p	1	2	3	4	5	6
dσ/dΩ	7.1	25	44.6	59	62.5	54.5

As a function of p, dσ/dΩ has a maximum due to competition between the factor κ^2 and the thermal factor.

The author would like to thank A. S. Davydov and V. M. Agranovich for discussions.

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EQUATION OF STATE FOR THE MgO CRYSTAL

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This letter is a report on the calculation of the energy of the MgO crystal by a statistical method. The dependence of energy on volume at absolute zero has been found for pressures from zero to 10^7 atmospheres (at high pressures, the effect of temperature is small[1]).

In calculations for lattices of the alkali halide type it is customary to use a potential derived from the electron density of an isolated ion, i.e., to ignore the deformation of the ions in the lattice. But an isolated oxygen ion is not, in general, stable; in this work the electron density chosen for oxygen was found for a lattice at zero pressure by a variational method.[2] The magnesium ion deforms very litte, and the Hartree-Fock electron density is used in this case.[3] The energy calculations took into account the first quantum correction,[4] assuming an overlap of about 20%.

According to the statistical theory, the energy of any system of electrons with a density ρ is equal to:

$$\varepsilon(\rho) = \int \left\{ \varkappa_k \rho^{5/3} + \left(V_k + \frac{1}{2} V_p\right)\rho - \varkappa_a \rho^{4/3} - K(\rho) + \frac{1}{72} \frac{(\nabla\rho)^2}{\rho} \right\} dv,$$

$$\varkappa_k = 2.871, \quad \varkappa_a = 0.7386,$$

i.e., the sum of the kinetic (Fermi) and potential (Thomas-Fermi) energies of the electrons in the nuclear field, the Dirac exchange energy, the Wigner-Macke correlation energy, and the quantum correction of Kompaneev and Kirzhnits.[4-6] Atomic units are used throughout.

The correlation energy,

$$K(\rho) = 0.0306\,\rho \left\{ \ln\left(1 + \frac{4}{\lambda}\right) - \frac{2}{1 + 2\lambda} \right\}, \quad 1/\lambda = 4.862\rho^{1/3}$$

in the region of density $\rho = 0.2$ to 0.02 which we consider here, is approximately equal to

$$K(\rho) \approx 0.113\,\varkappa_a \rho^{4/3}.$$

The ionic energy of the crystal is obtained by summing the interaction energy of one pair of ions over all the ion pairs in the lattice. The interaction energy of each pair of ions is equal to

$$U = \varepsilon(\rho_1 + \rho_2) - \varepsilon(\rho_1) - \varepsilon(\rho_2) = q_1 q_2 / r + U_s,$$

where q_1, q_2 are the charges on the ions, ρ_1, ρ_2 are the electron densities of the ions, and U_S is the energy required to remove the electron clouds from both ions.[5] The total energy of the crystal, referred to a single ion pair, has the form

$$E(\delta) = -\alpha q^2/\delta + 6U_s^{+-}(\delta) + 6U_s^{--}(\sqrt{2}\,\delta) + 6U_s^{++}(\sqrt{2}\,\delta),$$

where $\alpha = 1.7476$ for a face-centered lattice, δ is the shortest distance between unlike ions, and U_S^{+-}, U_S^{--}, U_S^{++} are the overlap energies of the corresponding neighboring like and unlike ions.

In order to facilitate the numerical calculations, the electron densities of the ions taken from the literature[2,3] were approximated by the formulas

$$\rho_1(r) = 45\exp(-4{,}9\,r) \quad \text{magnesium.}$$

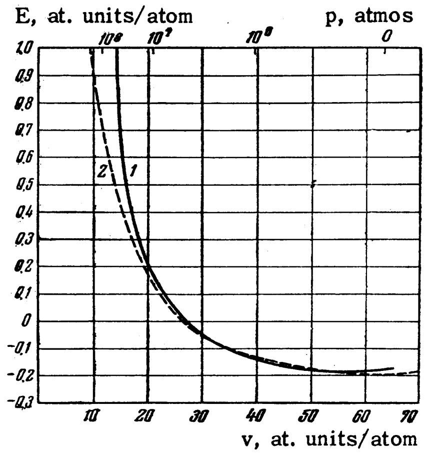
$$\rho_2(r) = \left\{ \begin{array}{lll} 280\exp(-15\,r) & \text{for} & r < 0.35 \\ 3.85\exp(-2.3\,r) & \text{"} & 0.35 < r < 1.6 \\ 1.54\exp(-1.8\,r) & \text{"} & r > 1.6 \end{array} \right\} \text{oxygen.}$$

Curves of crystal energy, referred to the energies of the free atoms, are shown in the figure (in atomic units). Curve 1 is the theoretical one. The lower part of Curve 2, where $p < 3 \times 10^4$ atmos, is based on Bridgman's experimental data[7] extrapolated to absolute zero; the portion of Curve 2 where $p > 3 \times 10^4$ atmos is an extrapolation of Bridgman's data to high pressures by Davydov's formula.[1]

In the range of pressures from zero to 10^6 atmospheres the theoretical Curve 1 can be approximated by the formula

$$E(v) = 93.7\exp(-1.69v^{1/2}) - -3.495v^{-1/2}+0.582 \text{ at. units/atom.}$$

The pressure is found from the formula $p = -dE/dv$. The equilibrium volume at zero pressure is calculated to be $v_0 = 55$ at. units/atom, and is found experimentally to be $v_0 = 63$. The calculated binding energy, referred to the energy of the free atoms, is 10.0 ev per molecule = 231 kcal/mole. The experimental value of this energy[8] is 242 kcal/mole. At pressures above 5×10^6 atmos the calculated curve 1 lies somewhat higher than curve 2. This might be explained by the onset of an energy storage due to the overlapping of the inner shells. In curve 2 it is only the overlapping of the outer shells which is extrapolated, whereas the calculations for curve 1 automatically take into account the overlapping of the inner shells as well.



I wish to express my thanks to B. I. Davydov for proposing this subject and discussing the results.

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EFFECT OF ELECTRIC POLARIZATION ON MAGNETIC PROPERTIES OF FERRITES

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If the spin-orbit interaction of the d electrons in ferrites is taken into account, the effective magnetic permeability becomes a function of the electric polarization of the electron shells of the atoms, i.e., of the dielectric constant. No such dependence is observed at radio frequencies in ferromagnetic metals, owing to the strong polarizability of the conduction electrons.

In certain types of ferrites one can expect the electric properties to affect not only the frequency dependence of the effective permeability, or the width, form, and position of the resonance-absorption line, but also the dependences of these effects on the dimensions and shapes of the specimens, dependences that cannot be accounted for by the method of demagnetizing factors.

The spin-orbit interactions, within the framework of the macroscopic theory, can be accounted for with the aid of the following closed system of equations:

$$\dot{\mathbf{M}} = \gamma \mathbf{M} \times \mathbf{H}_{\text{eff}}; \tag{1}$$

$$\ddot{\mathbf{P}}_j + \alpha_j \dot{\mathbf{P}}_j + \omega_j^2 \mathbf{P}_j = -(g/c)\,\partial \mathbf{A}/\partial t, \tag{2}$$

$$\Delta \mathbf{A} = -\frac{4\pi}{c}\left[c \operatorname{curl} \mathbf{M} + \dot{\mathbf{P}} - \frac{1}{4\pi c}\ddot{\mathbf{A}}\right], \tag{3}$$

$$\mathbf{P} = \sum_j \mathbf{P}_j, \quad \mathbf{H}_i = -4\pi\mathbf{M} + \operatorname{curl}\mathbf{A};$$

$$\mathbf{H}_{\text{eff}} = \mathbf{H} + aM_s^{-2}\Delta\mathbf{M} + \mathbf{H}_i,$$

H is the intensity of the external field, and $aM_s^{-2} \times \Delta\mathbf{M}$ are the fields of the exchange forces. The self-consistent internal field $\mathbf{H}_i$ is due to the spin-spin (source — c curl **M**) and spin-orbit (source — $\dot{\mathbf{P}}$) interactions.

The term **P** in Eq. (2) describes the polarization current due to the change in the electric dipole moment of the atom, a change caused by the vortical electric field due to the magnetization fluctuations. In other words, it is due to the changes in the spatial portion of the wave function of the d electrons, occurring upon change of orientation of the magnetic moments of the electrons.

Equations (2) describe the change in the polarization of a set of interacting atoms with an internal electromagnetic field.