



Fig.13 temperature dependence of (a) Thermal conductance, (b) Power Factor and (c) figure of merit for the rectangular single pore ASiNR structure

VII. CONCLUSION

In summary, we have investigated the influence of different pore shapes and its associated position on the thermoelectric performance of ASiNR-NP devices. Nanopores of different shapes i.e. circular, rectangular, triangular and rhombus have been introduced at varying positions of the nano structure so as to study their effect on the thermoelectric figure of merit. By optimizing the pore parameters, we have been able to achieve higher Figure of merit, which is approximately three times higher than pristine ASiNR. Further, the effect of pore passivation is observed, which has been successfully able to enhance ZT in case of Rectangular pores. Thus, our work extends the idea towards achieving better thermoelectric devices by optimal pore efficiency.

REFERENCES

- [1] H. Sadeghi, S. Sangtarash, and C.J. Lambert, "Enhanced thermoelectric efficiency of porous silicene nanoribbons", *Sci. Rep.* Vol. 5, 9514, March 2015.
- [2] Y. Liang, V. Wang, H. Mizuseki, and Y. Kawazoe, "Band gap engineering of silicene zigzag nanoribbons with perpendicular electric fields: a theoretical study", *J. Phys. Condens. Matter* Vol. 24, 455302, Oct. 2012.
- [3] Y.L. Song, Y. Zhang, J.M. Zhang, D.B. Lu, and K.W. Xu, "Modulation of the electronic and magnetic properties of the silicene nanoribbons by a single C chain.", *Eur. Phys. J. B* Vol. 79, No. 2, pp. 197–202, 2011.
- [4] C. Le'andri, G. Lay, B. Aufray, C. Girardeaux, J. Avila, M. E. Davila, M. C. Asensio, C. Ottaviani, and A. Cricenti, "*SiGe, Ge and related compounds 6: materials, processing and devices, ECS Transactions*", Vol. 64, 2005.
- [5] M.S. Hossain, F.A. Dirini, F.M. Hossain, and E. Skafidas, "High performance Silicenenano-ribbon thermoelectric devices by incorporation and dimensional tuning of nanopores", *Sci. Rep.* Vol. 5, 11297, June 2015.
- [6] L.D. Hicks and M.S. Dresselhaus, "Thermoelectric figure of merit of a one dimensional conductor", *Phys. Rev. B*, Vol. 47, pp. 16631–16634, June 1993.
- [7] S. Kaur, D.K. Randhawa, and S.B. Narang, "Theoretical investigation of effect of pore size and porepassivation on the thermoelectric performance of silicene nanoribbons", Vol. 32, pp. 3485-3493, Sept. 2017.
- [8] Z. Ni, H. Zhong, X. Jiang, R. Quhe, Y. Wang, J. Yang, J. Shi, and J. Lu, "Tunable band gap and doping type in silicene by surface adsorption: Towards tunneling transistors", *Nanoscale* Vol. 6, pp. 7609–7618, April 2014.
- [9] Y. Qi, Z. Wang, M. Zhang, F. Yang, and X. Wang, "Thermoelectric devices based on one dimensional nanostructures", *J. Mater. Chem. A* Vol. 1, pp. 6110–6124, Feb. 2013.
- [10] L. Pan, H. J. Liu, X. J. Tan, H. Y. Lv, J. Shi, X. F. Tang and G. Zheng, "Thermoelectric properties of armchair and zigzag silicene nanoribbons", *Phys. Chem. Chem. Phys.*, Vol. 14, pp. 13588–13593, Aug. 2012.
- [11] D. Kienle, J.I. Cerda, and A.W. Ghosh, "Extended Huckel theory for band structure, chemistry, and transport. Carbon nanotubes", *J. Appl. Phys.* Vol. 100, 043714, Aug. 2006.
- [12] R. Landauer, "Spatial variation of currents and fields due to localized scatterers in metallic conduction", *IBM J. Res. Dev.* Vol. 1, pp. 223–231, July 1957.
- [13] M.S. Hossain, F. Al-Dirini, F.M. Hossain, and E. Skafidas, "High performance Silicenenano-ribbon thermoelectric devices by incorporation and dimensional tuning of nanopores", *Sci. Rep.* Vol. 5, 11297, June 2015.
- [14] G.Q. Zhang, Q.X. Yu, W. Wang, and X.G. Li, "Nanostructures for thermoelectric applications, synthesis, growth mechanism & property studies", *Adv. Mater.* Vol. 22, pp. 1959–1962, April 2010.
- [15] K. Esfarjani, M. Zebarjadi, and Y. Kawazoe, "Thermoelectric properties of a nanocontact made of two-capped single-wall carbon nanotubes calculated within the tight binding approximation", *Phys. Rev. B: Condens. Matter Mater. Phys.* Vol. 73, 085406, Feb. 2006.
- [16] H. Sadeghi, S. Sangtarash, and C.J. Lambert, "Enhancing the thermoelectric figure of merit in engineered graphene nanoribbons", *Beilstein J. Nanotechnol.* Vol. 6, pp. 1176–1182, May 2015.
- [17] Atomistic Tool Kit Manual, Quantum wise Inc. Atomistix toolkit version 13.8.0, Quantum wise A/S [Online] Available: <http://quantumwise.com/>