

Reliable metal alloy contact for a $\text{Mg}_{3+\delta}\text{Bi}_{1.5}\text{Sb}_{0.5}$ thermoelectric device

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Table S1. Typical work functions of various metals, metal alloys, and TE materials.

	Work Function (eV)		Work Function (eV)
Ni	5.15	Sb	4.55~5.7
Fe	4.7	Bi	4.31
Al	4.3	Mg	3.66
Cr	4.5	Bi_2Te_3	5.4
Stainless steel	4.3~4.4	$\text{Bi}_{0.5}\text{Sb}_{1.5}\text{Te}_3$	4.5
NiFe (80:20 wt%)	4.8	PbTe	3.9
n-type $\text{Mg}_3\text{Sb}_{2-x}\text{Bi}_x$	3.85		

Table S2. Compositions of contact materials used in this study.

	wt %
NiFe	Ni/Fe = 80:20
Stainless steel	Fe/Cr/Ni/Mo = 67.5:17.0:13.0:2.5
NiCrFe	Ni/Cr/Fe = 72:14~18:12~16
NiCr	Ni/Cr = 80:20
Fe	>99%
Ni	>99%

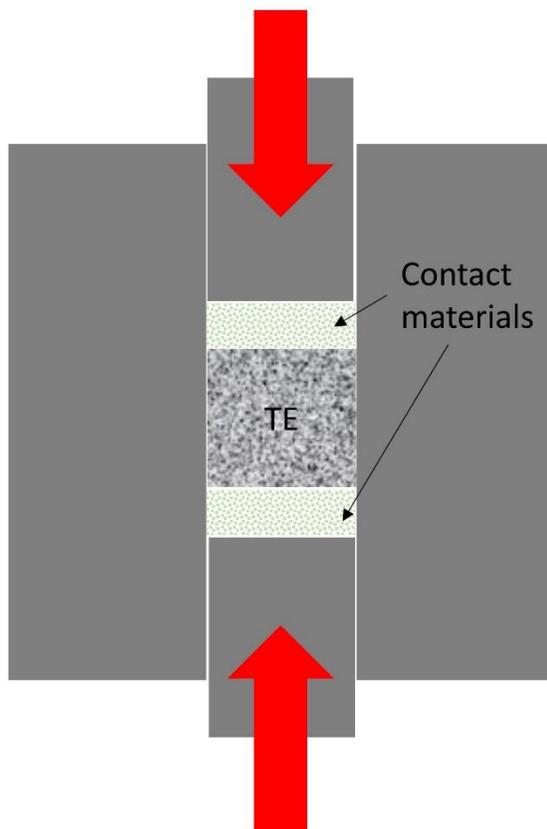


Figure S1. Schematic illustration of one-step hot-pressing to form a contact between a TE material and a metal or metal alloy.

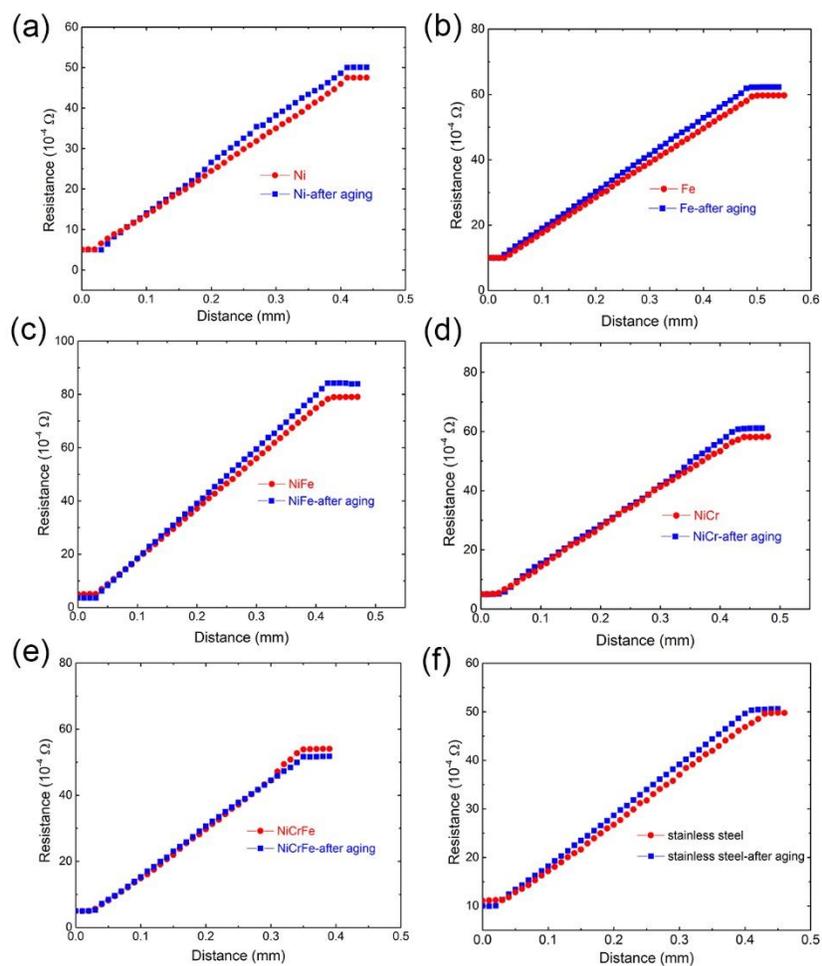


Figure S2. Comparison of measured contact resistivity curves before and after aging for $\sim 2,100$ h at 573 K for each as-prepared single TE leg sample.

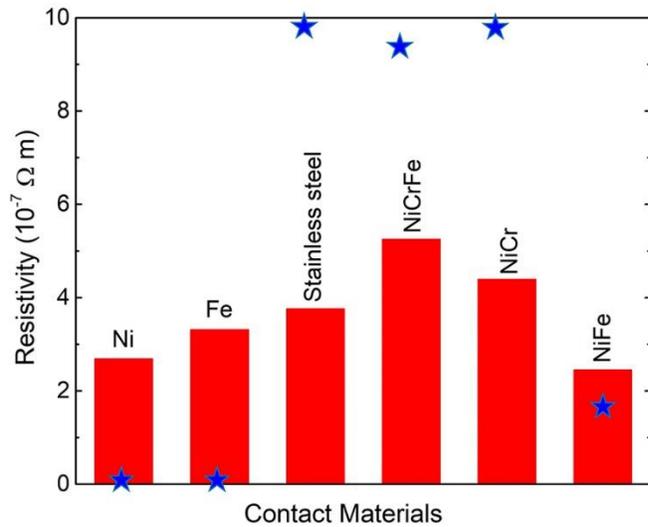


Figure S3. Resistivity of the metals and metal alloys used as contact materials in the single M/TE leg. The data with red pillars were extracted from their slopes in the measurement curve (Figure S2), and the data shown as blue stars were obtained through measurements on the commercial ULVAC ZEM-3 after hot-pressing following the procedure for preparing the single M/TE leg.

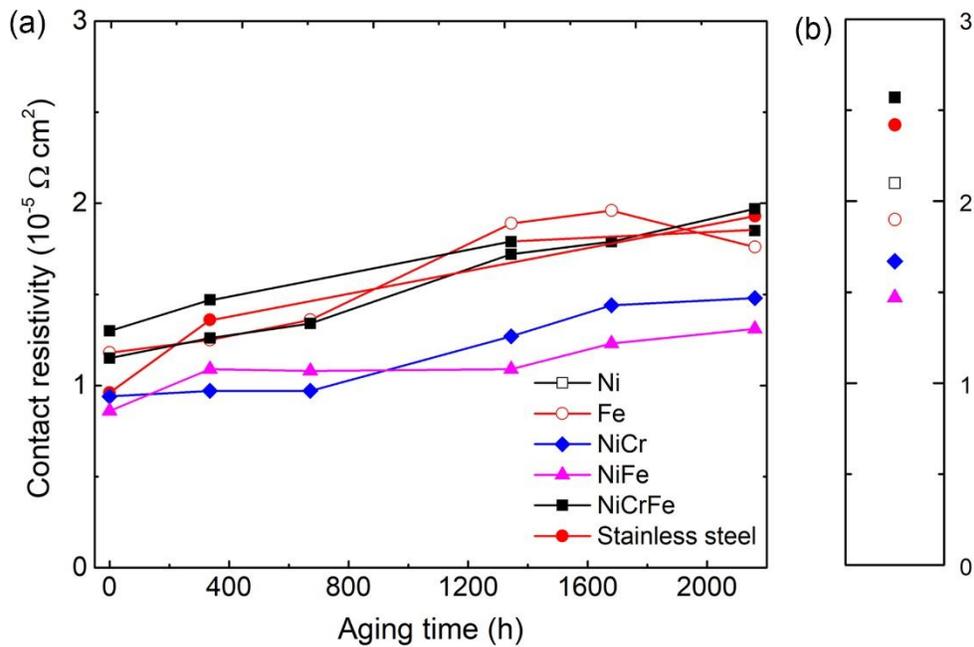


Figure S4. (a) Aging-time dependence of contact resistivity of single M/TE leg composed of n-type $\text{Mg}_{3+\delta}\text{Bi}_{1.5}\text{Sb}_{0.5}$ and different contact materials as specified. (b) Contact resistivity of single M/TE leg composed of n-type $\text{Mg}_{3+\delta}\text{Bi}_{1.5}\text{Sb}_{0.5}$ and different contact materials as specified after thermal failure testing. For clearer readability, error of 1.5%~2% is not shown.

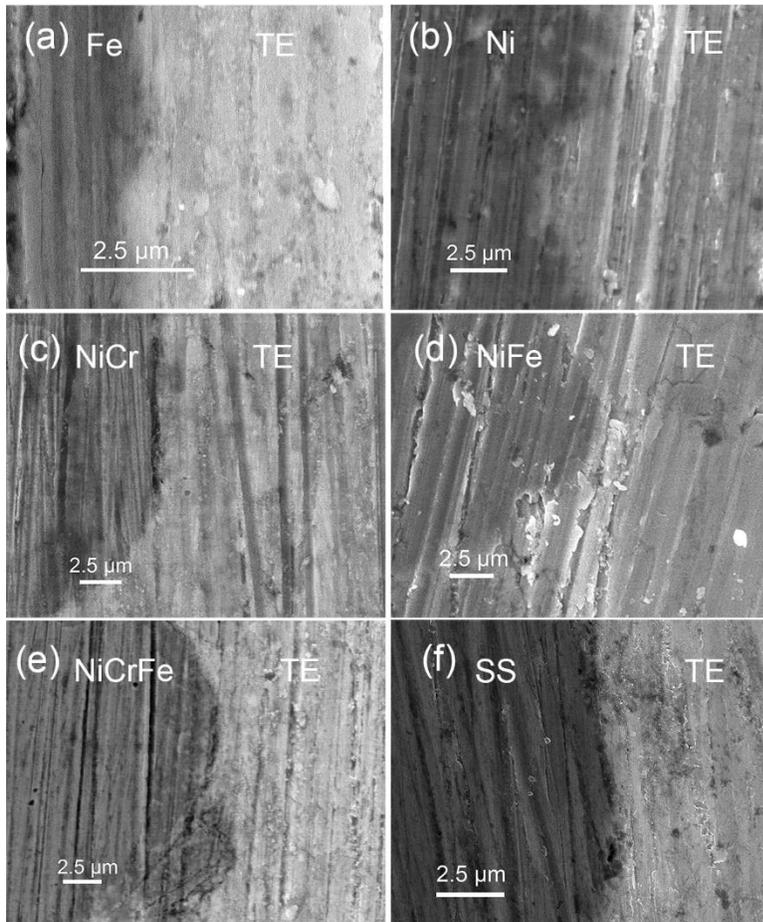


Figure S5. Microstructural morphology of the as-prepared contact interfaces in the single M/TE leg composed of $\text{Mg}_{3+\delta}\text{Bi}_{1.5}\text{Sb}_{1.5}$ and (a) Fe, (b) Ni, (c) NiCr, (d) NiFe, (e) NiCrFe, and (f) stainless steel (SS).

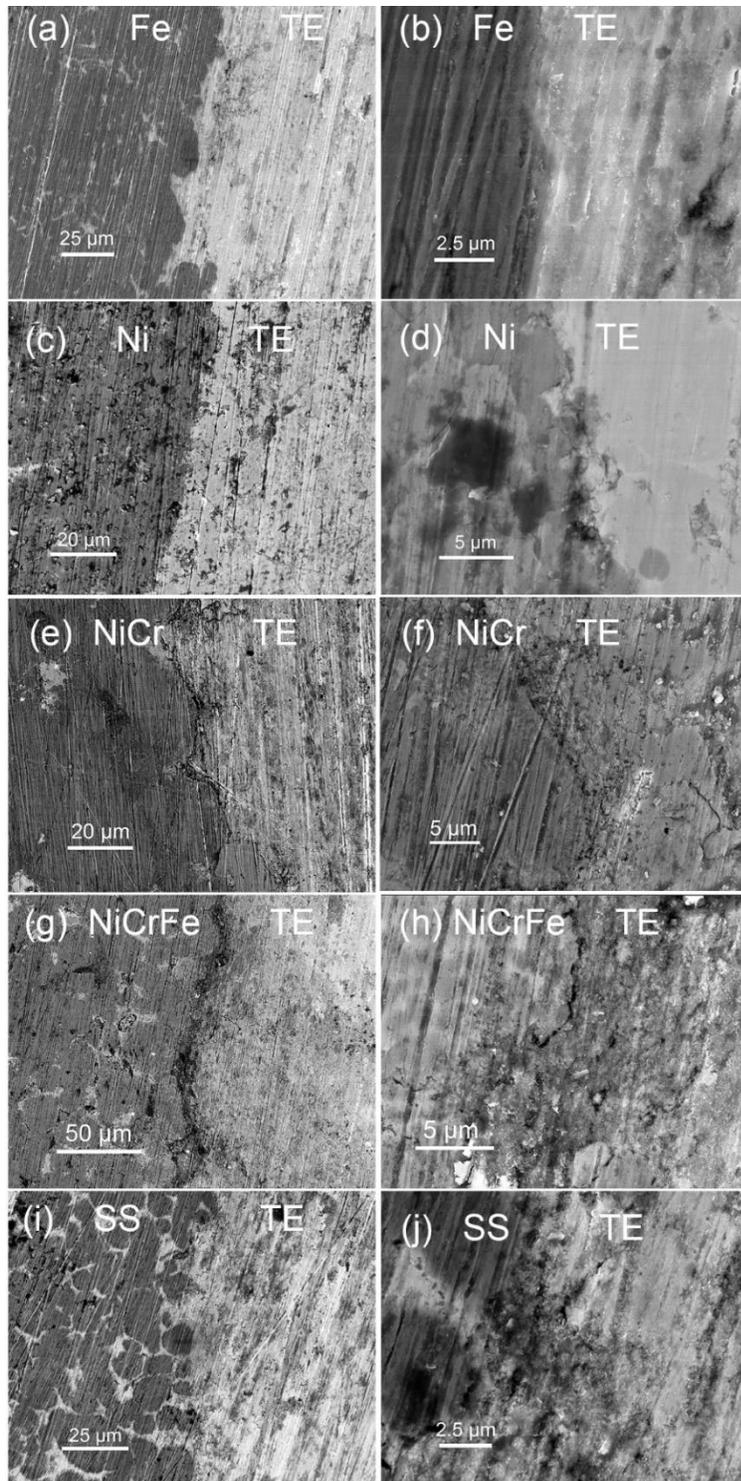


Figure S6. Microstructural morphology of the contact interfaces in the single M/TE leg composed of Mg_{3+δ}Bi_{1.5}Sb_{1.5} and (a,b) Fe, (c,d) Ni, (e,f) NiCr, (g,h) NiCrFe, and (i,j) stainless steel (SS) after aging and thermal cycling and quenching test.

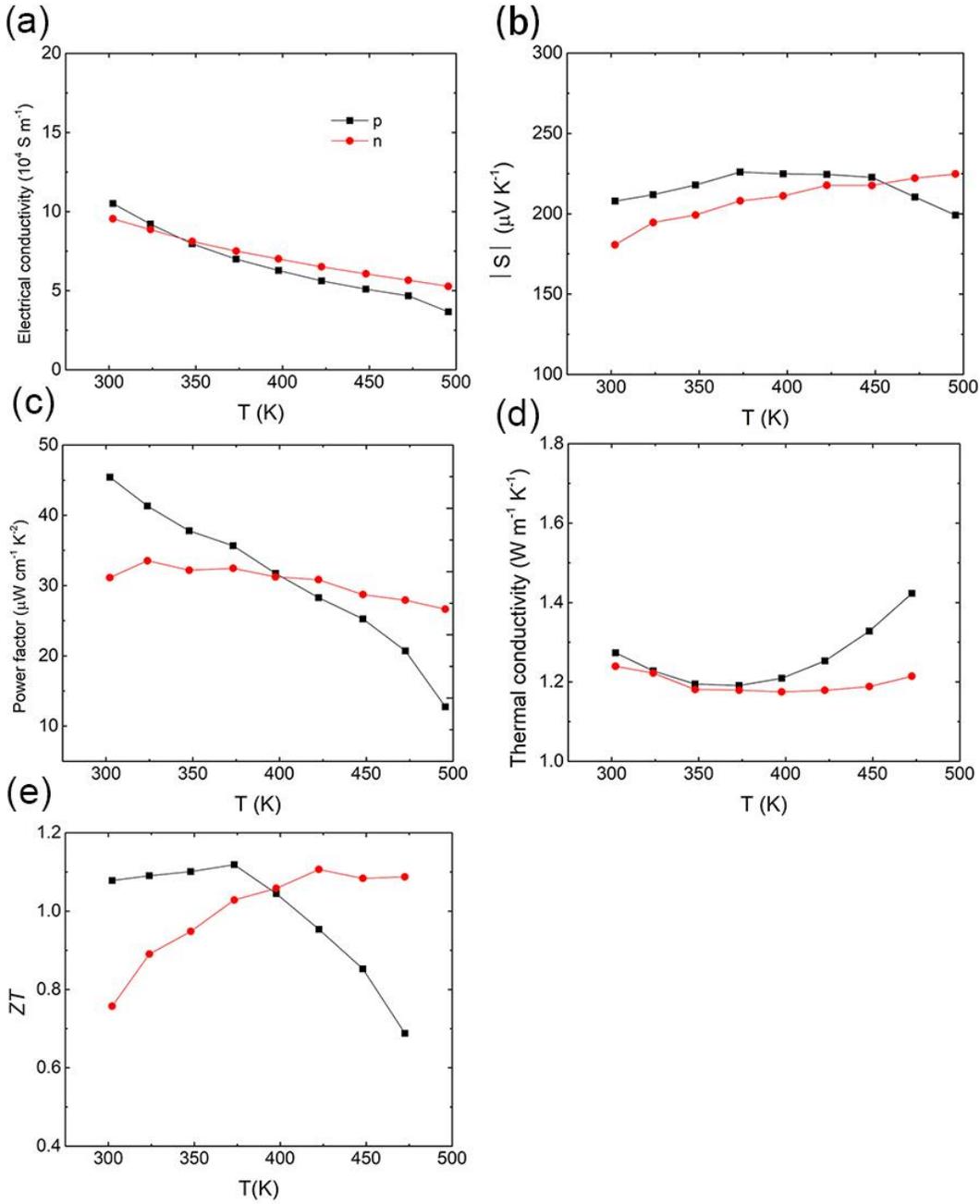


Figure S7. Thermoelectric properties of n-type $\text{Mg}_{3+\delta}\text{Bi}_{1.5}\text{Sb}_{0.5}$ and p-type $\text{Bi}_{0.4}\text{Sb}_{1.6}\text{Te}_3$.

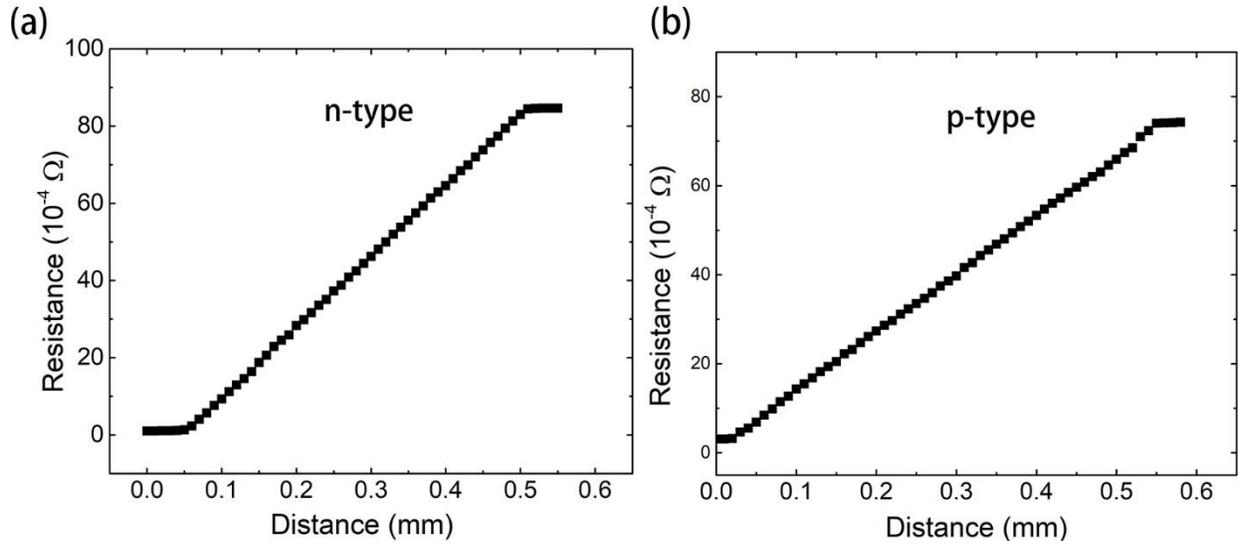


Figure S8. The measured contact resistance of (a) NiFe/Mg_{3+δ}Bi_{1.5}Sb_{0.5}/NiFe and (b) Fe/Bi_{0.4}Sb_{1.6}Te₃/Fe. The n-type NiFe/Mg_{3+δ}Bi_{1.5}Sb_{0.5}/NiFe exhibits the contact resistance of $7.6 \times 10^{-6} \Omega \text{ cm}^{-2}$ and p-type Fe/Bi_{0.4}Sb_{1.6}Te₃/Fe has the contact resistance of $1.25 \times 10^{-5} \Omega \text{ cm}^{-2}$.