Investigation of near-room and high-temperature thermoelectric properties of (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ composite system

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ABSTRACT

Polycrystalline composite samples of (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ with different concentrations of Bi$_2$Te$_3$ such as 5%, 10%, 15% and 20% were prepared by the solid-state reaction technique. The X-Ray diffraction analysis has shown the hexagonal composite crystal structure with space group of R$3\,m$. Field emission scanning electronic microscope shows secondary particles on the surface of the samples. All the samples have shown the usual semi-conducting behaviour throughout the temperature range. It is observed that bismuth has been coordinated with 6 selenium atoms in (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$ compound and it has enormous selenium vacancies. The electrical resistivity represents the noteworthy result of the grain boundaries leading to the higher content of scattering centres in the polycrystalline composite samples. It is found that the electronegativity differences of In and Te, In and Se are less than Bi and Se, Bi and Te is the reason for the decrease in Seebeck coefficient in the compound containing 15% and 20% of Bi$_2$Te$_3$.

1 Introduction

Bismuth telluride and bismuth selenide are the dominant thermoelectric compounds for the near-room temperature applications because of their inherently small thermal conductivity and large electronic weighted mobility. As a consequence of low energy gap (0.14 eV), the performance is finally imperfect by the harmful effects of thermally produced minority charges [1]. The impact is moderately mitigated by the heavy doping/composite in the matrix. Alloying of Bi$_2$Se$_3$ and Bi$_2$Te$_3$ along with the doping of indium can produce bipolar effects by enhancing the band gap. The task is found to be very challenging because carrier mobility is also disrupted during the composite alloying, while deviations in the electronic structure might prove advantageous [2].

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The ternary combination of alloy has an energy band gap extending from 0.2 to 0.3 eV. The crystal structure of Bi$_2$Te$_3$ and Bi$_2$Se$_3$ is represented by covalently bonded (Te,Se)$_1$-Bi-(Te,Se)$_1$ quintuple layers stalking of generally with the adjoining layers linked by feeble van der Waals bond [3]. These compounds have been investigated in earlier reports to improve the power factor. In order to increase the power factor of a material, a large Seebeck coefficient and low electrical resistivity values are required. It can be noticed that thermoelectric materials which shows a ZT value of more than unity can be considered as one of the best thermoelectric materials. Whereas thermoelectric materials strive on the efficiency with mechanical power generation and vigorous refrigeration when they attain the ZT values up to three [4].

Gion Lee et al. [5] investigated the thermoelectric performances of Bi$_2$Te$_3$–Bi$_2$Se$_3$ solid solutions by attrition milling and hot pressing and obtained the highest thermoelectric power of 170 $\mu$V/K at 300 K. Thermoelectric properties of Bi$_2$Te$_3$, Sb$_2$Te$_3$, and Bi$_2$Se$_3$ single crystals were investigated by Kalbuchinski et al. [6] obtained the highest electrical resistivity of 30,000 S/cm and the Seebeck coefficient of 150 $\mu$V/K at 300 K. The highest power factor 131 $\mu$W/m K$^2$ was recorded at 473 K for optimized thin films of (Bi$_2$Se$_3$)$_{1-x}$(Bi$_2$Te$_3$)$_x$ alloyed films by Adam et al. [7]. Khandi et al. [8] have successfully evaluated the structural stability, electronic structure, and transport coefficients of the Heusler compound Ru$_2$TaGa using semi-classical Boltzmann theory. They [9] have examined the electronic structure, mechanical, phonon, and thermoelectric properties of this chemical as well as the use of ab-initio calculations and Boltzmann transport theory to compare and forecast the overall physical properties. The electrical, dynamic, elastic, magnetic, and thermoelectric properties of FeRhCrGe alloy have been studied using density functional theory [10, 11].

To the best of our knowledge, doping on Bi$_2$Se$_3$ and Bi$_2$Te$_3$ has been studied vast, while the simultaneous doping and composite for these compounds have been investigated least. In the previous report, we have investigated low-temperature thermoelectric properties of (Bi$_{1-x}$In$_x$)$_2$Te$_{2.7}$Se$_{0.3}$, (Bi$_{1-x}$Sn$_x$)$_2$Te$_{2.7}$Se$_{0.3}$, (Bi$_{1-x}$In$_x$)$_2$Se$_{2.7}$Te$_{0.3}$, and (Bi$_{1-x}$In$_x$)$_2$Se$_{2.7}$Te$_{0.3}$ samples [12, 13]. In the present investigation, n-type (Bi$_{1-x}$In$_x$)$_2$Te$_{2.7}$Se$_{0.3}$ system’s carrier concentration is significantly affected by the development of antistructure defects. The bismuth telluride composite impurities and precipitants in the (Bi$_{1-x}$In$_x$)$_2$Te$_{2.7}$Se$_{0.3}$ crystal lattice develop flaws that scatter the charge carriers. Hence, in the present research work structural, surface morphological, and thermoelectric properties of novel composite materials systems of (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$ with different concentration of Bi$_2$Te$_3$ such as 5%, 10%, 15%, and 20% have been investigated in the high-temperature range of 30$^\circ$–450 $^\circ$C.

### 2 Experimental procedure

The conventional solid-state reaction method is used to prepare the polycrystalline sample of (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ for 95%/(wt 5%, wt 10%, wt 15%, and wt 20%), respectively.

#### 2.1 Synthesis of (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$

(Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$ has been synthesized by using a solid-state reaction approach, the precursors of bismuth (99.99%), indium (99.99%), selenium (99.995%), and tellurium (99.99%) were combined in a stoichiometric ratio and mixed for two hours, while being vigorously ground in an agate mortar. Pelletization of the combined powder was carried out using a 5 tonne compression force. The pellets were placed in a quartz ampoule and vacuum-sealed there for 30 h at 480 $^\circ$C. To increase the uniformity of the compounds, the grinding process is repeated for the sintered pellets. The pellets are again sintered for 15 h at 250 $^\circ$C.

#### 2.2 Synthesis of Bi$_2$Te$_3$

Precursors of Bismuth (99.99%), Tellurium (99.99%), Selenium (99.995%), and Indium (99.9%) were combined in a stoichiometric ratio and processed for two hours in an agate mortar. Utilizing a hydraulic press with a 5 tonne compression, the powder was formed into pellets. The pellets were sintered at 420 $^\circ$C for 24 h under vacuum at 10$^{-6}$ torr in a quartz tube with a 12 mm diameter. To achieve the appropriate homogeneity in the compound, the grinding procedure was repeated for the sintered samples for an hour. This powder was sintered for 12 h at 200 $^\circ$C after being pelletized.
2.3 Composition of \((\text{Bi}_{0.98}\text{In}_{0.02})\text{Se}_{2.7}\text{Te}_{0.3}/\text{Bi}_2\text{Te}_3\) for 95%/wt 5%, wt 10%, wt 15%, wt 20%)

The prepared \(\text{Bi}_2\text{Te}_3\) was added separately to \((\text{Bi}_{0.98}\text{In}_{0.02})\text{Se}_{2.7}\text{Te}_{0.3}\) in composition of 5%, 10%, 15%, and 20%, respectively, and grounded thoroughly in an agate mortar for 2 h to get the proper homogeneity mixture. The samples were sealed at same vacuum and sintered for about 12 h to densify the grains. The pellets of dimension \(10 \times 2 \times 5 \text{ mm}^3\) were subjected to various experimental characterization.

3 Characterization

To verify the purity, crystallinity, and phase formation of the compounds, an X-ray diffraction (XRD) investigation was conducted using an X-ray diffractometer (Rigaku Miniflex) and CuK\(\alpha_2\) rays. Using the “JEOL JSM-7100F”, field emission scanning electron microscopy (FESEM) has been carried out at a magnification of 35 kX and a voltage of 15 kV. To identify the components of the chemical, Energy-Dispersive X-Ray Analysis of Spectra (EDS) has been carried out with the same apparatus.

The temperature-dependent Electrical resistivity and Seebeck coefficient were measured simultaneously by Steady-state DC method using instrument “Linesis LSR3” in the temperature range 30\(^\circ\)C–450 \(^\circ\)C.

4 Results and discussion

4.1 Powder X-ray diffraction studies

To recognize the purity, crystalline phase, and crystallinity of \((\text{Bi}_{0.98}\text{In}_{0.02})\text{Se}_{2.7}\text{Te}_{0.3}/\text{Bi}_2\text{Te}_3\) powder X-ray diffraction study has been taken between 20\(^\circ\) and 80\(^\circ\) at the scan rate of 2\(^\circ\)/min. Figure 1a signifies \((\text{Bi}_{1-x}\text{Sn}_x)\text{Se}_{2.7}\text{Te}_{0.3}\) powder XRD patterns which exhibit hexagonal structure with space group \(R\overline{3}m\), prominent aligned XRD peak plane (015) were detected for all samples. The present XRD patterns match with the JCPDS data sheet [Fig. 2] has been given in Fig. 2, which are in good agreement with the present XRD patterns. The sudden increase in crystallite size, XRD peak broadening in \((\text{Bi}_{0.98}\text{In}_{0.02})\text{Se}_{2.7}\text{Te}_{0.3}/\text{Bi}_2\text{Te}_3\) (80% / 20%) is due to the increasing \(\text{Bi}_2\text{Te}_3\) content. The change in the ratio of the host and composite compound had a significant effect on the strain which influenced XRD patterns in the composite structure [14] [Fig. 3]. The crystallite sizes were estimated using Williamson–Hall formula, where the crystallite size of the sample was found to be decreasing with the composite concentration till 15% \(\text{Bi}_2\text{Te}_3\). EXPO 2014 has been utilized to know the deviation between theoretical and calculated XRD peak patterns which is shown in Fig. 4 [15]. The characterizability factors such as \(R_p, R_{wp}, R_{ep}\), and \(\chi^2\) values are presented in Table 1.

4.2 Field emission scanning electron microscopy (FESEM) and energy-dispersive analysis of spectra (EDS)

Figure 5 shows the Field emission scanning electron microscopic images of \((\text{Bi}_{0.98}\text{In}_{0.02})\text{Se}_{2.7}\text{Te}_{0.3}/\text{Bi}_2\text{Te}_3\) composite samples. The sample \((\text{Bi}_{0.98}\text{In}_{0.02})\text{Se}_{2.7}\text{Te}_{0.3}/\text{Bi}_2\text{Te}_3\) of 95%–5% shows few porosity with compact structure which is depicted in Fig. 5 (a) [16]. The dopant particles of tellurium atoms have been found
surface of (Bi0.98In0.02)2Se2.7Te0.3/BiTe3 with 80%–20% shows the homogeneous distribution of the composites in the grains (Fig. 5d) [17, 18].

The existence of the added elements of the samples was examined by the EDS, and the images are shown in Fig. 6a–d. All the (Bi0.98In0.02)2Se2.7Te0.3/BiTe3 samples indicate the presence of bismuth, selenium, indium, tellurium, and selenium. Beside the EDS elemental mapping shows that the added elements have been homogeneously distributed on the surface of the sample.

4.3 Electrical resistivity

The electrical resistivity of (Bi0.98In0.02)2Se2.7Te0.3/Bi2Te3 composites were measured in the temperature range 30–450 °C [Fig. 8]. All the samples have shown n-type semi-conducting behaviour entire temperature range. It is observed that bismuth has co-ordinated with 6 selenium atoms in (Bi0.98In0.02)2Se2.7Te0.3 compound and it has huge selenium vacancies [19, 20]. Such coordination is disturbed by indium dopant in the compound. In the host lattice, the sites which have indium coordination with selenium are seeming to have larger volume than that of the host [21]. The decrease in electrical resistivity with the increase in temperature can be attributed to the reduction in Se vacancies. Some of the bismuth site in the samples were observed to be substituted by indium, gives a partial coordination between indium, selenium, and tellurium atoms. Beside the negative trending behaviour of the electrical resistivity from 5 to 20% of composite is observed due to the antisite defects like BiTe, SnTe, BiSe, and SnSe formed during
Because of the super stoichiometry, Bi atoms can arrive sublattice and form selenium vacancies in the interstitial site [22, 23]. Initially, there is an enhancement in the value of electrical resistivity with a rise in temperature from 10 to 220 K due to the low mobility of the opposing charges around another donor atom of composite Bi$_2$Te$_3$, which causes direct cation–cation interaction of homopolar Bi–Bi bonds with (Bi$_{1-x}$In$_x$)$_2$Te$_{2.7}$Se$_{0.3}$. The electrons fail to conduct significantly up to 220°C. The negative charge mingles with extra electrons of all the donor atoms, leading to the usual semi-conducting behaviour from metallic semi-conductor behaviour above 220 °C[24, 25]. The creation of antistructure defects in the n-type (Bi$_{1-x}$In$_x$)$_2$Te$_{2.7}$Se$_{0.3}$ system has a significant impact on the carrier concentration, which is closely related to the electrical conductivity and Seebeck coefficient. Tellurium has two distinct crystallographic sites, Te (1) and Te (2), and as a result, different antistructure defects, such as Bi–In–Te (1) and Bi–In–Te (2), are developed. These potential antistructures have

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**Table 1** Powder X-ray diffraction data of (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ composite samples

| Sample  | $R_p$  | $R_{wp}$ | $R_{ep}$ | $\chi^2$ | Crystallite size (nm) | $a = b$ (Å) | $c$ (Å) | Lattice strain (%) |
|---------|--------|---------|---------|---------|-----------------------|-------------|-------|---------------|
| BIS/BT 5% | 5.6 | 7.3 | 7.2 | 1.1 | 15 ±0.0092 | 4.16 | 28.89 | 4.2 |
| BIS/BT 10% | 5.1 | 7.1 | 6.8 | 1.0 | 16 ±0.0086 | 4.15 | 28.80 | 8.4 |
| BIS/BT 15% | 6.23 | 8.0 | 4.5 | 1.5 | 18 ±0.0077 | 4.12 | 28.70 | 2.7 |
| BIS/BT 20% | 7.4 | 9.7 | 8.2 | 1.3 | 25 ±0.0055 | 4.17 | 28.90 | 6.9 |

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![Fig. 4](https://example.com/fig.png)

The Rietveld refinement plots of (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ composite samples.
distinct formation energies from one another, which led to irregular fluctuations in the effective masses of different composite concentrations\footnote{26}. However, there is a minor distortion due to incorporation of indium atom into the selenium and tellurium sublattice which lowers the influence of super-stoichiometric bismuth content in Bi,Se, and Bi,Te \footnote{27, 28}. The activation energy of all the samples were calculated using the Small polaron hopping model (SPH) (Fig. 9). For electrical resistivity data between

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig5}
\caption{The FESEM images of (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ composites}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig6}
\caption{Energy-dispersive X-ray analysis of spectra of (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ composites}
\end{figure}
33 and 350 °C, the small polaron hopping model (SPH) is used at high temperatures and is represented by

$$\rho = \rho_0 T \exp \left( \frac{E_A}{k_B T} \right),$$

where $E_A$ is the activation energy [29, 30]. Figure 9 shows a linear relationship between $\ln(\rho / T)$ and $1 / T$, indicating that thermally activated small polarons are responsible for the hopping mechanism between nearest neighbouring sites in the $(\text{Bi}_{1-x}\text{In}_x)_2\text{Se}_{2.7}\text{Te}_{0.3}/\text{Bi}_2\text{Te}_3$ system in the high-temperature region. $E_A$ values are found to vary inconsistently with the doping concentration due to the variation in the composition of selenium atoms after sintering [31, 32], which leads to the higher content of scattering centres in $(\text{Bi}_{0.98}\text{In}_{0.02})_2\text{Se}_{2.7}\text{Te}_{0.3}/\text{Bi}_2\text{Te}_3$ samples [33].

### 4.4 Seebeck coefficient

Temperature-dependent Seebeck coefficient was measured in the temperature range of 30–450 °C for the synthesized polycrystalline samples and is shown in Fig. 10. In the n-type $(\text{Bi}_{1-x}\text{In}_x)_2\text{Se}_{2.7}\text{Te}_{0.3}/\text{Bi}_2\text{Te}_3$ alloys, the electrons are created by the antistructure defects by the occupation of Te/Se sites with Bi and In atoms [33]. The reduction in the difference of the electronegativity among the component atoms found to be favourable for increase in the antistructure defects. Hence, carrier (holes) concentration in $(\text{Bi}_{1-x}\text{In}_x)_2\text{Se}_{2.7}\text{Te}_{0.3}/\text{Bi}_2\text{Te}_3$ decreases with increasing $\text{Bi}_2\text{Te}_3$ content. It is found that the differences in the electronegativity of In and Te, In and Se are lesser than Bi and Se, Bi and Te [34, 35]. This could be the reason for the decrease in Seebeck coefficient in the compound containing 15% and 20% of $\text{Bi}_2\text{Te}_3$. Similar phenomena were also observed in $\text{Bi}_x\text{Sb}_{2-x}\text{Te}_3$ [36]. With the increased Te in the $(\text{Bi}_{1-x}\text{In}_x)_2\text{Se}_{2.7}\text{Te}_{0.3}/\text{Bi}_2\text{Te}_3$ system there is a rise of carrier concentration or band structure change in turn there is a variation in both the electrical resistivity and Seebeck coefficients. This is because Se has a higher evaporation pressure than Te and hence easily forms donor-like vacancies.
in the Bi$_2$Te$_3$-type lattice [37]. The theoretical carrier concentration is calculated using equation

$$S(T) = \frac{8k_B^2 \pi^2 m^*}{3e^2 h^2} \left( \frac{n}{3n} \right)^{2/3} T,$$

where $m^*$ is the effective mass of the electron, $e$ is the elementary charge of an electron, $h$ is the Plank’s constant, $n$ is the carrier concentration, and $T$ is the absolute temperature, where $S(T)$ is the temperature-dependent Seebeck coefficient, $k_B$ is the Boltzmann’s constant [38]. The mobility can be calculated using

$$\mu = \frac{1}{ne\rho}$$

### 4.5 Power factor

Figure 11 shows the temperature-dependent power factor ($PF = S^2/\rho$) of the studied (Bi$_{1-x}$In$_x$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ composites. The highest power factor of about 500 $\mu$W/mK$^2$ was observed in (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ (95%/5%), whereas the pristine (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ (80%/20%) has the lowest $PF$ of 250 $\mu$W/mK$^2$ at 300 $^\circ$C. Table 3 shows the comparison of thermoelectric properties of other reported bismuth chalcogenide thermoelectric materials [16, 39, 40].

### 5 Conclusion

In this work, we report investigation of thermoelectric properties of the (Bi$_{1-x}$In$_x$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ composite system with composition (95/5%, 90/10%, 85/15%, 80/5%). The XRD analysis confirms the hexagonal crystal system with space group of $R3m$. Field emission scanning electronic microscope shows secondary particles on the surface of the sample which is triggered by covering of the atomic layer of tellurium or selenium. All the samples have shown semi-conducting behaviour throughout the temperature range. It is observed that Bi has been coordinated with 6 Se atoms in (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$ compound and it has huge Se vacancies. The observed electrical resistivity represents the noteworthy result of the grain boundaries on the electrical properties of the samples, which leads to the higher content of scattering centres in the composites. It is found that the differences in the electronegativity of In and Te, In and Se are lesser than Bi and Se, Bi and Te is the reason for the decrease in Seebeck coefficient in the compound containing 15% and 20% of Bi$_2$Te$_3$. 

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Table 2: Theoretical charge density ($n_{Th}$), mobility ($\mu_{Th}$), activation energy ($E_A$), and scattering factor ($\gamma_{Th}$) of (Bi$_{0.98}$In$_{0.02}$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ nanocomposites

| Sample | $n_{Th}$ (10$^25$ m$^{-3}$) | $\mu_{Th}$ (10$^{-3}$ m$^2$/Vs) | $\gamma_{Th}$ | $E_A$ (meV) |
|--------|-----------------|-----------------|----------|----------|
| Bi$_2$Te$_3$  | 9.25            | 2.7             | 59.83    | 57       |
| Bi$_2$Te$_3$.7Se$_0$.3  | 8.5             | 1.9             | 52.97    | 65       |
| (Bi$_{0.98}$In$_{0.02}$)$_2$Te$_{2.7}$Se$_0$.3  | 8.5             | 2.1             | 59.65    | 61       |
| (Bi$_{0.96}$In$_{0.04}$)$_2$Te$_{2.7}$Se$_0$.3  | 8.6             | 1.6             | 59.74    | 65       |

Table 3: Comparison of thermoelectric properties of other reported bismuth chalcogenide composites

| S. No | Composites                      | Electrical resistivity (Ωm) | Seebeck coefficient (µV/K) | Power factor (µW/mK$^2$) | Temperature (°C) |
|-------|---------------------------------|-----------------------------|---------------------------|---------------------------|------------------|
| 1     | Bi$_2$Te$_3$ nanocomposite      | $3 \times 10^{-5}$          | $-150$                    | 650                        | 160 [39]         |
| 2     | Bi$_2$Te$_3$.Bi$_2$Se$_3$       | $25 \times 10^{-6}$         | $-100$                    | 500                        | 449 [16]         |
| 3     | Bi$_2$Te$_3$.Bi$_2$Se$_3$       | $10 \times 10^{-6}$         | $-140$                    | 196                        | 450 [40]         |
| 4     | (Bi$_{1-y}$In$_y$)$_2$Se$_{2.7}$Te$_{0.3}$/Bi$_2$Te$_3$ | $30 \times 10^{-6}$         | $-110$                    | 450                        | 450              |

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Author contributions

GSH: methodology, writing—original draft, and formal analysis. ANP: supervision and validation. AR: writing, review, and editing. KG and DSU: data curation.

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Data availability

The thermoelectric data were generated at Centre for Clean Energy, Department of Physics, Manipal Institute of Technology derived data supporting the findings of this study are available from the corresponding author [ANP] on request.

Declarations

Competing interest All authors certify that they have no affiliations with or involvement in any organization or entity with any financial interest or non-financial interest in the subject matter or materials discussed in this manuscript.

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