

The third generation CALPHAD databases: segmented model for pure Al, Cr, Ge, Ir, Mo, Nb, Re, W, Fe, Ni and Ta

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A novel physically-based model for the description of the thermodynamic properties of the pure elements down to 0K has been proposed. The proposed model based on the fitting of the heat capacity data and considered physical several contributions (e.g. electronic, vibrational, etc.) [1]. Since these contributions appear in different temperature ranges and can be described by different functions, the segmented regression methodology [2] has been applied for the contraction of the physically-based mathematical model for the heat capacity of pure elements. The thermodynamic properties of pure Cr, Al and Fe have been modelled by the proposed segmented model and the obtained results have been presented during annual CALPHAD 2014 meeting [3]. Currently, we extended the proposed segmented approach for the description of the heat capacity data [4] of such pure elements as Ir, Mo, Nb, Re, W, Ni and Ta. The obtained results show a good agreement between experimental data for the entire temperature range down to 0K. Moreover we validate the consistency of underlying fitting results, by calculating other physical properties of interest, such as the enthalpy and the entropy and compared them to the available experimental data. The obtained results fit well the data on the S_{298} and the enthalpy.

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[3] I. Roslyakova, B. Sundman, H. Dette, Modeling of thermo-physic properties for pure elements using segmented regression methodology. CALPHAD XLIII, Changsha, China, 2014.

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