Enhancement of thermoelectric properties of Zintl phase SrMg$_2$Bi$_2$

by Na-doping

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The single parabolic band (SPB) model:
The Seebeck coefficient:

$$ S(\eta) = \frac{k_B}{e} \left[ \frac{(r + 5/2)F(r + 3/2)(\eta)}{(r + 3/2)F(r + 1/2)(\eta)} - \eta \right] $$

The Hall carrier concentration:

$$ n_H = \frac{1}{eR_H} \frac{(2m^*k_BT)^{3/2}(r + 3/2)^2F(r + 1/2)(\eta)}{3\pi^2h^3 (2r + 3/2)F(2r + 1/2)(\eta)} $$

The Hall mobility:

$$ \mu_H = \left[ \frac{\pi \hbar^4}{\sqrt{2(k_BT)^3/m^*}} \right] \frac{m^*E_{def}^2}{m_1^*} \frac{C_1}{C_1} \left[ \frac{(2r + 3/2)F(2r + 1/2)(\eta)}{(r + 3/2)F(r + 1/2)(\eta)} \right] $$

Lorenz Factor:

$$ L = \frac{k_B}{e} \left[ \frac{(r + 7/2)F(r + 5/2)(\eta)}{(r + 3/2)F(r + 3/2)(\eta)} \right] \left[ \frac{(r + 5/2)F(r + 3/2)(\eta)}{(r + 3/2)F(r + 1/2)(\eta)} \right] $$

Where $F_j(\eta) = \int_0^\infty \frac{\xi f(\xi - \eta)}{1 + \exp(\xi - \eta)} d\xi$ is the Fermi integral, $m^* = \frac{k_B^2}{2e^2} \left[ \frac{n \times r_H}{4mF_{1/2}(\eta)} \right]^{2/3}$ is the density-of-states effective mass.

In the above equations, $k_B$ is the Boltzmann constant, $h$ is the reduced Plank constant, $C_1$ is the elastic constant for longitudinal vibrations, $E_{def}$ is the deformation potential coefficient characterizing the strength of carriers scattered by acoustic phonons, $m^*_I$ is the inertial effective mass, $m^*_b$ is the band effective mass and $\eta$ is the reduced Fermi level. When charge carriers are scattered by the acoustic phonons, $r=-1/2$. 

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Figure S1 XRD patterns for SrMg₂Bi₂ kept in air for 0 and 1 day.