Contributions of electron to thermal expansions of gold and platinum

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P-V-T equations of state (EOS) of gold and plutinum are often used as pressure calibrants in in situ high-temperature and high-pressure experiments of Earth's interior. It has been pointed out that these EOS of metals possibly underestimate pressure values under high-temperature conditions, since electronic thermal pressures (ETPs) were not taken into account. In this study ETP of metal Au and Pt and their volume dependence are predicted by the first-principles electronic structure calculations with the full-relativistic treatment in order to correct their thermal equations of state (EOS). The ETPs of Au and Pt are predicted as

[26.6-1.55ln(V/V0)](V/V0)**{-0.2-0.04ln(V/V0)}T**2 (Pa)

and

[221.4-463.5ln(V/V0)](V/V0)**{0.05-2.2ln(V/V0)}T**2 (Pa),

respectively, as increasing with increasing temperature and pressure. Therefore, corrections of ETP for the previous EOS of metal Au and Pt are necessary under high-temperature and high-pressure of the Earth's mantle condition. However, we find the large difference between the ETPs of Au and Pt, which can be attributed to the different positions of the Fermi level, and ETP for Au is considerably smaller than it for Pt. These calculated properties support a recent experimental study of Hirose et al. (2001).