Thermal expansion as the cause of the temperature dependence of the magnetic susceptibility of metals

V. M Zverev and V. P. Silin
P. N. Lebedev Physics Institute, Academy of Sciences of the USSR, Moscow

(Submitted 28 February 1986, resubmitted 8 April 1986)
Pis'ma Zh. Eksp. Teor. Fiz. **43**, No. 9, 450–452 (10 May 1986)

Thermal expansion has an important effect on the temperature dependence of the magnetic susceptibility of a metal, $\chi(T)$. Experimental data are compared with the theoretical behavior $\chi(T)$ for the paramagnetic metals Pt, Ph, Mo, and Ir.

The temperature dependence of the magnetic susceptibility of metals has attracted the interest of theoreticians for a long time now (Ref. 1, for example). Among the various theoretical approaches which have been taken there is the conventional one,[2] in which the temperature dependence $\sim T^2$ is determined by the usual small thermal spreading of the Fermi level, and there is the new approach of Ref. 3, where the fine details of the Fermi distribution of electrons are taken into account. The latter approach leads to a behavior more complex than T^2.

In the present letter we wish to propose an approach which is an alternative to that of Ref. 3, in which we perceive thermal expansion to be the main reason for the temperature dependence of the magnetic susceptibility of several metals. Following Ref. 2, we begin from the conventional expansion for the paramagnetic susceptibility χ of a metal in a magnetically disordered phase:

$$\chi^{-1}(T, V, N) = \frac{1}{2\beta^2 \nu}\left\{1 + 2\psi\nu - \frac{(\pi\kappa T)^2}{6\nu^2}\left[\nu\nu'' - (\nu')^2\right]\right\}. \qquad (1)$$

This expression is written as a function of the temperature T, the volume V, and the number of electrons, N. Here κ is the Boltzman constant, β is the magnetic moment of the electron, $\nu = \nu(\eta)$ is the density of energy states of the electrons, ν' and ν'' are their derivatives, and $\eta = \eta(N/V)$ is the chemical potential, given by the equation

$$\int_0^\eta d\epsilon\nu(\epsilon) = N/2V.$$

Finally, ψ is the constant of the exchange interaction.

Since we need to interpret experimental data expressed in terms of the variables T (the temperature), P (the pressure), and N (the number of electrons), we write the pressure of the metal as $P = P_0(V, N) + \Delta P(T, V, N)$, where ΔP is an increment in the pressure which vanishes at $T = 0$. This expression[4] allows us to express the volume V in terms of the pressure: $V = V_0(P, N) + \Delta V(T, P, N)$, where V_0 is the solution of the equation $P = P_0(V, N)$. Using a relation of this sort, we can easily switch from the variable V to the pressure in expression (1). As a result, we find

$$\chi^{-1}(T,P,N) = \frac{1+2\bar{\psi}\bar{\nu}}{2\beta^2\bar{\nu}}\left\{1 - \frac{(\pi\kappa T)^2}{6\bar{\nu}^2}\,\frac{[\bar{\nu}\bar{\nu}'' - (\bar{\nu}')^2]}{1+2\bar{\psi}\bar{\nu}} - \frac{\Delta V(T,P,N)}{V_0(P,N)}\left[\overline{\frac{\partial \ln \chi(0,V,N)}{\partial \ln V}}\right]\right\}. \tag{2}$$

The bar over a function means a transition from the variable V to the pressure.

We will attempt to show the importance of thermal expansion to an understanding of the temperature dependence of the magnetic susceptibility. For this purpose, we compare experimental data with (2), in which we will completely ignore the conventional contribution $\sim T^2$, in contrast with Ref. 2.

An important point is that $\Delta V/V_0$ is well known for many metals (Ref. 5, for example). The information on $[\partial \ln \chi(0)/\partial \ln V]$ is considerably less reliable. We will accordingly illustrate the importance of thermal expansion by several examples.

Figures 1–3 show the temperature dependence of the magnetic susceptibility. The solid curves are calculated from

$$\chi^{-1}(T) = \chi^{-1}(0)\left\{1 - \frac{\Delta V(T)}{V_0}\left[\frac{\partial \ln \chi(0)}{\partial \ln V}\right]\right\}, \tag{3}$$

and the dashed curves from

$$\chi(T) = \chi(0)\left\{1 + \frac{\Delta V(T)}{V_0}\left[\frac{\partial \ln \chi(0)}{\partial \ln V}\right]\right\}. \tag{4}$$

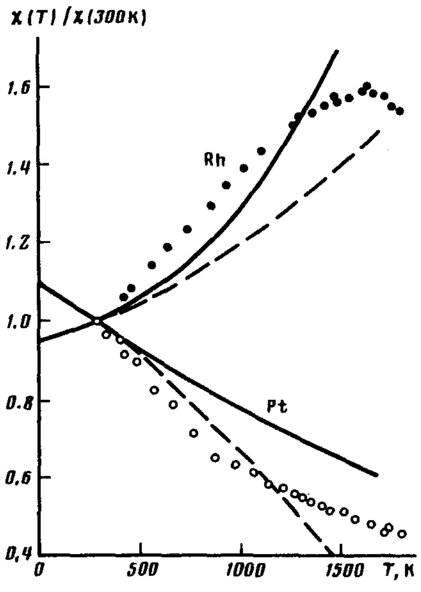

FIG. 1. Temperature dependence of the paramagnetic susceptibility of Pt and Rh. The experimental data are taken from Ref. 6.

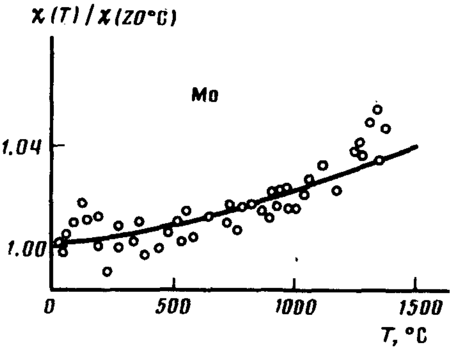

FIG. 2. Temperature dependence of the paramagnetic susceptibility of Mo. The experimental data are taken from Ref. 6.

The experimental data are taken from Ref. 6. In plotting the theoretical curves we took $[\partial \ln \chi(0)/\partial \ln V]$, to have the values -15, 9.6, 1.2, and 22 for Pt, Rh, Mo, and Ir, in accordance with Refs. 7 and 8. We selected these examples with the purpose of finding a qualitative (Fig. 1) and quantitative (Figs. 2 and 3) description of the various temperature dependences on the basis of a common phenomenon: thermal expansion. To simplify the comparison of the behavior which we found with the types of behavior discussed in the ordinary approach, which ignores thermal expansion, we follow Ref. 2 and require that the experimental and theoretical curves pass through the same point at $T = 300$ K (cf. Figs. 11 and 12 of Ref. 2).

In the case in Fig. 2, the dashed line coincides with the solid line. In the other figures, in contrast, these curves are markedly different, indicating that thermal expansion has an exceedingly strong effect. The most important piece of information we need for a quantitative comparison of the theoretical curves with the experimental data is an accurate value of $[\partial \ln \chi(0)/\partial \ln V]$. If this derivative is determined from a measurement of only the longitudinal paramagnetostriction, the result may be a larger error, amounting to even the wrong sign, as follows from Refs. 7 and 8. On the other hand, at high temperatures, the terms $\sim T^2$ in expression (2) become important; they may compete with the thermal-expansion effect and give rise to a maximum on the curve, as in the case of Rh, for example, at $T \approx 1600$ K. Second, the discrepancy between the experimental data and the curve plotted from (3) for Ir (Fig. 3) at high temperature, $T \gtrsim 1000$ °C, may be due to an extremely strong effect of thermal expan-

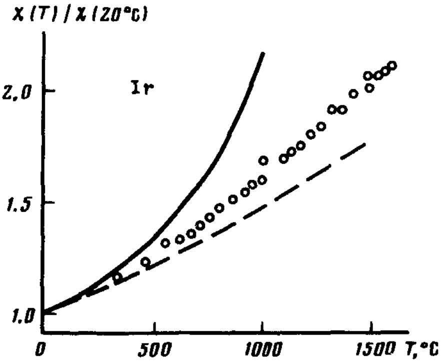

FIG. 3. Temperature dependence of the paramagnetic susceptibility of Ir. The experimental data are taken from Ref. 6.

sion on the paramagnetic susceptibility, in which case approximate expression (3) would no longer apply.

Finally, we note that in a model which ignores the dependence of the constant of the exchange interaction (ψ) on the volume (or pressure) the sign of the temperature dependence of the paramagnetic susceptibility will be determined by the sign of ν'— the first derivative of the density of energy states at the Fermi level.

In summary, this study has shown that thermal expansion has a strong effect on the temperature dependence of the magnetic susceptibility of metals. It may be that under certain conditions a similar effect may be important for metals in a magnetically ordered state.

[1]S. V. Vonsovskiĭ, Magnetizm, Nauka, Moscow, 1971 (Magnetism, Halsted, New York, 1975).
[2]M. Shimizu, Rep. Prog. Phys. **44**, 329 (1981).
[3]Yu. P. Irkhin, L. M. Noskova, and E. V. Rozenfel'd, Fiz. Tverd. Tela (Leningrad) **26**, 787 (1984) [Sov. Phys. Solid State **26**, 475 (1984)].
[4]L. D. Landau and E. M. Lifshitz, Statisticheskaya fizika, Nauka, Moscow, 1973, Part I (Statistical Physics, Addison-Wesley, Reading, Mass.).
[5]S. I. Novikova, Teplovoe rasshirenie tverdykh tel (Thermal Expansion of Solids), Nauka, Moscow, 1974.
[6]H. Kojima, R. S. Teblle, and D. E. G. Williams, Proc. R. Soc. **260**, 237 (1961).
[7]E. Fawceett, Phys. Rev. B **2**, 3887 (1970).
[8]E. Fawceett and V. Pluzhnikov, Physica B + C **119**, 161 (1983).

Translated by Dave Parsons