Supporting Information

Silicon-based thermoelectrics made from a boron-doped silicon dioxide nanocomposite

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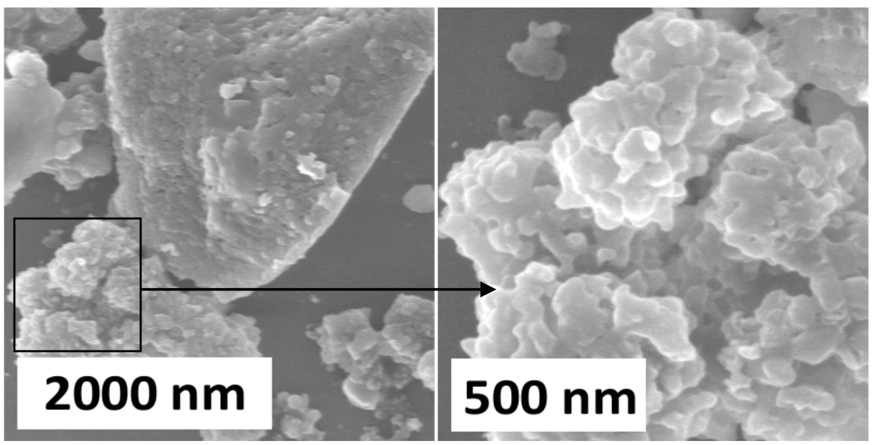

Figure S1. SEM image of a representative region of the powder mixture obtained after the magnesiothermic reduction.

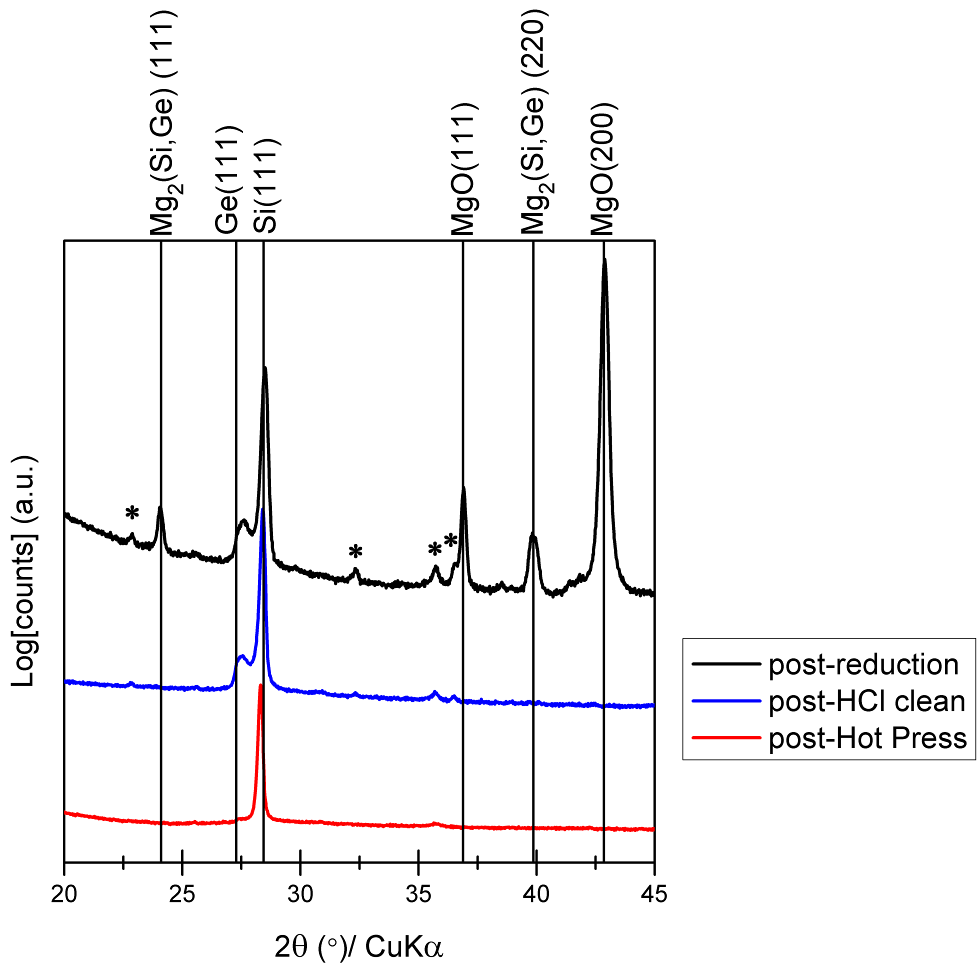

Figure S2. X-ray diffraction patterns of the SiGe composite after the magnesiothermic reduction, the SiGe composite after the magnesia & silicide-germanide impurity phases are removed with hydrochloric acid, and the $Si_{80}Ge_{20}$ alloy after being hot pressed. The impurity phase marked with the asterisks is assumed to be a magnesium germanium oxide phase that forms due to the high local temperature during the magnesiothermic reduction. This magnesium germanium oxide phase is assumed to transform to magnesium fluoride during the hydrofluoric acid clean which precedes the hot pressing step.

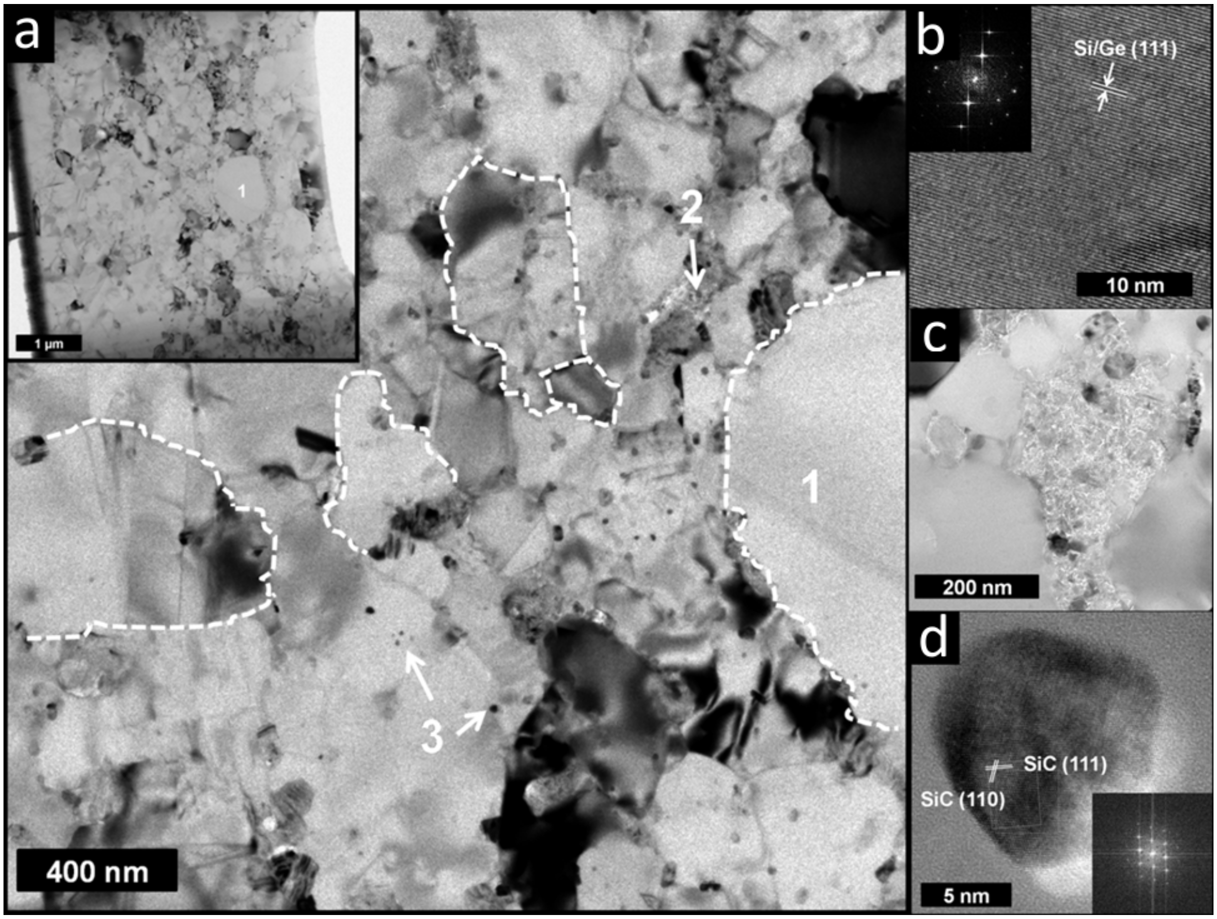

Figure S3. (a) TEM image of lamella prepared from a $Si_{90}Ge_{10}$ pellet by focused ion beam etching with an inset image at lower magnification and (b) HR-TEM image of the large SiGe grain marked "1", (c) a magnified image of region "2" which contains magnesium and fluorine, and (d) an HR-TEM image of the SiC nanoparticle that is embedded in the SiGe grain shown in region "3". Both of the HR-TEM images include a Fast Fourier Transform of the image as an inset.

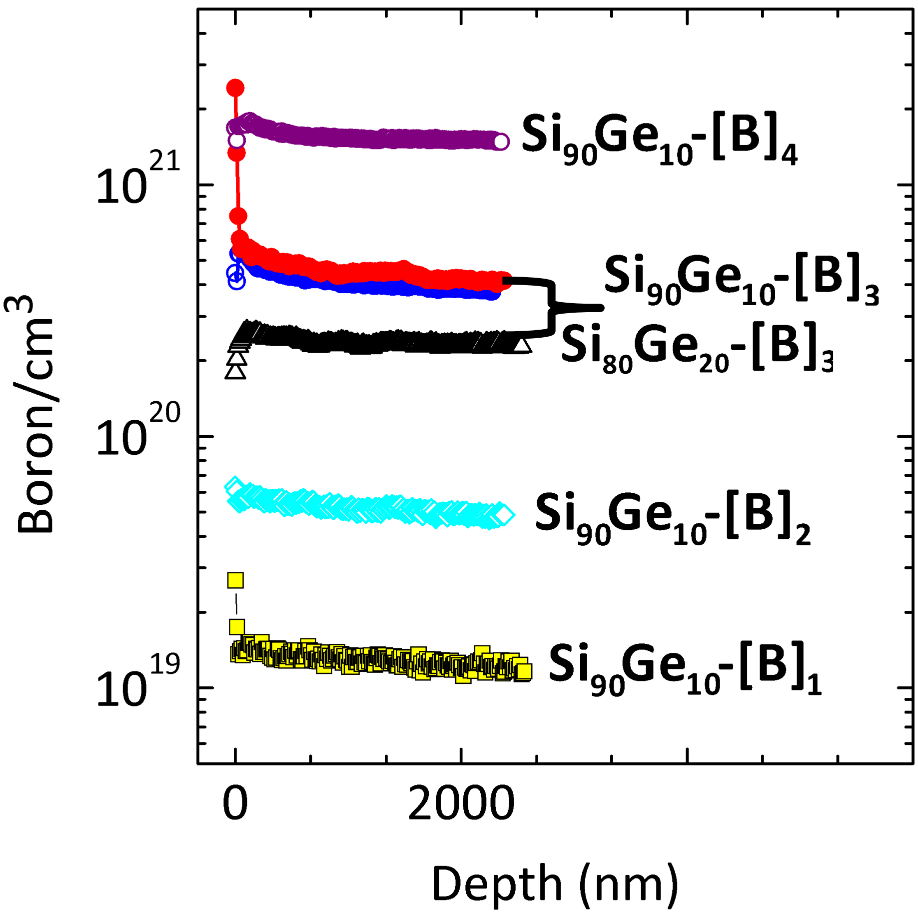

Figure S4. Secondary ion mass spectrometry depth profiles of boron in the $Si_{1-x}Ge_x$ nanocomposites that were prepared with varying boron content. Two $Si_{90}Ge_{10}$ w/ $[B]_3$ samples were measured in order to check doping reproducibility.

Effective medium model for electrical conductivity:

References:
Bergman, D.J.; Levy, O. *J. Appl. Phys.* **1991**, 70, 6821.
Landauer, R., **Electrical Transport and Optical Properties of Inhomogeneous Media**, American Institute of Physics, New York, **1978**, pp. 2–45
Lee, H.; Vashaee, D.; Wang, D.Z.; Dresselhaus, M.S.; Ren, Z.F.; Chen, G. *J. Appl. Phys.* **2010**, *107*, 094308.

$$\sigma_{effective} = \sigma_{host}\frac{2-3\Phi}{2} \qquad \Phi \equiv \frac{pore\ volume}{total\ volume}$$

$$\Phi_{Si_{90}Ge_{10}-[B]_2} \approx 0.04$$

$$\Phi_{Si_{90}Ge_{10}-[B]_4} \approx 0.02$$

$$\frac{\sigma_{effective,\ Si_{90}Ge_{10}-[B]_2}}{\sigma_{effective,\ Si_{90}Ge_{10}-[B]_4}} = \frac{\sigma_{host,\ Si_{90}Ge_{10}-[B]_2}}{\sigma_{host,\ Si_{90}Ge_{10}-[B]_4}} \times 0.969$$

$$\sigma_{effective,\ Si_{90}Ge_{10}-[B]_2}(T = 300\ K) \approx 2.2 \times 10^4\ S/m$$

$$\sigma_{effective,\ Si_{90}Ge_{10}-[B]_4}(T = 300\ K) \approx 6.0 \times 10^4\ S/m$$

$$\frac{2.2 \times 10^4\ S/m}{6 \times 10^4\ S/m} = 0.367 \approx \frac{\sigma_{host,\ Si_{90}Ge_{10}-[B]_2}}{\sigma_{host,\ Si_{90}Ge_{10}-[B]_4}} \times 0.969$$

$$\boxed{\frac{\sigma_{host,\ Si_{90}Ge_{10}-[B]_2}}{\sigma_{host,\ Si_{90}Ge_{10}-[B]_4}} \approx 0.378}$$

$\therefore$ The electrical conductivity of the $Si_{90}Ge_{10} - [B]_2$ host matrix (i.e. the conducting phase) is about 38% of the electrical conductivity of the $Si_{90}Ge_{10} - [B]_4$ host matrix at room temperature. Variation in the thermoelectric properties of our samples is not due to a density/porosity effect. The modulation of the electronic properties was achieved by tuning the carrier density.

Consider our results from the room temperature Hall effect measurements:

$$\boxed{\frac{\sigma_{effective,\ Si_{90}Ge_{10}-[B]_2}}{\sigma_{effective,\ Si_{90}Ge_{10}-[B]_4}} = \frac{p_{Si_{90}Ge_{10}-[B]_2}\ \mu_{Si_{90}Ge_{10}-[B]_2}}{p_{Si_{90}Ge_{10}-[B]_4}\ \mu_{Si_{90}Ge_{10}-[B]_4}} = 0.386}$$

The discrepancy between the effective electrical conductivities and host electrical conductivities of the two samples with the most different densities (94.7% vs. 98.0%) is due to different carrier densities in the conducting SiGe host matrix. The ~2% discrepancy between effective and host electrical conductivities may be attibuted to a difference in densities or sample quality.