The database TEFIS for thermophysical properties of substances

E.S. Ivanchenko, N.N. Kalitkin, I.A. Kozlitin, L.V. Kyzmina, I.A. Panin
kalitkin@imamod.ru, ioannkozlitin@gmail.com
Institute for mathematical modeling of RAS, Moscow

The database TEFIS has been created during the last 50 years. It is destined for calculating different thermophysical properties of substances under extreme conditions. The last 5 years we revised this database. The new models permit to improve physical and mathematical accuracy of all results. Moreover the new programming codes were composed. They were so effective that now the database uses personal computers.

TEFIS includes the next physical models.

1. Plasma microfield lies in the base of models of optical and thermodynamical properties in TEFIS. Our original microfield model is called Quasi-Independent Particles model (QUIP). The QUIP model is based only on the fundamental principles. Nevertheless it is very simple and consists of a few formulas. Its physical accuracy is perhaps better than APEX and other model of database SESAM (Los-Alamos).
2. Thermodynamic of gaseous substances are described by ionization equilibrium model. This model is treat gases as a mixture of classic ion cores and partly degenerated free electrons. The main improvement is that the charged particles interaction is described not by the Debye type model, but the original microfield non-ideality model. It is based on the QUIP microfield model mentioned above. This model does not contend any plasma phase transitions. It is applicable even at huge densities if temperature is high enough. The important result is that strongly coupled gaseous plasma can't exist.
3. For condensed matter we use the quantum-statistical model (the Thomas-Fermi model with quantum and exchange corrections). This model excellently describes main hugoniots at $P>25$Mbar. The joint treatment of experimental and theoretical data permits us to construct wide-range hugoniots of high precision at $0<P<1$Gbar. A special high accuracy 0.2% was reached for Cu and Fe (it is 5-10 times better of world level).
4. Electrical and heat conductivities are described by the original semi-quantum model of electron transfer. Physical and mathematical accuracy of this model is about 1%. This model has no analogs in literature.