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Ultra-high power factor of *p*-type Bi_2Se_3 for room temperature thermoelectric applications

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Polycrystalline alloys of $Bi_{2-x}Mn_yGa_zSe_3$ (x = y+z; y = 0.015, 0.03, 0.045; z = y/0.03, x/0.06, x/0.09) compounds were prepared by melting of high purity elemental Bi (rod, 6N, Wako, Japan), Se (shots, 5N, Wako, Japan), Mn (metal powder, 99.999%, Sigma Aldrich) and Ga (shots, 99.999%, Wako, Japan) in high vacuum (10^{-6}) evacuated quartz tubes. The tubes were slowly heated up to 1073 K over 10 h and maintained at this temperature for 5 h. Then, it was allowed to cool down naturally. Further, the obtained ingots were ground into powders and then densified by uni-axial hot-press under the pressure of 70 MPa at 858 K for 15 min in a graphite die, and the samples are named BGMS 0, BGMS 0.015, BGMS 0.03 and BGMS 0.045 for the $Bi_{2-x-y}Mn_xGa_ySe_3$ (x = 0.015, 0.03, 0.045; y = x/0.03, x/0.06, x/0.09) alloys respectively. The relative densities of all the pellets were more than 98%. The grinding process for all the samples is maintained for 20 mins to study the randomly oriented texturing effect of the as-prepared alloys

on thermoelectric properties. XRD pattern of the samples characterized by the PANalytical X'Pert pro (Netherland) using Cu Kα radiation (λ = 1.5406 Å) at room temperature. Rietveld refinement of all the samples was done by using GSAS II software. The morphology and the elemental mapping were carried out by HR-SEM (ThermoFisher Apreo S) equipped with an EDS. The thermal conductivity of the samples was measured by LFA 467 HT Hyper Flash instrument (NETZSCH, Germany). Pyroceram 9606 sample was used as a reference for all the as-prepared samples. Room temperature Hall carrier density and Hall mobility were obtained by HMS 5300 under the Van der Pauw four-probe setup. Seebeck coefficient and electrical resistivity were simultaneously measured using ADVANCE RIKO ZEM-3 (Japan).

Sample code	**a**	**c**	**c/a**
BGMS 0	4.137	28.636	6.922
BGMS 0.015	4.108	29.112	7.086
BGMS 0.03	4.159	28.946	6.959
BGMS 0.045	4.166	28.860	6.928

Table.S1. calculated lattice parameters of as prepared pure Bi_2Se_3 and Mn & Ga co doped samples.

Sample code	Γ_m **(×10^{-2})**	Γ_s **(×10^{-2})ε**	**(γ)**
BGMS 0.015	0.307	0.137	47.5
BGMS 0.03	0.615	0.271	48.3
BGMS 0.045	0.924	0.402	48.8

Table.S2. Disorder scattering parameters Γ_m- mass fluctuation, Γ_s – strain field fluctuation and scattering factor (γ) of Mn and Ga co-doped Bi_2Se_3 alloys.

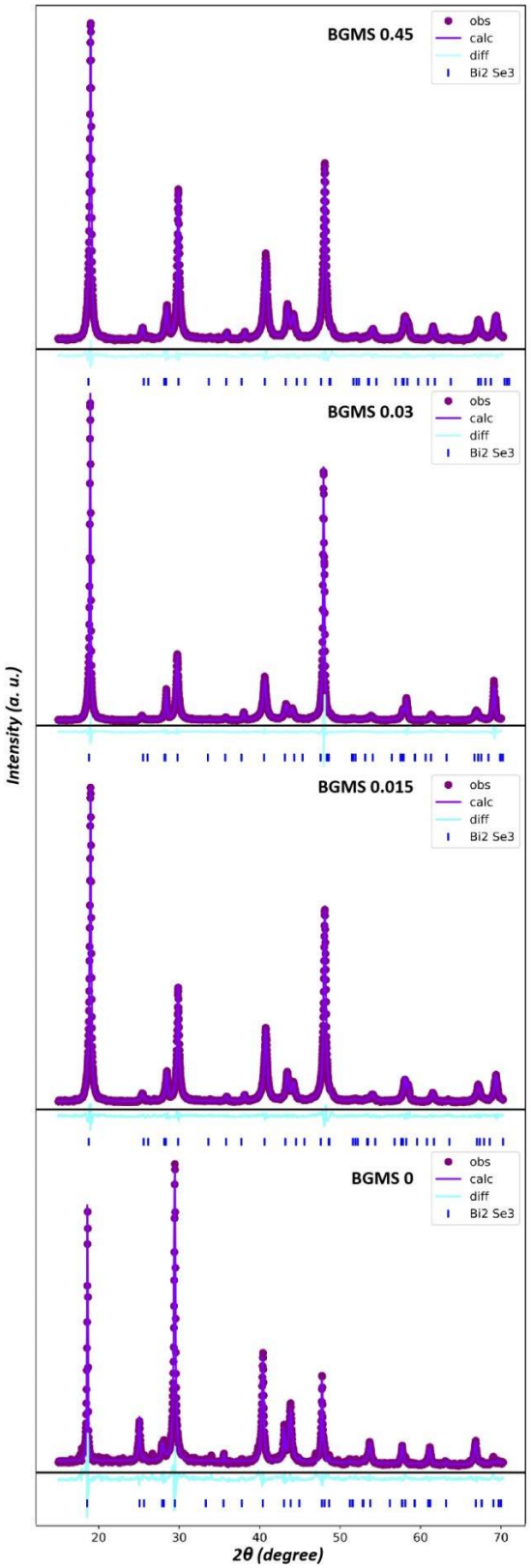

Figure.S1. Rietveld refinement of as prepared pure Bi_2Se_3 and Mn & Ga co substituted samples.

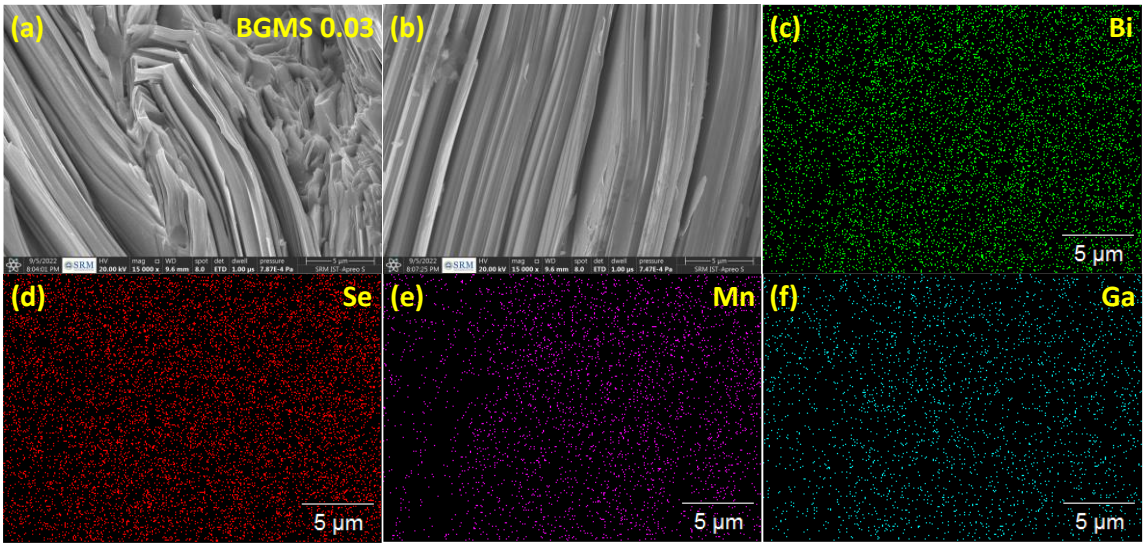

Figure. S2. Hi-Resolution SEM image with the corresponding elemental quantification analysis of BGMS 0.03 sample.

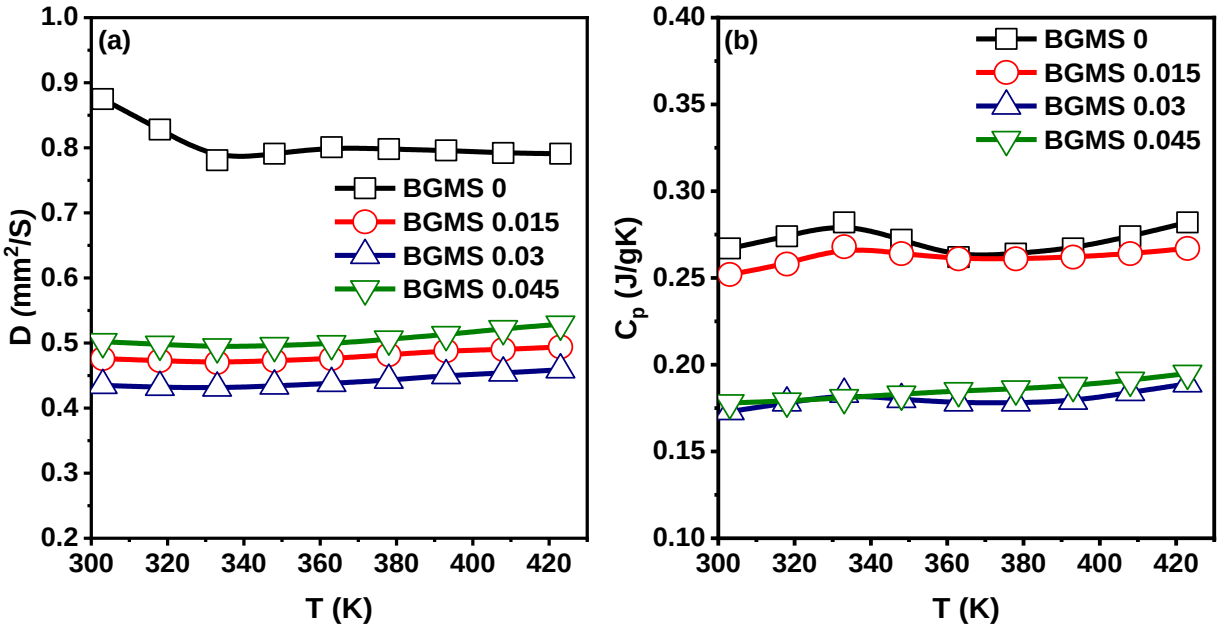

Figure.S3. Temperature dependence of thermal diffusivity (a), and Specific heat capacity of as prepared pure Bi_2Se_3 and Mn & Ga co substituted samples.

The Lorenz number L calculated from the measured Seebeck values from the following semi-empirical equation, $L = 1.5 + exp\left(-\frac{|S|}{116}\right)$.

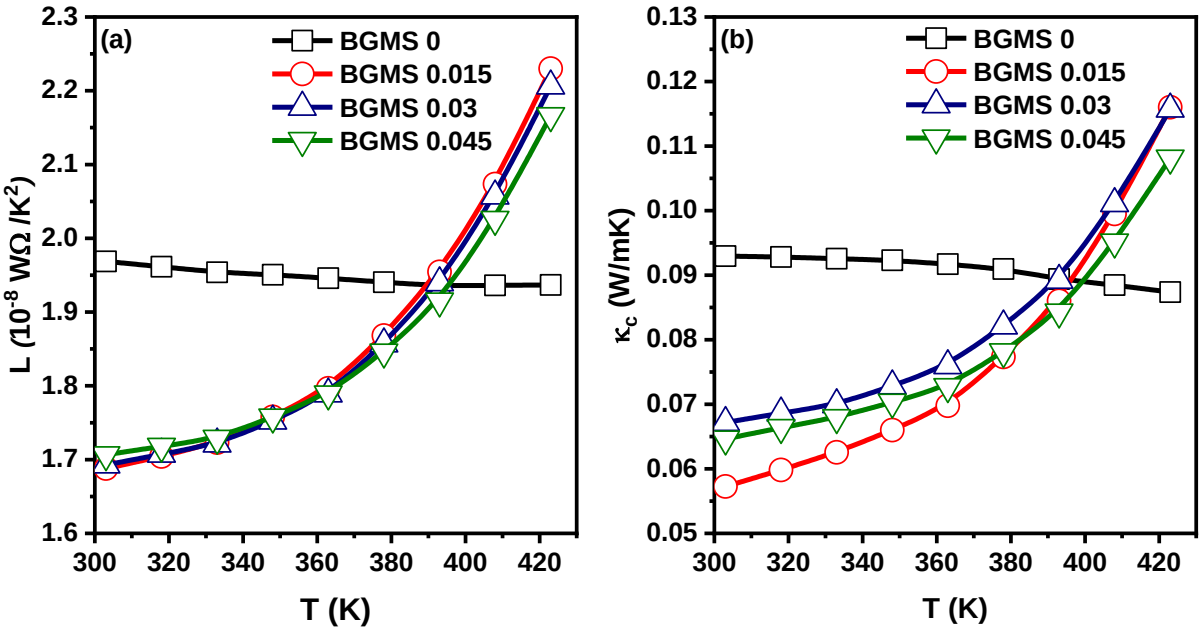

Figure.S4. (a) calculated Lorenz number and (b) carrier thermal conductivity as a function of temperature for as prepared pure Bi_2Se_3 and Mn & Ga co substituted samples.

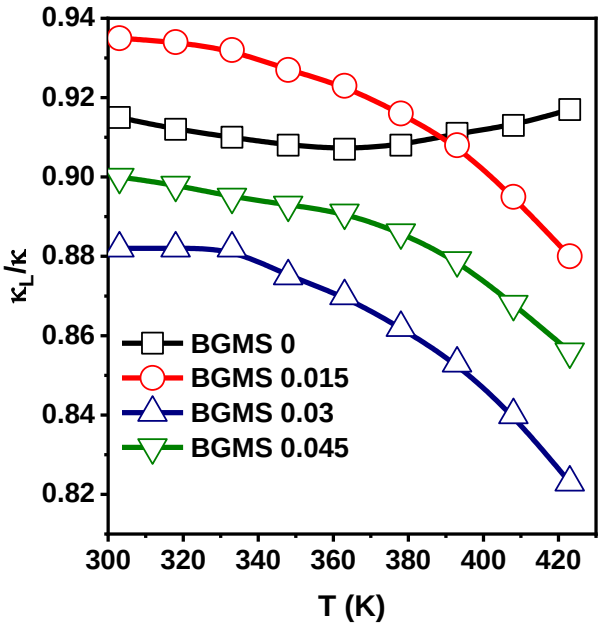

Figure.S5. The calculated ratio of κ_L/κ as a function of temperature for as prepared pure Bi_2Se_3 and Mn & Ga co substituted samples. which exhibits the importance of lattice thermal conductivity reduction in total thermal conductivity.

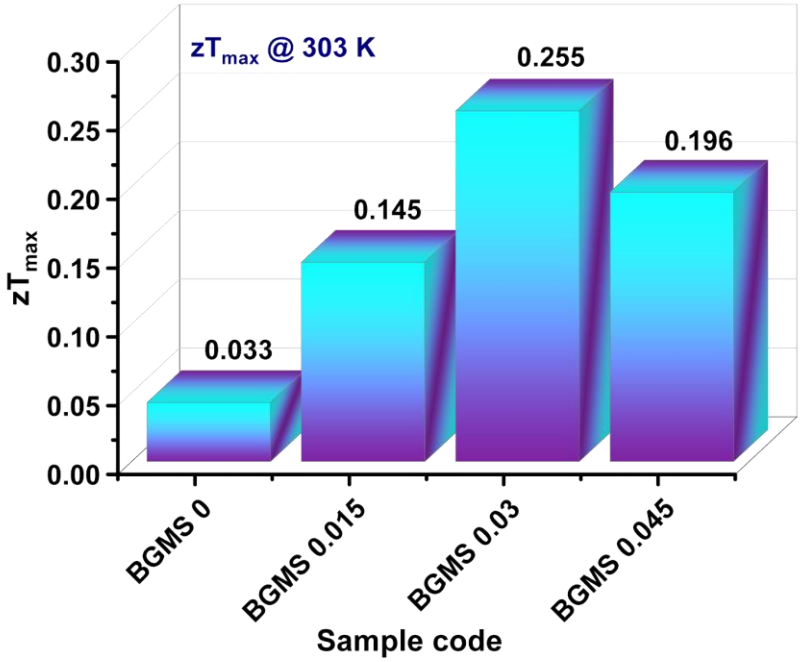

Figure.S6. The peak zT of as prepared pure Bi_2Se_3 and Mn & Ga co substituted samples.

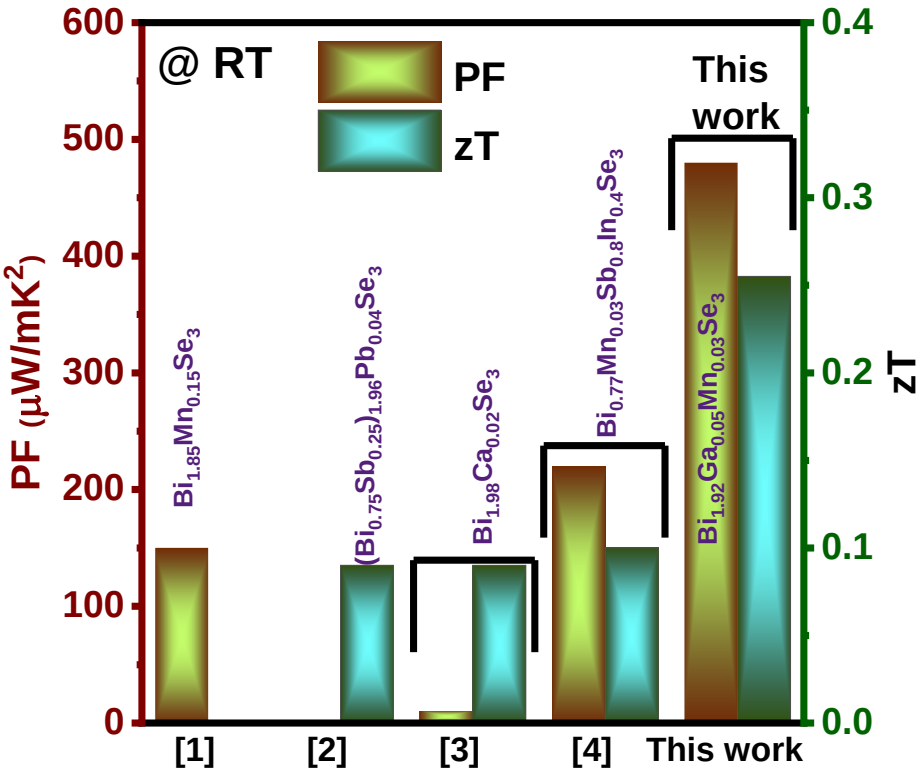

Figure.S7. Comparison of reported power factor and figure of merit with this work at room temperature [1–4].

References:

1 C. M. Kim, S. H. Kim, T. Onimaru, K. Suekuni, T. Takabatake and M. H. Jung, *Curr. Appl. Phys.*, 2014, **14**, 1041–1044.

2 J. Kašparová, Č. Drašar, A. Krejčová, L. Beneš, P. Lošťák, W. Chen, Z. Zhou and C. Uher, *J. Appl. Phys.*, 2005, **97**, 2–6.

3 Y. S. Hor, A. Richardella, P. Roushan, Y. Xia, J. G. Checkelsky, A. Yazdani, M. Z. Hasan, N. P. Ong and R. J. Cava, *Phys. Rev. B - Condens. Matter Mater. Phys.*, 2009, **79**, 2–6.

4 F. Jiang, C. Xia, Y. Zhu, Z. Han, C. Liu, J. Xia, Y. Chen and W. Liu, *Appl. Phys. Lett.*, 2021, **118**, 4–9.