Supporting Information

Simultaneous optimization of thermoelectric and mechanical properties in p-type NbFeSb via entropy engineering

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1. Supplemental Equations

For an n-element alloy with a disordered ideal solid solution structure, its configurational entropy can be expressed by **Eq. S1:**[1,2]

$$\Delta S = -R\sum_{i=1}^{n} x_i ln x_i \tag{S1}$$

where R and x_i represent the gas constant and the mole fraction of the i-th element, respectively.

Based on the single parabolic band (SPB) model, the Lorentz number (L) can be approximated by **Eq. S2:**[3]

$$L = 1.5 + exp(\frac{-|S|}{116}) \tag{S2}$$

Where S represents the Seebeck coefficient, L ranges between 1.45 and 2.45×10^{-8} W Ω K^{-2}, and it is related to the scattering factor and Fermi level.

To quantitatively assess the point-defect scattering strength, we calculated the disorder scattering parameters using **Eqs. S3, S4, and S5:**[4-8]

$$\Gamma_m = \frac{1}{3}\left(\frac{M_x}{M_{ave}}\right)^2 \sum f_i \left(1 - \frac{M_i}{M_x}\right)^2 \tag{S3}$$

$$\Gamma_s = \frac{1}{3}\left(\frac{M_x}{M_{ave}}\right)^2 \sum \varepsilon f_i \left(1 - \frac{r_i}{r_x}\right)^2 \tag{S4}$$

$$\Gamma_{total} = \Gamma_m + \Gamma_s \tag{S5}$$

where M_x, M_{ave}, and M_i denote the average atomic weight on a certain element site, that of all constituent elements, and the atomic weight of a single element, respectively. Similarly, r_i and r_x correspond to the atomic radius of a single element and the average radius on a certain element site, respectively. The subscript i indicates the number of substitutional elements at a certain element site. The parameter ε is a phenomenological adjustable parameter, typically ranging from 10 to 100.[6-8]

2. Supplemental Figures

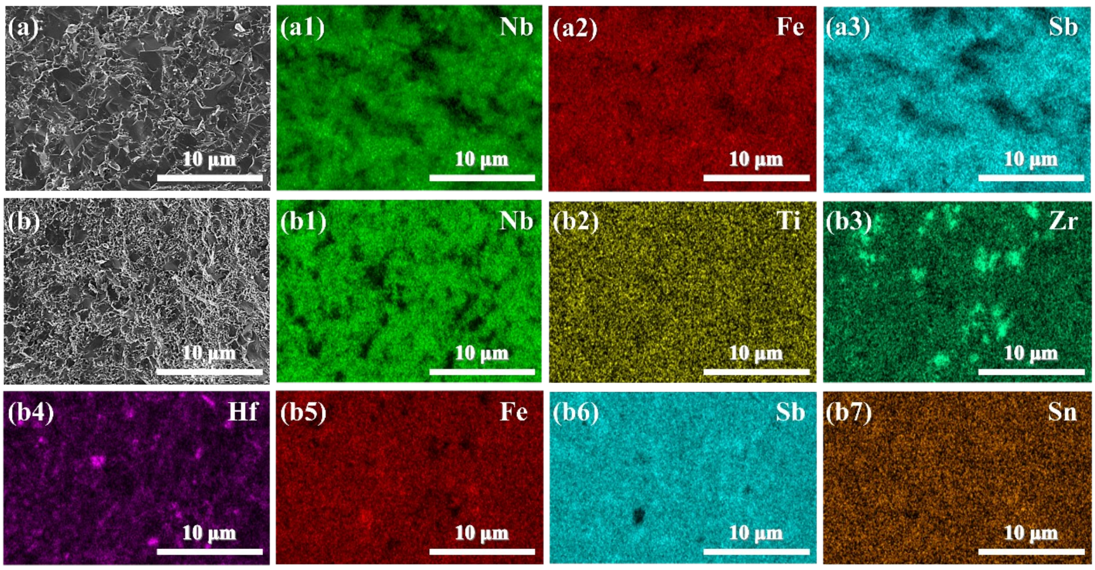

Fig. S1. Elemental mappings of the fracture surfaces for (a) NbFeSb and (b) $Nb_{0.82}M_{0.18}FeSb_{0.98}Sn_{0.02}$.

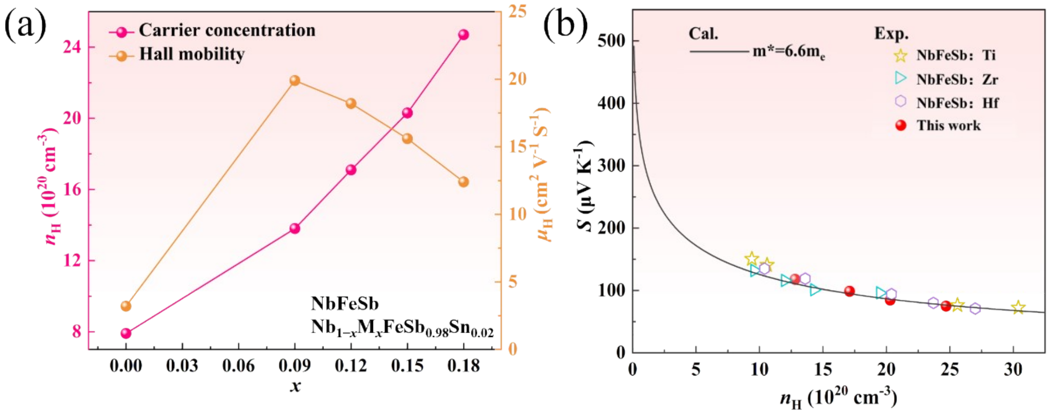

Fig. S2. (a) Room temperature carrier concentration (n_H) and Hall mobility (μ_H). (b) Room temperature Pisarenko plot with $m^* = 6.6\ m_e$, where m_e is the electron effective mass.

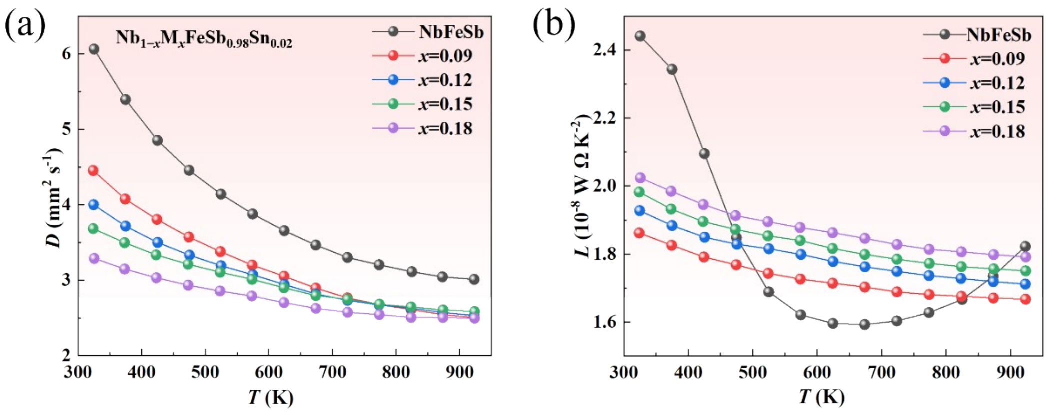

Fig. S3. Temperature dependence of thermal transport parameters for NbFeSb and $Nb_{1-x}M_xFeSb_{0.98}Sn_{0.02}$ (x = 0.09, 0.12, 0.15, and 0.18): (a) Thermal diffusivity (D) and (b) Lorenz number (L).

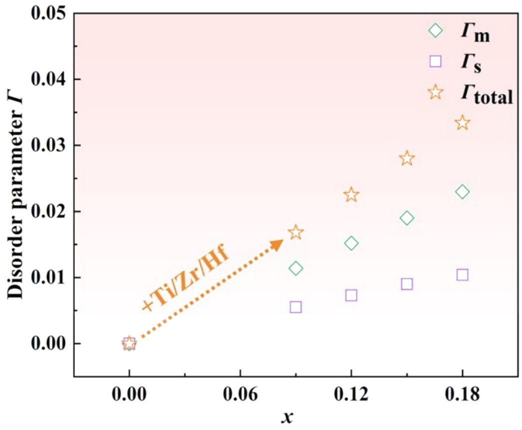

Fig. S4. Calculated disorder parameters of Γ_{m}, Γ_{s}, and Γ_{total} of NbFeSb and $Nb_{1-x}M_xFeSb_{0.98}Sn_{0.02}$ (x=0.09, 0.12, 0.15, and 0.18).

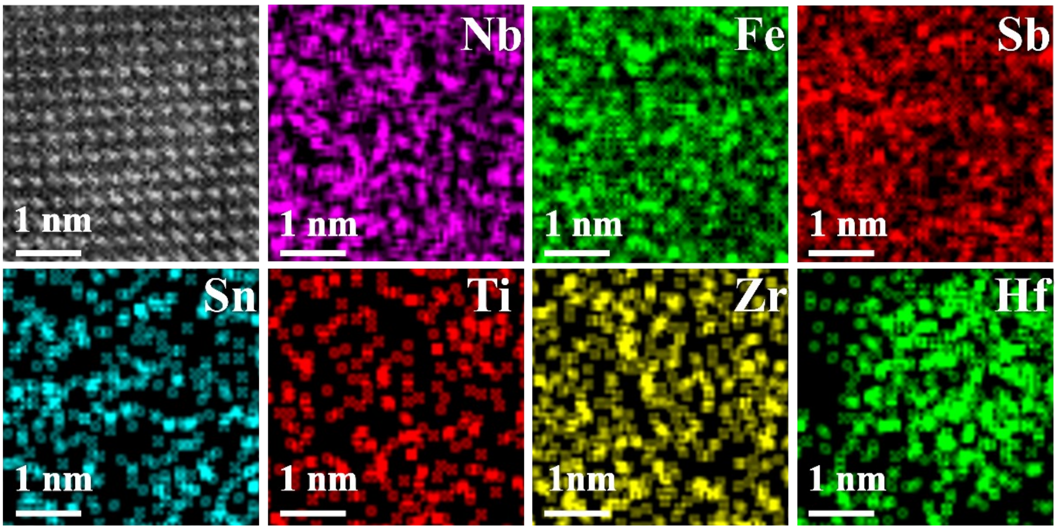

Fig. S5. Elemental mappings of Hf-enriched nanodomains.

Reference

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