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Local structure in ball-milled and Ni substituted $Nd_yFe_{4-x}Ni_xSb_{12}$[1] FRANK BRIDGES, FELIPE RIVAS, MARKUS SHORT, TREVOR KEIBER, Physics Dept. UC Santa Cruz, Santa Cruz CA 95064., PETER ROGL, Institute of Physical Chemistry, University of Vienna, Austria — We report EXAFS measurements at the Nd L_{III}, Fe, and Sb K edges in $Nd_yFe_{4-x}Ni_xSb_{12}$. Recent measurements show that ball-milled $Nd_yFe_4Sb_{12}$, with $\sim$ 150 nm size particles, significantly improved the figure of merit (ZT) by 22 %, compared to material with 10 μm sized particles. Since ball milling can produce significant disorder and even amorphization, which would lower the thermal conductivity, we compared the local structure for ball-milled and hand ground samples. We find that the average local structure is essentially unchanged by ball milling; the reduced particle size reduces the phonon mean free path, thereby reducing the thermal conductivity. When Ni is substituted on the Fe site, together with a decreased concentration of Nd, we find the largest changes in disorder are about the Nd atoms; there is little disorder of the first few neighbors about the Fe site. Further the local distortions are not uniform; the lattice constant decreases with Ni concentration, but the Nd-Sb bond length slightly expands while the Sb-Sb contracts more than expected. Some consequences are discussed.

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