Quantum-statistical calculations of equation of state of refractory metals

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Abstract

We use the Hartree–Fock–Slater mode with taking into account the band structure to calculate the thermal contribution of electrons to the equation of state of refractory metals (Ti, Cr, Nb, Mo, Re) in a wide range of densities (from 0.1 to 100 g/cm^3) and temperatures (from 0 to 100 keV). The calculated dependences are used to construct the Hugoniots of solid samples of these metals in the pressure range from 1 to 10^7 GPa. The comparison with the experimental data is given. This work is supportedby the Russian Science Foundation (grant No. 19-19-00713).

Quantum-statistical approach

The simplest quantum-statistical model is the Thomas–Fermi (TF) model, which is based on the semiclassical approximation for electrons. Considering of the exchange and the quantum effects within the framework of the TF approximation leads to the Thomas–Fermi with corrections (TFC) model [1]. The separation of electrons into continuous spectrum, recorded in semiclassical form, and discrete energy spectrum, recorded in a wave function form, and taking into account the exchange energy in the semiclassical approximation gives the equations of the Hartree–Fock–Slater (HFS) model [2].

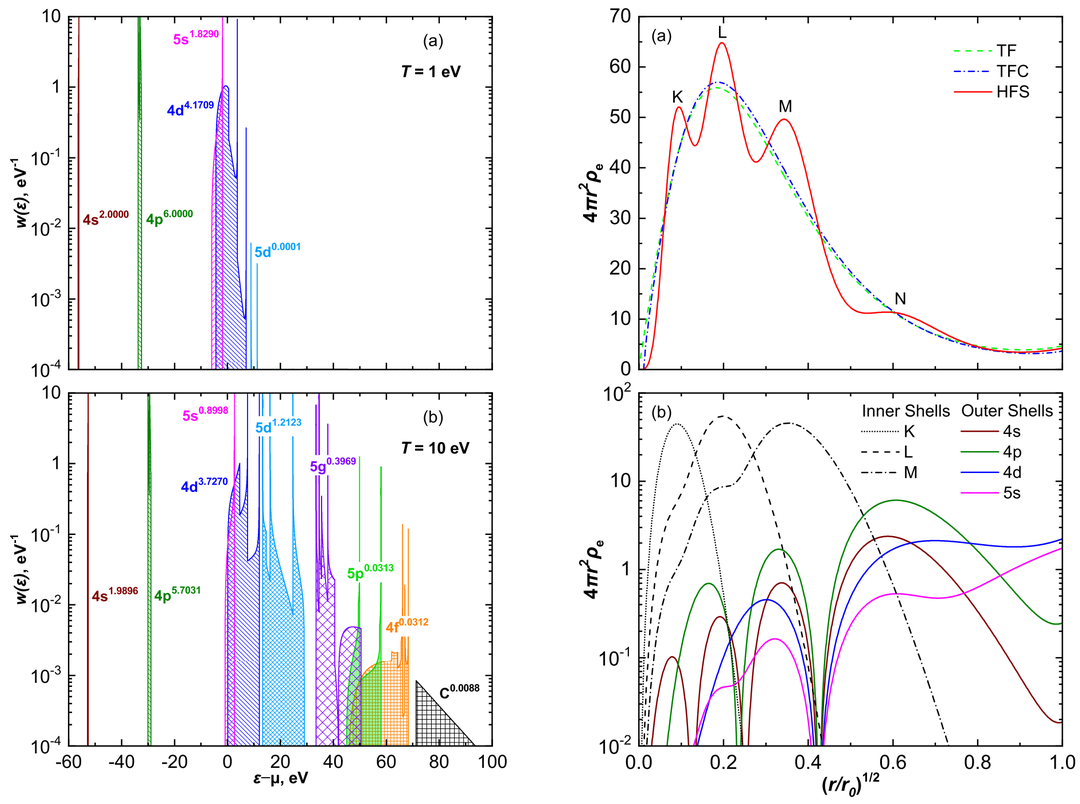


Figure 1: The density of states for outer electron shells of Mo ($\rho = 10.22$ g/cm^3) at temperatures (a) $T = 1$ eV (here the chemical potential $\mu = 1.3587$ eV) and (b) $T = 10$ eV ($\mu = -1.6297$ eV) calculated in the framework of the HFS model [3].

Figure 2: Dependence of the radial electron density $4\pi r^2 \rho_\mathrm{e}$ upon $x = \sqrt{r/r_0}$ for Mo in atomic cell at temperature $T = 1$ eV and density $\rho = 10.22$ g/cm^3. (a) Calculations for different ways to take into account electronic subsystem: green dashed curves—TF; blue dash-dot curves—TFC; red solid curves—HFS. (b) Separate contributions of electrons in different configurations according to the HFS model [3].

Electron heat capacity calculations

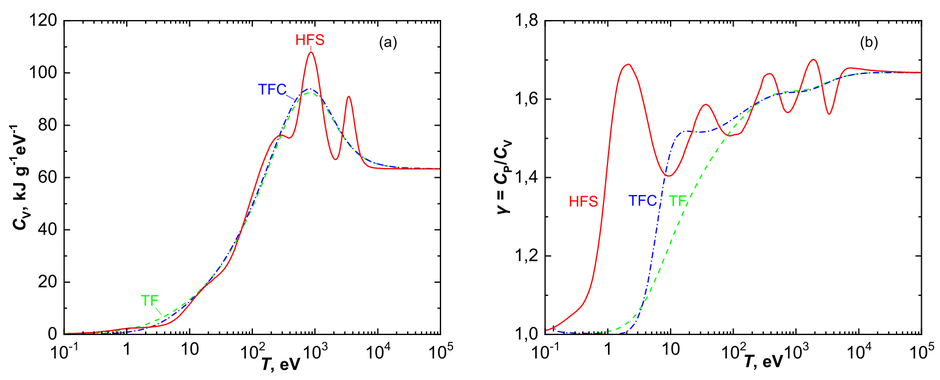


Figure 3: (a) Electron heat capacity at constant volume C_V and (b) adiabatic index $\gamma = C_\mathrm{P}/C_\mathrm{V}$ as functions of the temperature T for Mo at constant density $\rho = 10.22$ g/cm^3 according to different models: green dashed curves—TF; blue dash-dot curves—TFC; red solid curves—HFS [3].

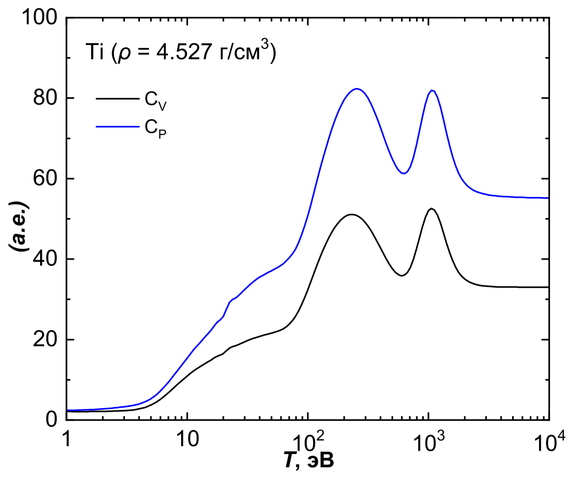
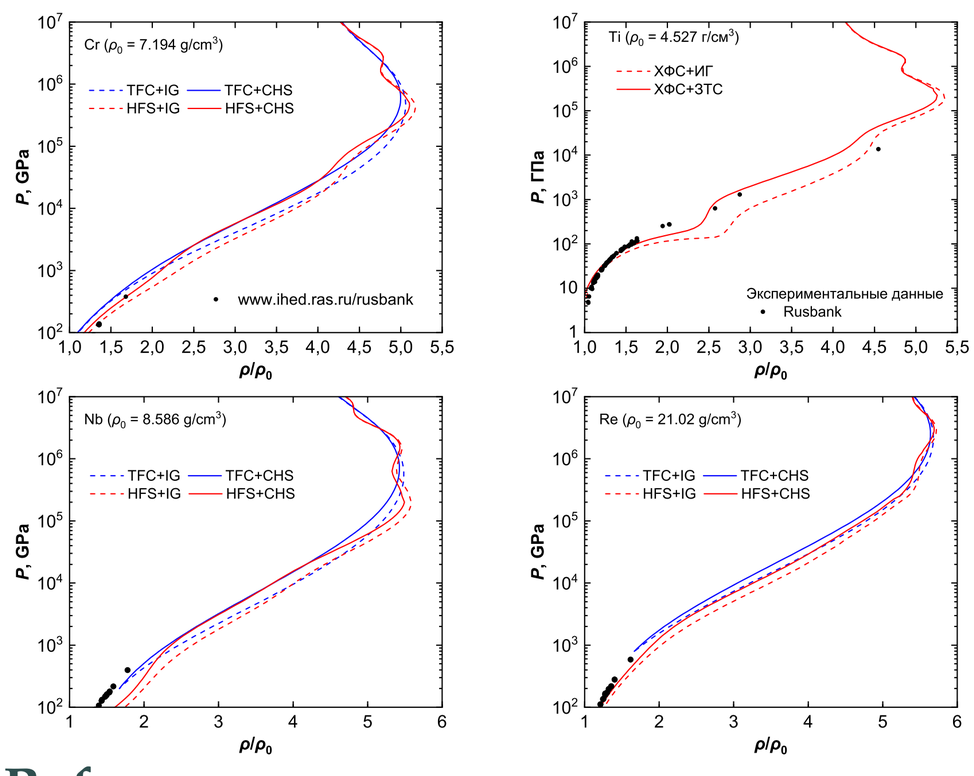


Figure 4: Electron heat capacity at constant volume C_V and pressure C_P as functions of the temperature T for Ti at constant density $\rho = 4.527$ g/cm^3 according to HFS model.

Hugoniot calculations



References

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