Modeling thermoelectric transport coefficients of multicomponent solid solutions

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We describe two approaches to compute the Seebeck coefficient (or thermopower) and the electrical resistivity of the Nickel-based alloys containing Cr, Si and small amounts of Al, Co, Fe, Mn, Mg, Cu, P and C.

We first benchmark the applicability of the Gorter-Nordheim law to describe the experimental measurements of those multicomponent alloys. We find a good agreement between the calculated and the measured values of the Seebeck coefficient with a deviation of less than 2.5 %.

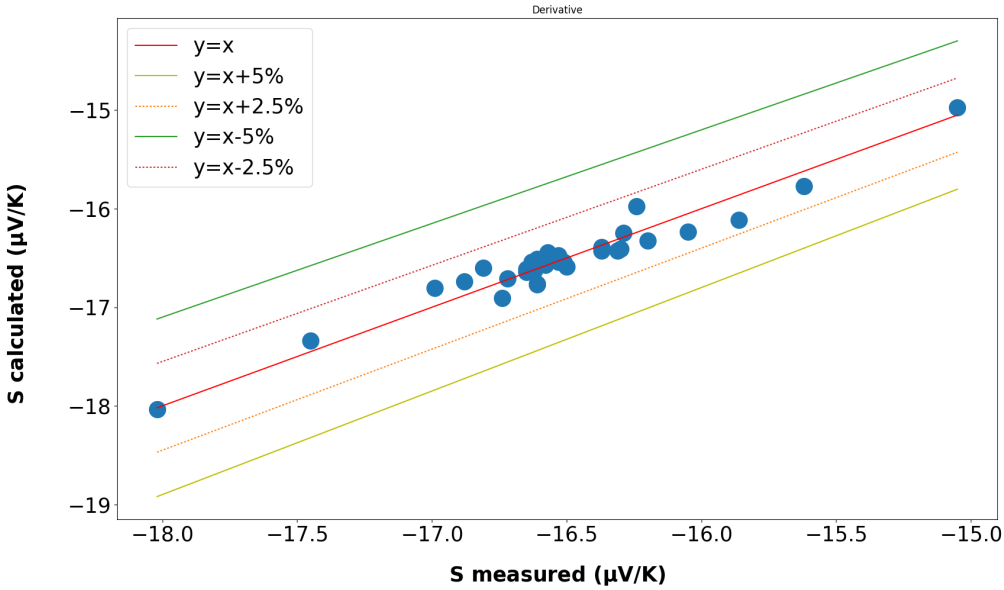

Figure 1: Calculated Seebeck vs. measured Seebeck

Then, we present some preliminary results of the thermopower and the electrical resistivity directly calculated with an *ab initio* method, using the Density Functional Theory (DFT) within the Local Density Approximation (LDA), called the Korringa-Kohn-Rostoker Green's function method in the Coherent Potential Approximation (KKR-CPA)[1].

[1] Swihart, J. C., Butler, W. H., Stocks, G. M., Nicholson, D. M. and Ward, R. C. First-Principles Calculation of the Residual Electrical Resistivity of Random Alloys. Phys. Rev. Lett. 57, 1181–1184 (1986)