher than that of the p-AlGaAs/AlGaAs/GaAs/AlGaAs/n-AlGaAs system as shown in figure 2. The refrigeration power dependence on voltage is explained as follows. When $V_{\text{bias}}$ increases, the carrier densities in the well increase. From equations (4) and (5), it can be seen that the Auger recombination rate increases faster than the radiative recombination rate. Thus the refrigeration power increases with the increase in $V_{\text{bias}}$ and then decreases with further increase in $V_{\text{bias}}$. Therefore, the opto-thermionic refrigeration dependence on $V_{\text{bias}}$ is the competition between the radiative recombination and the Auger recombination process.

$Q_{\text{refrig}}$ versus $V_{\text{bias}}$ at various doping densities is also calculated and the results are plotted in figure 3. The donor density in the n-doped region is set to be equal to the acceptor density in the p-doped region for simplicity, that is $N_{\text{donor}} = N_{\text{acceptor}}$. The calculated results show that there exists a doping density of about $N_{\text{donor}} = N_{\text{acceptor}} = 3.6 \times 10^{19}\,\text{cm}^{-3}$ with a maximum value of refrigeration power of $33\,\text{W cm}^{-2}$. This maximum value of refrigeration power is the result of the competition between the Auger recombination and the radiative recombination processes.

The optimal doping density dependence on the refrigeration power for p-BTO/BTO/STO/BTO/n-BTO is shown in figure 4. It can be seen that the optimal doping density is $2.0 \times 10^{19}\,\text{cm}^{-3}$ and $1.0 \times 10^{18}\,\text{cm}^{-3}$ for the p-doped and n-doped regions, respectively. The maximum refrigeration power with the optimal doping density is $39\,\text{W cm}^{-2}$ at $V_{\text{bias}} = 3.06\,\text{V}$.

The cooling efficiency is defined as the ratio of the useful output energy to the input energy. For laser cooling in heavy-metal-fluoride glass doped with trivalent ytterbium ions, the cooling efficiency is 2% [16]. For opto-thermionic cooling in the p-BTO/BTO/STO/BTO/n-BTO system at $V_{\text{bias}} = 3.06\,\text{V}$, the cooling efficiency, which is defined as the ratio of the net cooling power to the input power and written as $\eta = P_{\text{cool}}/P_{\text{total}} = Q_{\text{refrig}}/JV_{\text{bias}}$, is 2.1%.

## 4. Summary

In summary, the refrigeration power of the p-BTO/BTO/STO/BTO/n-BTO system is obtained based on the analysis of the opto-thermionic refrigeration process. It is found that refrigeration power of the p-BTO/BTO/STO/BTO/n-BTO system is much higher than that of the p-AlGaAs/AlGaAs/GaAs/AlGaAs/n-AlGaAs system under the same conditions. For a well width of 40 nm, the refrigeration power of $39\,\text{W cm}^{-2}$ is theoretically obtained with the doping density of $2.0 \times 10^{19}\,\text{cm}^{-3}$ and $1.0 \times 10^{18}\,\text{cm}^{-3}$ for p and n regions, respectively. The results indicate that the perovskite oxide structures have potential for application in opto-thermionic refrigeration, and an experimental study on the proposed structure of p-BTO/BTO/STO/BTO/n-BTO is highly expected.

## Acknowledgment

This work has been supported by the National Natural Science Foundation of China and National Basic Research Programme of China.

## References

[1] Mal'shukov A G and Chao K A 2001 *Phys. Rev. Lett.* **86** 5570
[2] Han P, Jin K J, Zhou Y L, Wang X, Ma Z S, Ren S F, Mal'shukov A G and Chao K A 2006 *J. Appl. Phys.* **99** 074504
Han P, Jin K J, Zhou Y L, Lu H B and Yang G Z 2007 *J. Appl. Phys.* **101** 014506

[3] Abakumov V N, Perel V I and Yassievich I N 1991 *Nonradiative Recombination in Semiconductors* (Amsterdam: North-Holland)
[4] Strauss U, Rühle W W and Köhler K 1993 *Appl. Phys. Lett.* **62** 55
[5] Yasuda H and Kanemitsu Y 2008 *Phys. Rev.* B **77** 193202
[6] Ahn C H, Rabe K M and Triscone J M 2004 *Science* **303** 488
[7] Lee H N, Christen H M, Chisholm M F, Rouleau C M and Lowndes D H 2005 *Nature* **433** 395
[8] Reyren N *et al* 2007 *Science* **317** 1196
[9] Wang N, Lu H B, Chen W Z, Zhao T, Chen F, Peng H Y, Lee S T and Yang G Z 1999 *Appl. Phys. Lett.* **75** 3464
[10] Yang G Z, Lu H B, Chen F, Zhao T and Chen Z H 2001 *J. Crystal Growth* **227–228** 929
[11] Zhou M J, Zhu Y L, Ma X L and Lu H B 2006 *Appl. Phys. Lett.* **88** 071905
[12] Horio K and Yanai H 1990 *IEEE Trans. Electron Devices* **37** 1093
[13] Lundstrom M S and Schuelke R J 1983 *IEEE Trans. Electron Devices* **30** 1151
[14] Sze S M 1981 *Physics of Semiconductor Devices* (New York: Wiley)
[15] Rubano A, Paparo D, Miletto F, Scotti di Uccio U and Marrucci L 2007 *Phys. Rev.* B **76** 125115
[16] Epstein R I, Buchwald M I, Edwards B C, Gosnell T R and Mungan C E 1995 *Nature* **377** 500