Title: 3G_TDB software for automated generation of TDB files using modified segmented regression (MSR) model: pure Mn as an example

Abstract:

There has been a rising interest in novel modelling approaches that can describe thermo-physical properties more accurately and for wider temperature ranges. New applications such as thermoelectric materials [1] require the re-assessment of related thermodynamic systems down to temperatures lower than the room temperature. With the introduction of the so-called 3rd generation CALPHAD databases, it became possible use the newly proposed physically based models to get more accurate and reliable descriptions. A novel and robust modelling approach proposed by Roslyakova et al. [2] used a combination of Debye and a segmented function to achieve a better agreement with experimental data for temperatures down to 0 K. This model was later modified [3] to expand the temperature range above the melting point without the addition of any new fitting parameters. The results for pure Mn compared with other available thermodynamic models [4-6] can be seen in Figure 1. Be that as it may, there is an increasing supply-demand gap for such re-assessments that require a more robust and genuine solution to make these models more available to the CALPHAD community members. The 3G_TDB software has been developed to systematically analyse different types of available experimental or DFT data and fit them accordingly using the MSR model, enabling the user to compare the validity of the obtained results using statistical goodness of fit criteria, and to compare the results obtained by one set of data versus another. It would also allow the user to the TDB file that can be further used in available computational thermodynamic software. This presentation will show the progress of the 3G_TDB when used to re-assess the pure Mn unary system.

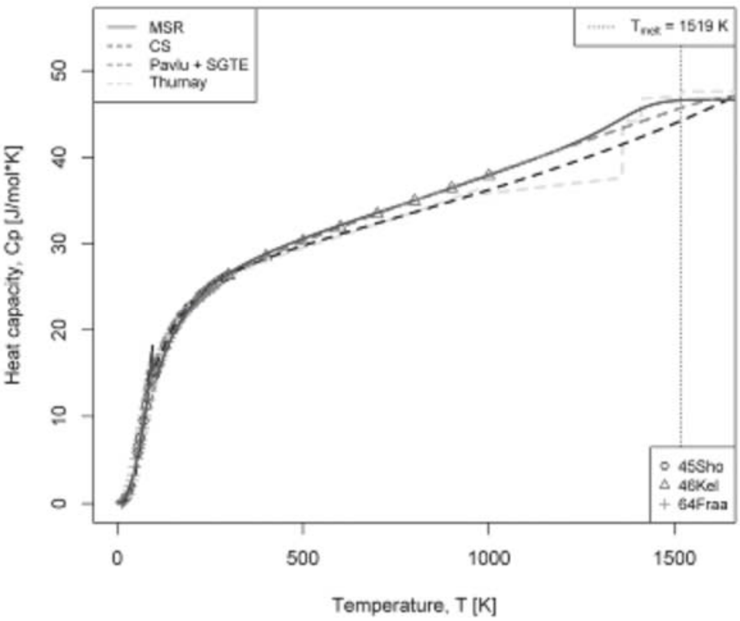

Fig. 1: Comparison of the heat capacity of the modified SR model and other assessments for pure Mn

References:
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