

MULTIPHASE SEMI-EMPIRICAL WIDE-RANGE EQUATION OF STATE OF IRON

I. N. Arapov, A. A. Kayakin, A. S. Danilov, D. G. Gordeev

FSUE «RFNC – VNIIEF», Sarov, Russia

The report describes a model that enables the development of multiphase equations of state of different materials by “cross-linking” individual (local) equations of state of their phases. The cross-linking can be done both in the equilibrium approximation and taking into account interfacial kinetics when switching from one phase of the solid to another.

The effectiveness of the model is tested by the case of developing an equation of state of iron, since this substance is well studied, including in the range of phase transitions in the solid. We developed two local equations of state to describe the thermodynamic properties of iron. The first describes the α -phase of the solid, and the second, the ε -phase of the solid, liquid and vapor phases. The cross-linked phases are described using the ROSA-MFI model [1, 2]. We show that the use of the developed multiphase equation of state improves the accuracy of describing experimental data in the range of the α - ε phase transition. The figures presented in the report provide a comparison of the calculations using the developed EOS with experimental data and calculations by other models.

References

1. **Arapov, I. N.** Semi-empirical wide-range equation of the state of copper in the form of the ROSA-MFI model [Text] / I. N. Arapov, A. A. Kayakin, A. S. Danilov, D. G. Gordeev, L. F. Gudarenko // Sat. tez. doc. inter. conf. “XVI Zababakhinsky scientific readings”. – 2023. – P. 147.
 2. **Danilov, A. S.** Algorithms and features of software implementation in the URS-OF software package of the ROSA-MFI semi-empirical model of wide-range equations of state [Text] / A. S. Danilov, D. G. Gordeev, O. N. Shumilina, I. N. Arapov // VANT. Ser. “Mathematical modeling of physical processes”. – 2024. – Iss. 1. – P. 64–77.
-