THE 3rd-GENERATION CALPHAD MODEL FOR SOLID AND LIQUID Ge AND THE BINARY Ge-Si SYSTEM

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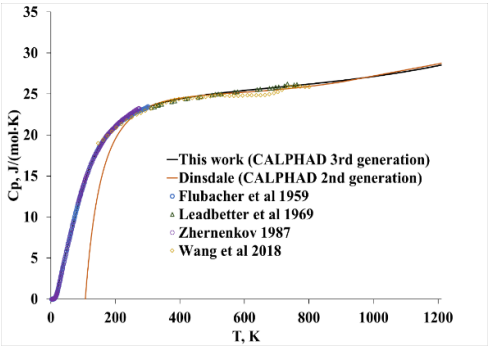
Germanium and silicon-germanium alloys serve as key materials in several advanced in technologies such as microelectronics, photonics and optoelectronic as well as solar cell elements especially in space technology. In response to improvements in experimental measurement and analysis methods and computational capabilities, it has become important to make new databases on the thermodynamic properties of pure germanium, silicon, and their alloys.

Third-generation CALPHAD models offer a superior alternative to the previously widespread polynomial expressions in existing databases. Based on modern thermodynamic data, these models provide an accurate description of thermodynamic function from absolute zero (0 K) up to temperatures above the melting point.

Critical review of available data for solid and liquid phases of Ge and Ge-Si were performed.

The stable crystalline modification with the diamond cubic structure type was described with two characteristic temperatures and two polynomial terms. The results of heat capacity modelling are shown in the figure below.



Experimental data and and calculation results of heat capacity of pure crystalline germanium in the temperature range 0-T_{fus}

A two-state model has been proposed to definition the liquid phase of Ge with two characteristic Einstein temperatures.

Combining thermodynamic models, including a liquid phase model with two characteristic temperatures developed for pure silicon and germanium, allows to describe the interaction in a binary system and obtain a more accurate prediction of the properties of the binary system in a supercooled liquid state.

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