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the thermodynamics of the formation of (p, c, and m)-rich phases in the laves phase fe-c alloy is studied by means of the thermodynamic model proposed by guyer and rabe for the decomposition of the iron-carbon compound fe2c. the model is used to predict the formation of (mg, c, and p)-rich phases in a fe-8 wt.% c-8 wt.% mg-1 wt.% p alloy. the experimental data of the phase compositions obtained by x-ray diffraction and electron backscatter diffraction are shown to be well reproduced by the model. the solid solution formation energies of mg and c in the solid solution fe-c are shown to be positive due to the large repulsive mg-c and fe-c interactions. the theoretical results are in qualitative agreement with the experimental data of the phase compositions obtained by the melt-spinning technique. the model allows the determination of the thermodynamic parameters of formation of the (fe, c, and p) and (fe, c, p, and mg) phases as well as of the (p, c, and mg)-rich phases in the alloy and its decomposition as function of the chemical composition and temperature. the decomposition model shows that these phases are thermodynamically stable in the alloy. pep tos is a toolbox for automated and interactive analysis of molecular materials. it contains the ability to perform molecular simulation of engineered materials (msme) to analyze the energetics, properties, and kinetics of materials and microstructures. the pep tos package is implemented using the c# programming language and is accessed through a graphical user interface (gui) and a command-line interface (cli). the gui is developed using c# xaml, and the cli is developed using c# console applications. these tools are implemented on windows, mac os x, and linux.

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gem-selektor v.3 is a software tool for interactive thermodynamic modeling and analysis of chemical systems. the package consists of various modules (tools) including a chemical thermodynamics database and code for numerical implementation of thermodynamic equations, graphical user interface (gui) for system setup, data analysis, and interpretation, and computational modules for gem-selektor. it is available for windows and linux, with no need for a java virtual machine (jvm). the gem-selektor package includes an underlying c code, which provides the numerical subroutines for the thermodynamic equations, while the gui and the other modules are written in the python scripting language. gem-selektor is a code package for interactive thermodynamic modeling of heterogeneous aqueous and non-aqueous chemical systems, especially those involving metastability and dispersity of mineral phases, solid solution - aqueous solution equilbria, and adsorption/ion exchange. includes a built-in psi-nagra chemical thermodynamic database 12/07 in both thermochemical and reaction formats, and an advanced multi-widget gui (graphical user interface) with a context-sensitive help system. enhanced with the cemdata thermodynamic database, gem-selektor is widely used in the cement-chemistry community since 2007, where it is promoted by prof. barbara lothenbach (empa) and her colleagues, who also maintain and provide the cemdata tdb. professor bhattacharjee is also known for his inspiring lectures to undergraduate students. he has given a series of lectures on thermodynamics at st. xavier's college, kolkata. he also lectures on thermodynamics at the indian institute of technology, delhi and is actively involved with the national council of teacher education, new delhi. professor bhattacharjee also consults and lectures on thermodynamics for the national science academy. he has given lectures at many institutions and is a frequent contributor to the international journal of heat transfer. 5ec8ef588b

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