Atomistic explanation of the Gough-Joule-effect

B. Schweizer[a] and J. Wauer

Institut für Technische Mechanik, Universität Karlsruhe, Kaiserstr. 12, 76128 Karlsruhe, Germany

Abstract. An interpretation of the Gough-Joule-Effect from an atomistic point of view is given by a special investigation of lattice vibrations using a non-interacting model. The calculations are restricted to crystals with ideal crystal structure built up of only one kind of particles. Approximate analytical formulas are derived. A comparison between the classical macroscopic theory and the here presented microscopic calculations is drawn.

PACS. 05.45.-a Nonlinear dynamics and nonlinear dynamical systems – 63.70.+h Statistical mechanics of lattice vibrations and displacive phase transitions – 46.25.Hf Thermoelasticity and electromagnetic elasticity (electroelasticity, magnetoelasticity)

1 Introduction

Thermomechanic problems are mathematically described by two field equations, namely the mechanical and the thermal field equation [1,2]. The mechanical field equation results from a combination of the equation of motion and the constitutive equation. The mechanical field equation yields the displacement field. The thermal field equation is derived from the balance of energy, the constitutive entropy equation and Fourier's law of heat conduction. The thermal field equation yields the temperature field. The mechanical and the thermal field equation are fully coupled, that means in both equations occur the field variables of both field equations.

Regarding thermoelastic materials, one can detect two coupling effects. The first effect is the the well-known effect of thermal expansion. Solid bodies respond to an increase and decrease of temperature with expansion and contraction, respectively. Due to this phenomenon, the mechanical field equation is coupled with the thermal field equation, hence in the mechanical field equation appears a thermal coupling term.

The second effect describes the reversible heating or cooling of a body by means of a deformation. If one, for instance, transfers a body in a hydrostatic state of stress by a reversible adiabatic change of state, the body will cool off in the case of a tensile state of stress and will heat up in the case of a compressive state of stress. After unloading, the body takes up the original temperature. The effect of reversible heating and cooling is also known as Gough-Joule-effect [3,4]. The consequence is that the thermal field equation is coupled with the mechanical field equation, thus in the thermal field equation appears a

mechanical coupling term. For most materials, the temperature changes due to the Gough-Joule-effect are comparatively small [5]. For metals, we observe temperature changes in the magnitude of one kelvin [6].

It remains to mention that if dissipation is taken into account, we obtain a thermoviscoelastic material [1]. We detect heating due to dissipation and another coupling term in the mechanical field equation. If we further note that the parameters are functions of the temperature, one can perceive additional coupling effects between the two field equations [7,8]. Discussions on the Gough-Joule-effect in viscoelastic fluids can be found in [9]. In [10,6] investigations are carried out on nonlinear thermomechanic problems, which also consider plasticity.

The main objective of this paper is to give an atomistic explanation of the mechanical coupling term in the thermal field equation, which causes the Gough-Joule-effect. We restrict ourselves to the most simple case that is an ideal crystal built up of only one kind of particles (Debye solid). The microscopic explanation of the Gough-Joule-effect for non-crystalline solids, such as polymers, is probably another than that given here for crystals. The microscopic explanation of the thermal expansion is well known. It originates in the unsymmetry of the potential curve and the displacement of the center of oscillation with varying temperature [11,12]. To the authors' knowledge, a microscopic interpretation of the Gough-Joule-effect does not exist in the literature. A detailed description of experimental works on the Gough-Joule-effect can be found in [13].

2 Macroscopic theory

For a comparison with the microscopic calculations in Section 3, we first recall the macroscopic results. We consider

a e-mail: schweiz@itm.uni-karlsruhe.de

an isotropic thermoelastic solid. The linearized balance and constitutive equations are (see [14,1])
the balance of momentum

$$\rho\,\dot{\mathbf{u}} = \boldsymbol{\nabla}\cdot\boldsymbol{\sigma}^T + \rho\,\mathbf{k} \qquad (\boldsymbol{\sigma} = \boldsymbol{\sigma}^T)\ \ , \tag{1}$$

the balance of energy

$$\rho\,T\,\dot{s} = -\boldsymbol{\nabla}\cdot\mathbf{q} + \rho\,r\ \ , \tag{2}$$

the constitutive equation

$$\boldsymbol{\sigma} = 2\,\mu\,\boldsymbol{\epsilon} + \lambda\,(\boldsymbol{\epsilon}\cdot\cdot\mathbf{I})\,\mathbf{I} - \gamma\,(T - T_0)\,\mathbf{I}\ \ , \tag{3}$$

the constitutive entropy equation

$$\rho\,s = \gamma\,(\boldsymbol{\epsilon}\cdot\cdot\mathbf{I}) + \rho\,\frac{c_V}{T_0}\,(T - T_0) \tag{4}$$

and Fourier's law of heat conduction

$$\mathbf{q} = -\kappa\cdot\boldsymbol{\nabla}(T - T_0)\ . \tag{5}$$

As usual, the linearized stress tensor is denoted as $\boldsymbol{\sigma}$ and the linearized strain tensor as $\boldsymbol{\epsilon}$. ρ is the density, $\dot{\mathbf{u}}$ is the time derivative of the displacement vector $\mathbf{u}$ and $\mathbf{k}$ collects the volume forces. T denotes the absolute temperature, T_0 terms the ambient temperature, s represents the specific internal entropy and c_V the specific heat capacity. Further, $\mathbf{q}$ denotes the heat flux, r represents internal sources of heat. κ is the coefficient of thermal conduction. The Lamé constants μ und λ can be expressed in terms of Young's modulus of elasticity E, Poisson's ratio ν and the bulk modulus K

$$\mu = \frac{E}{2(1+\nu)}\ ,\quad \lambda = \frac{\nu\,E}{(1+\nu)(1-2\nu)}\ ,\quad K = \frac{(3\lambda+2\mu)}{3}\ . \tag{6}$$

Assuming small changes in temperature, the relationship between the constant γ and the linear coefficient of thermal expansion α is given by

$$\gamma \approx (3\lambda + 2\mu)\,\alpha = 3\,K\,\alpha = \frac{E}{(1-2\nu)}\,\alpha. \tag{7}$$

Combining the balance of momentum (1) and the constitutive equation (3) and taking into account the strain-displacement relationship $\boldsymbol{\epsilon} = \frac{1}{2}\,[(\boldsymbol{\nabla}\mathbf{u})^T + \boldsymbol{\nabla}\mathbf{u}]$, the mechanical field equation results in

$$\mu\,\boldsymbol{\nabla}^2\mathbf{u} + (\lambda+\mu)\,\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\mathbf{u}) + \rho\,\mathbf{k} = \rho\,\ddot{\mathbf{u}} + \gamma\,\boldsymbol{\nabla}T\ . \tag{8}$$

Differentiation of equation (4) with respect to t and substituting the result into the balance of energy (2), we get with Fourier's law of heat conduction and after a linearization the thermal field equation

$$\kappa\,\boldsymbol{\nabla}^2\cdot T - \rho\,c_V\,\dot{T} - T_0\,\gamma\,(\dot{\boldsymbol{\epsilon}}\cdot\cdot\mathbf{I}) = -\rho\,r\ . \tag{9}$$

The term $T_0\,\gamma\,(\dot{\boldsymbol{\epsilon}}\cdot\cdot\mathbf{I})$ in equation (9) describes the reversible heating effect.

In order to analyze this effect, we assume, that a body is isentropically changed from an unstressed state with the temperature T_0 in a hydrostatic state of stress and strain. A linearized consideration according to equation (3) with a tensile stress of $\sigma_{11} = \sigma_{22} = \sigma_{33} = p$ leads to a volumetric extension of

$$\begin{aligned}\epsilon_{kk} &= \frac{\sigma_{kk}}{3K} + \frac{\gamma}{K}\,(T - T_0) \\ &= \frac{p}{K} + \frac{\gamma}{K}\,(T - T_0).\end{aligned} \tag{10}$$

Assuming a reversible adiabatic change of state, the entropy equation (4) results in

$$\gamma\,\epsilon_{kk} = -\rho\,\frac{c_V}{T_0}\,(T - T_0) \tag{11}$$

and with equation (10) it reads

$$\gamma\,\left(\frac{p}{K} + \frac{\gamma}{K}\,(T - T_0)\right) = -\rho\,\frac{c_V}{T_0}\,(T - T_0)\ . \tag{12}$$

Solving this equation for $(T - T_0)$ and reminding (7), we obtain for the difference of temperature

$$\Delta T_{\mathrm{makr.}} = (T - T_0) = -\frac{p}{\frac{E\alpha}{(1-2\nu)} + \frac{\rho c_V}{3\alpha T_0}}\ . \tag{13}$$

Assuming a hydrostatic state of stress with $p = 200\,\frac{\mathrm{N}}{\mathrm{mm}^2}$ and an ambient temperature of $T_0 = 273$ K, we get with equation (13) and the data in Appendix C the following differences of temperature

iron:

$$\Delta T_{\mathrm{makr.}} = -0.5750\ \mathrm{K}\ , \tag{14}$$

aluminium:

$$\Delta T_{\mathrm{makr.}} = -1.5933\ \mathrm{K}\ , \tag{15}$$

gold:

$$\Delta T_{\mathrm{makr.}} = -0.9583\ \mathrm{K}\ . \tag{16}$$

3 Microscopic theory

In this section, we give an atomistic explanation of the Gough-Joule-effect. The considerations are based on investigations of lattice vibrations. We consider the most simple case that is an ideal crystal built up of only one kind of particles (Debye solid [15]).

The basis of the approach is a simple model of statistically independent oscillating particles. The application of the model of statistically independent particles is a common method to reduce the complex oscillations in a solid on the motion of a single atom. The hypothesis of independent motion is used in several connections. For instance, the coefficient of thermal expansion can be calculated with a non-interacting model [11,12]. Also, approximate calculations of the heat capacity using the hypothesis of non-correlation are known (e.g. the Einstein-model [12]).
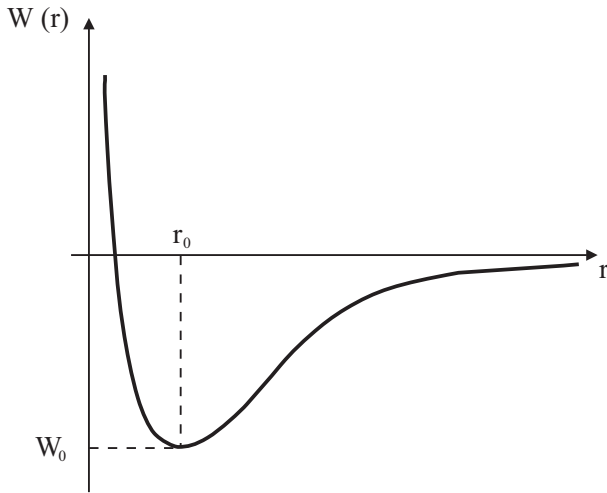
Fig. 1. Potential curve $W(r)$.

Moreover, the model of independent atomic motions is applied in the theory of diffraction [16]. For instance, the theory of Bragg scattering is essentially the same for an interacting and a non-interacting model.

The Gough-Joule-effect (strain or stress induces a temperature change) can be regarded as the inverse effect of the thermal expansion (temperature change induces strain or stress). Since the model of statistically independent particles is used for an approximate calculation of the thermal expansion, it seems likely that this model can also be used to analyse the Gough-Joule-effect. The main objective of the below investigation is to illustrate the Gough-Joule-effect in a simple model. Based on the authors judgment, a more detailed analysis, which takes phonons into account, leads to very sophisticated calculations.

The particles of the crystal are assumed to be oscillating point masses, rotatory degrees of freedom are neglected. The calculations are carried out classically, that means we presume that the temperature of the crystal is much higher than the Debye temperature.

The particles of the crystal oscillate in a potential field which has its origin in the attraction and repulsion forces of the particles. Figure 1 shows a typical graph of such a potential curve. r_0 is the distance of equilibrium, $W(r_0) = W_0$ is the lattice binding energy.

By reason of the theorem of the equipartition of energy, in the state of thermal equilibrium the oscillating particle has as much kinetic as potential energy. Since we neglect rotatory degrees of freedom, the particle has 6 degrees of freedom, 3 kinetic and 3 potential degrees of freedom. In the state of thermal equilibrium each degree of freedom has the same mean energy $\frac{1}{2} k T_0$ (T_0 is the temperature of the crystal and k is Boltzmann's constant). Hence, at a temperature of T_0, the particle has the kinetic energy $E_0 = \frac{3}{2} k T_0$ and consequently oscillates in a height of E_0 over the bottom (minimum) of the potential curve.

Because of the unsymmetry of the potential curve, the center of oscillation of the free oscillation for the particle lies right of the minimum of the potential curve. The higher the temperature, the larger the distance between the center of oscillation and the minimum of the potential curve. The consequence is the thermal expansion. If we assume a moderate ambient temperature, the particle oscillates in a low height over the bottom of the potential curve. Therefore, the potential curve near by the minimum is approximated by a polynomial of degree 3

$$W(r) = W_0 + \frac{1}{2} W_0''(r - r_0)^2 - \frac{1}{6} W_0'''(r - r_0)^3 . \quad (17)$$

Defining the zero level so that $W(r) \to 0$ for $r \to \infty$, the constant W_0 is assumed to be negative. By reason of the typical unsymmetric graph of the potential, the constants W_0'' and W_0''' are both assumed to be positive [12]. The iterative determination of these constants from macroscopic data is shown next. As mentioned before, at a constant temperature T_0, the particle performs a free oscillation at a height of $E_0 = \frac{3}{2} k T_0$ over the bottom of the potential curve. The energy equation for this free oscillation is given by

$$\frac{1}{2} m_A \dot{r}^2 + (W(r) - W_0) = E_0 . \quad (18)$$

Let a, b and c ($a > b > c$) be the roots of the polynomial $(W(r) - W_0) - E_0$. If E_0 is not too large, this polynomial has three real roots. Note that for larger values of E_0, the approximation of the potential curve by a polynomial of degree 3 is no longer valid and the roots became complex. Consequently, we have $(W(r) - W_0) - E_0 = \frac{1}{6} W_0'''(r - a)(r - b)(r - c)$. By separation, we get from equation (18)

$$\mathrm{d}t = \sqrt{\frac{m_A}{2}} \frac{1}{\sqrt{E_0 - (W(r) - W_0)}} \mathrm{d}r . \quad (19)$$

Thus, the half period time $\bar{T}$ (time from c to b) of the oscillation is given by

$$\bar{T} = \sqrt{\frac{3 m_A}{W_0'''}} \int_c^b \frac{1}{\sqrt{(r - a)(r - b)(r - c)}} \mathrm{d}r$$
$$= \sqrt{\frac{3 m_A}{W_0'''}} \frac{2}{\sqrt{a - c}} F(1, \sqrt{\frac{b - c}{a - c}}) . \quad (20)$$

$F(p, q)$ denotes the elliptic integral of the first kind. The center of oscillation is determined by

$$r_m = \frac{1}{\bar{T}} \int_0^{\bar{T}} r(t) \, \mathrm{d}t = \frac{1}{\bar{T}} \int_c^b \frac{r}{\dot{r}} \, \mathrm{d}r . \quad (21)$$

With the potential function (17), one gets

$$r_m = \frac{1}{\bar{T}} \sqrt{\frac{3 m_A}{W_0'''}} \int_c^b \frac{r}{\sqrt{(r - a)(r - b)(r - c)}} \mathrm{d}r$$
$$= a - \frac{E(1, \sqrt{\frac{b - c}{a - c}})}{F(1, \sqrt{\frac{b - c}{a - c}})} (a - c) . \quad (22)$$
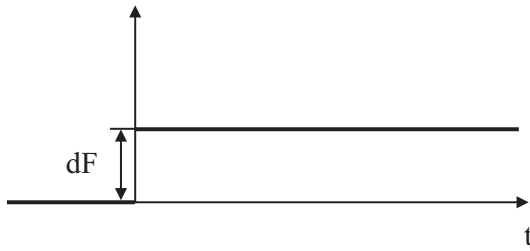
Fig. 2. Jump force $\mathrm{d}F$.

$E(p, q)$ represents the elliptic integral of the second kind. So, for the ideal lattice the coefficient of thermal expansion is found to be

$$\alpha = \frac{(r_m - r_0)}{r_0 \ T_0} \ . \tag{23}$$

Young's modulus E is associated with the curvature of the potential curve at the minimum. For the idealized crystal, one gets [11]

$$\left.\frac{\mathrm{d}^2 W}{\mathrm{d}r^2}\right|_{r=r_0} = W_0'' = E \ r_0 \ . \tag{24}$$

Knowing the macroscopic data α and E, the constant W_0'' is determined by equation (24) and W_0''' can be calculated iteratively using equation (23). An initial value for the iteration of W_0''' is given by the approximate formula (see [12])

$$W_0''' \approx \frac{4}{3} \ \frac{W_0''^2 \ \alpha \ r_0}{k} \ . \tag{25}$$

Now, the Gough-Joule-effect is analyzed. The crystal has to be transfered in a hydrostatic state of stress by a reversible adiabatic change of state. Since the change of state is reversible adiabatic, the hydrostatic force F has to be applied infinitely slow. Therefore, we apply a series of differential jump forces (step loads) $\mathrm{d}F$ (see Fig. 2).

We consider a crystal on which surfaces a differential tensile stress $\mathrm{d}p$ acts so that the crystal is in a hydrostatic state of stress. On each particle which takes the area r_0^2, there acts the differential force $\mathrm{d}F = \mathrm{d}p \ r_0^2$. The potential function of the tensile force $\mathrm{d}F$ is approximately linear (see Appendix B)

$$U_{\mathrm{d}p}(r) = -\mathrm{d}p \ r_0^2 \ r \ . \tag{26}$$

After applying the force $\mathrm{d}F$, the particle oscillates in the potential field $W(r) + U_{\mathrm{d}p}(r)$ given by

$$W_{\mathrm{d}p}(r) = W_0 + \frac{1}{2}W_0''(r - r_0)^2 - \frac{1}{6}W_0'''(r - r_0)^3 - \mathrm{d}p \ r_0^2 \ r. \tag{27}$$

The graph of the function $W_{\mathrm{d}p}(r)$ is shown in Figure 3. We now investigate the effect on the oscillating particle if a differential jump force $\mathrm{d}F$ is applied. The solid line in Figure 4 shows the potential curve $W(r)$, the dashed
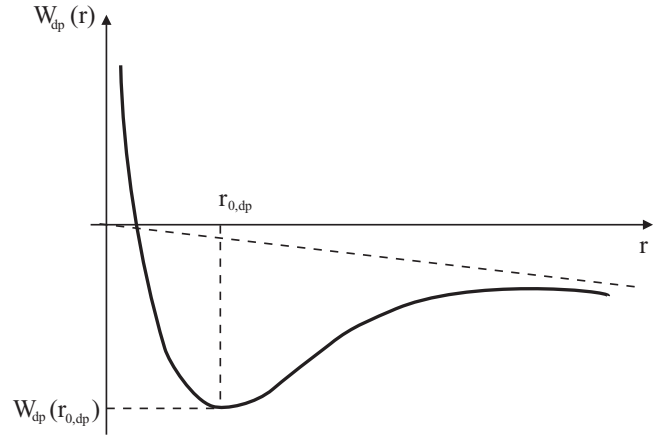

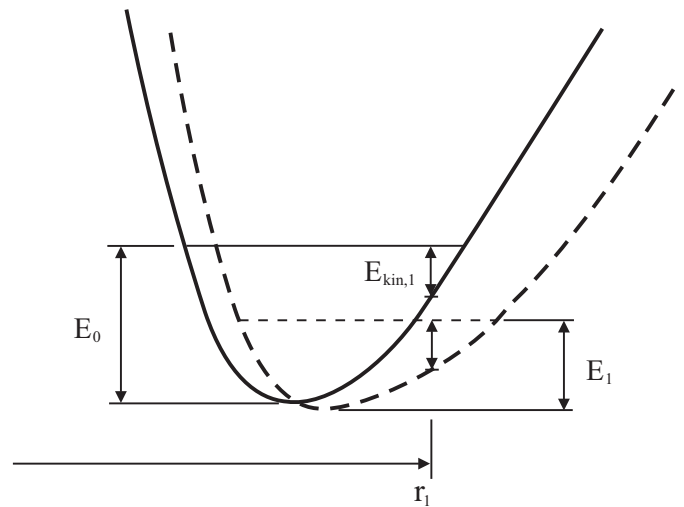**Fig. 3.** Potential curve $W_{\mathrm{d}p}(r)$.

Fig. 4. Jump force in the range $r_0 < r_1 < b$.

line the potential curve $W_{\mathrm{d}p}(r)$. The figure only shows the zone near the minima of the potential curves. Before the jump force $\mathrm{d}F$ acts, the particle oscillates in the potential field $W(r)$ in the height of E_0 over the minimum of the potential curve. First we assume that directly before $\mathrm{d}F$ acts, the particle is in the range $r_0 < r_1 < b$, that means right of the minimum of the potential curve. Applying a jump force implies that the acceleration jumps and the velocity shows a discontinuity. Hence, directly after $\mathrm{d}F$ has being applied, the particle rests at the same place r_1 and has the same velocity $\dot{r}(r_1)$, but now it oscillates in the potential field $W_{\mathrm{d}p}$. Before the jump force $\mathrm{d}F$ was applied, the particle oscillated in the height E_0 over the bottom of the potential curve $W(r)$, but after the jump force $\mathrm{d}F$ has being applied, the particle oscillates in the height E_1 over the bottom of the potential curve $W_{\mathrm{d}p}$. It is easy to construct the new height E_1. Because the velocity remains unchanged, the new height is obtained by fixing the line $E_{\mathrm{kin},1} = \frac{1}{2} m_A \dot{r}^2(r_1) = E_0 - |W_0 - W(r_1)|$ over the curve $W_{\mathrm{d}p}$ at r_1. It can be seen that the new height E_1 is lower than the old one, E_0. As a result, the temperature (the kinetic energy of the particle) decreases, if the jump force is applied, when the particle is in the range $r_0 < r_1 < b$.
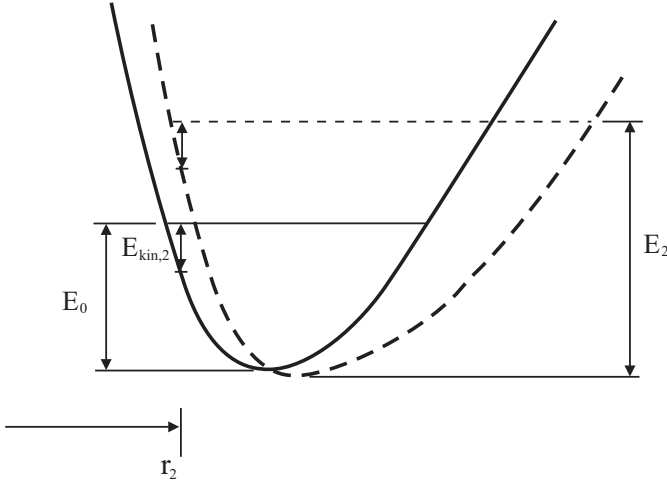
Fig. 5. Jump force in the range $c < r_2 < r_0$.

Next, we consider the case, that the particle is in the range $c < r_2 < r_0$, i.e., left of the minimum of the potential function when the differential jump force dF is applied. Figure 5 illustrates the situation. Once again, the particle keeps the position (r_2) and the velocity $(\dot{r}(r_2))$ immediately after the jump force has been applied. The new height E_2 after the jump force dF is applied is constructed in the same way as before. At the point $(r_2, W_{dp}(r_2))$ of the potential function $W_{dp}(r)$ the line $E_{\mathrm{kin},2} = \frac{1}{2} m_A \dot{r}^2(r_2) = E_0 - |W_0 - W(r_2)|$ is fixed as shown in the figure. One can observe that the new height E_2 is larger than the old one, E_0. Consequently, the temperature will increase if the jump force is applied and the particle is in the range $c < r_2 < r_0$. Recapitulating, the energy and therefore the temperature will decrease if the jump force is applied and the particle is right of the minimum of the potential curve. Energy and temperature will increase if the jump force is applied and the particle is left of the minimum. By reason of the unsymmetry of the potential curve $W(r)$ at a fixed point of time, there are statistically more particles of the crystal right of the minimum of the potential curve than left of it. Thus, applying a tensile hydrostatic state of stress, the temperature of the crystal will decrease. Analogous considerations for the case of a compressive hydrostatic state of stress can be carried out. Then, the temperature of the crystal will increase as predicted by the macroscopic theory.

We now quantify the above considerations. First, we calculate the change of the minimum of the potential curve due to the potential U_{dp}, i.e., we have to calculate the difference of the minimum of $W(r)$ and the minimum of $W_{dp}(r)$. The position $r_{0,dp}$ of the minimum of $W_{dp}(r)$ is

$$r_{0,dp} - r_0 = \frac{W_0''}{W_0'''} - \frac{W_0''}{W_0'''}\sqrt{1 - 2\,\frac{W_0'''}{W_0''^2}\,r_0^2\,dp}$$

$$= \frac{1}{W_0''}\,r_0^2\,dp + O(dp^2) \qquad (28)$$

and the minimum is found to be

$$\begin{aligned}
W_{dp}(r_{0,dp}) &= W_0 + \frac{1}{2}W_0''\left[\frac{1}{W_0''}\,r_0^2\,dp + O(dp^2)\right]^2 \\
&\quad - \frac{1}{6}W_0'''\left[\frac{1}{W_0''}\,r_0^2\,dp + O(dp^2)\right]^3 \\
&\quad - dp\,r_0^2\left[\frac{1}{W_0''}\,r_0^2\,dp + O(dp^2) + r_0\right] \\
&= W_0 - r_0^3\,dp + O(dp^2)\,. \qquad (29)
\end{aligned}$$

The difference of energy, that is the difference of the height of the free oscillation over the bottom of the potential curve before and after applying the jump force dF, can be calculated as a function of r

$$\begin{aligned}
dE(r) &= W_{dp}(r) - W(r) - (W_{dp}(r_{0,dp}) - W_0) \\
&= -r_0^2\,dp\,(r - r_0) \qquad (30)
\end{aligned}$$

where $c < r < b$. $dE(r)$ is the difference of energy if the oscillating particle is at the place r when the jump force dF is applied. At an instance of time, there are not all particles of the crystal at the same place r. Thus, we have to average and calculate the mean value dE of the difference of energy. In our simple model we assume that the particles oscillate in the same mean height over the bottom of the potential curve. Regarding all particles of the crystal, there are statistically

$$\rho_s = \frac{dt}{\overline{T}} = \frac{1}{\overline{T}}\frac{dr}{\dot{r}(r)} \qquad (31)$$

in the range $[r, r + dr]$. Hence, the resultant differential difference of energy, when dF is applied, can be calculated by weighting with ρ_s and integrating as

$$dE = \frac{1}{\overline{T}}\int_c^b \frac{dE(r)}{\dot{r}(r)}\,dr = -\frac{1}{\overline{T}}\,r_0^2\,dp\int_c^b \frac{(r - r_0)}{\dot{r}(r)}\,dr\,. \qquad (32)$$

With $\dot{r}$ from equation (18), we get

$$\begin{aligned}
dE &= -\frac{1}{\overline{T}}\,r_0^2\,dp\,\sqrt{\frac{3\,m_A}{W_0'''}} \\
&\quad \times \int_c^b \frac{(r - r_0)}{\sqrt{(r-a)(r-b)(r-c)}}\,dr \\
&= -r_0^2\left[a - r_0 - \frac{E(1, \sqrt{\frac{b-c}{a-c}})}{F(1, \sqrt{\frac{b-c}{a-c}})}\,(a - c)\right]dp\,. \qquad (33)
\end{aligned}$$

Equation (33) is the formula for the differential difference of energy when the initial state is stress-free. The general expression for the differential difference of energy, when the initial state is not stress-free, is carried out in Appendix A.

Applying the total load p, one has to note that the roots a, b and c as well as the position of the minimum of the potential curve are functions of p. Because of this fact, an analytical integration of equation (33) or the general expression (A.6) in Appendix A is not possible. Furthermore, equation (33) is not the exact expression for the differential difference of energy. Due to the fact, that not all particles of the crystal have the same temperature T_0 (T_0 is only the mean temperature), we would have to average over the temperature. This is also analytically not possible, but numerical calculations show that such an average determination has only little influence on the results. An approximate expression according to equation (33) is given by

$$\Delta E \approx -r_0^2 \left[a - r_0 - \frac{E(1, \sqrt{\frac{b-c}{a-c}})}{F(1, \sqrt{\frac{b-c}{a-c}})} \, (a - c) \right] p \, . \quad (34)$$

This formula was obtained under the assumption that the roots a, b and c are constant. This is not true. If the load p is applied, the particle oscillates in the potential $W_p(r)$. Consequently, the roots a, b and c are functions of p. A more detailed analysis, which takes into account this fact is carried out in Appendix A. The result is equation (A.7), which cannot be integrated analytically. Some numerical calculations of the difference of energy ΔE according to equation (A.7) show, that the results obtained by equation (A.7) are close to the results given by equation (34). The reason therefore is that a, b and c change little when p is applied. Thus, in the following we only use formula (34).

With equation (34) and with $\Delta E = \frac{3}{2} \, k \, \Delta T$, the temperature difference is found to be

$$\Delta T_{\text{mikr.}} = (T - T_0) \approx \frac{2 \, \Delta E}{3 \, k} = -\frac{2 \, r_0^2 \, p}{3 \, k}$$
$$\times \left[a - \frac{E(1, \sqrt{\frac{b-c}{a-c}})}{F(1, \sqrt{\frac{b-c}{a-c}})} \, (a - c) \right] \, . \quad (35)$$

Assuming a hydrostatic state of stress with $p = 200 \, \frac{\text{N}}{\text{mm}^2}$ and an ambient temperature of $T_0 = 273$ K, we get with equation (35) and the data in Appendix C the following differences of temperature

iron:

$$\Delta T_{\text{mikr.}} = -0.5307 \text{ K} \, , \quad (36)$$

aluminium:

$$\Delta T_{\text{mikr.}} = -1.5548 \text{ K} \, , \quad (37)$$

gold:

$$\Delta T_{\text{mikr.}} = -0.9602 \text{ K} \, . \quad (38)$$

4 Conclusion

Comparing the calculations of Sections 2 and 3, one can observe that the macroscopic and the above presented microscopic results show close agreement. The percentage error is

for iron:

$$\frac{(\Delta T_{\text{makr.}} - \Delta T_{\text{mikr.}})}{\Delta T_{\text{makr.}}} \times 100 = 7.7 \ \% \, , \quad (39)$$

for aluminium:

$$\frac{(\Delta T_{\text{makr.}} - \Delta T_{\text{mikr.}})}{\Delta T_{\text{makr.}}} \times 100 = 2.4 \ \% \, , \quad (40)$$

and for gold:

$$\frac{(\Delta T_{\text{makr.}} - \Delta T_{\text{mikr.}})}{\Delta T_{\text{makr.}}} \times 100 = -0.2 \ \% \, . \quad (41)$$

We only examined the probably simplest case, an ideal crystal with one kind of particles. The investigations are based on a simple model of statistically independent oscillating particles. Since the results of the macroscopic theory and the presented microscopic considerations are pretty close, the non-interacting model is adequate to describe the Gough-Joule-effect qualitatively and quantitatively. A more exact model, which takes phonons into account, would be preferable, but then, the calculations are much more complicated.

Calculations for crystals which do not consist only of one kind of particles (e.g. sodium chloride), should be possible to be carried out in a similar way as shown in Section 3. But then, additional average determinations will be necessary. For non-crystalline solids, the situation is more complicated. Perhaps, the main cause for the Gough-Joule-effect for non-crystalline solids is another one than that presented here for ideal crystals.

Appendix A

In Section 3 we only derived the linearized expression for the difference of energy. Equation (30) yields the differential difference of energy $\mathrm{d}E$ due to the differential jump force $\mathrm{d}F$ when the initial state is unstressed ($p = 0$). Generally, $\mathrm{d}E$ is not only a function of r but also a function of p. With analogous considerations which led to equation (30), we find the general expression (see Fig. 6)

$$\mathrm{d}E(r, p) = W_p(r, p + \mathrm{d}p) - W_p(r, p)$$
$$- \frac{\partial W_p(r_{0,p}, p)}{\partial p} \, \mathrm{d}p$$
$$= \frac{\partial W_p(r, p)}{\partial p} \, \mathrm{d}p - \frac{\partial W_p(r_{0,p}, p)}{\partial p} \, \mathrm{d}p \, , \quad (A.1)$$

where

$$W_p(r, p) = W_0 + \frac{1}{2} W_0''(r - r_0)^2$$
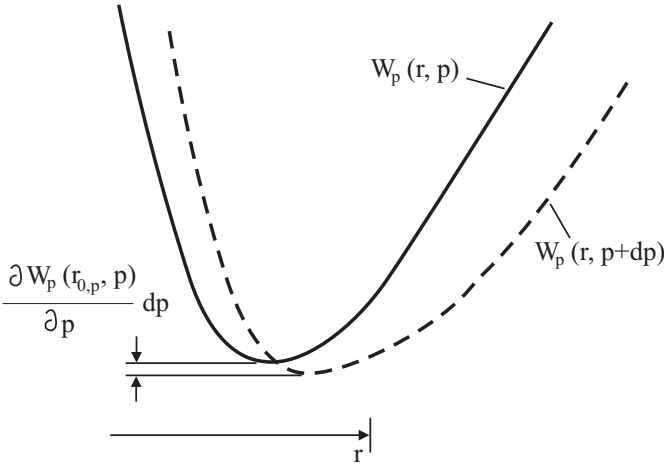$$- \frac{1}{6} W_0'''(r - r_0)^3 - p \, r_0^2 \, r \quad (A.2)$$

Fig. 6. Potential curves $W_p(r, p + \mathrm{d}p)$ and $W_p(r, p)$.

and

$$
W_p(r_{0,p}, p) = W_0 + \frac{1}{2} W_0''(r_{0,p} - r_0)^2
$$
$$
- \frac{1}{6} W_0'''(r_{0,p} - r_0)^3 - p\, r_0^2\, r_{0,p} \; . \quad \text{(A.3)}
$$

In equation (A.1) the term $W_p(r, p + \mathrm{d}p) - W_p(r, p)$ represents the difference between the curves $W_p(r, p + \mathrm{d}p)$ and $W_p(r, p)$ for a fixed r. The term $\frac{\partial W_p(r_{0,p}, p)}{\partial p}\, \mathrm{d}p$ is the difference between the minimum of $W_p(r, p + \mathrm{d}p)$ and the minimum of $W_p(r, p)$.

The position of the minimum $r_{0,p}$ of the potential curve W_p is given by

$$
r_{0,p} - r_0 = \frac{W_0''}{W_0'''} - \frac{W_0''}{W_0'''} \sqrt{1 - 2\, \frac{W_0'''}{W_0''^2}\, r_0^2\, p} \; . \quad \text{(A.4)}
$$

Substituting equation (A.4) into (A.3) and differentiating with respect to p leads to

$$
\frac{\partial W_p(r_{0,p}, p)}{\partial p} = \frac{r_0^2\, W_0''}{W_0'''} \times \left[\frac{1}{\sqrt{1 - 2\, \frac{W_0'''}{W_0''^2}\, r_0^2\, p}} - 1 \right]
$$
$$
\times \left[1 - \sqrt{1 - 2\, \frac{W_0'''}{W_0''^2}\, r_0^2\, p} \right]
$$
$$
- \frac{r_0^2\, W_0''}{2\, W_0''' \sqrt{1 - 2\, \frac{W_0'''}{W_0''^2}\, r_0^2\, p}}
$$
$$
\times \left[1 - \sqrt{1 - 2\, \frac{W_0'''}{W_0''^2}\, r_0^2\, p} \right]^2
$$
$$
- \frac{r_0^4\, p}{W_0'' \sqrt{1 - 2\, \frac{W_0'''}{W_0''^2}\, r_0^2\, p}} - r_0^3 \; .
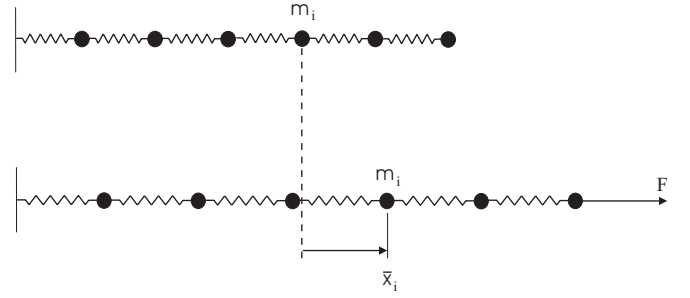$$
$$
\text{(A.5)}
$$

Fig. 7. 1D array of springs.

Thus, weighting according to (32), the differential difference of energy is found to be

$$
\mathrm{d}E = \frac{1}{\overline{T}(p)} \int\limits_c^b \frac{\mathrm{d}E(r, p)}{\dot{r}(r, p)}\, \mathrm{d}r \; . \quad \text{(A.6)}
$$

Note, if we apply the load p, the form of the potential curve and therefore the position of the roots a, b and c will change. Hence, a, b and c are functions of p. Moreover, the velocity $\dot{r}$ and $\overline{T}$ are functions of p. The general expression for the difference of energy due to applying the load p is given by

$$
\Delta E = \int\limits_0^p \frac{1}{\overline{T}(p)} \int\limits_{c(p)}^{b(p)} \frac{1}{\dot{r}(r, p)}
$$
$$
\times \left(\frac{\partial W_p(r, p)}{\partial p} - \frac{\partial W_p(r_{0,p}, p)}{\partial p} \right) \mathrm{d}r\, \mathrm{d}p \; . \quad \text{(A.7)}
$$

This integral can not be solved analytically. For $p = 0$, equation (A.1) leads to equation (30) and equation (A.6) leads to equation (33). Strictly speaking, equation (A.7) is not the exact expression for the energy difference since not all particles have the same mean temperature. Further average calculations would have to be carried out.

Appendix B

The calculations in Section 3 are based on the model of statistically independent oscillating particles. Due to this hypothesis, the hydrostatic force $\mathrm{d}F$ can approximatively be taken into account by a linear potential (see Eq. (26)). Also, the same approach is applied in the determination of the modulus of elasticity with the non-interacting model [11].

Why a hydrostatic force gives (approximatively) rise to a linear potential can be illustrated by a simple 1D spring model (see Fig. 7). The particles m_i are connected with linear springs (spring constant c). The position of the particles is determined by the coordinates x_i. If a constant force F is applied at the right end of the array, the particles take a new position of equilibrium characterized by the coordinates $\bar{x}_i$.

According to the non-interacting model, we fix all particles except the particle m_i. On this particle acts the force
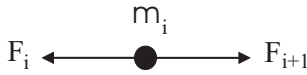
Fig. 8. Forces acting upon particle m_i.

$F_i = c\,(x_i - \bar{x}_{i-1})$ due to the left spring and the force $F_{i+1} = c\,(\bar{x}_{i+1} - x_i)$ due to the right spring (Fig. 8), so that the resultant force is given by $F_R = -2\,c\,x_i + c\,(\bar{x}_{i-1} + \bar{x}_{i+1})$. Since $\bar{x}_{i-1}$ and $\bar{x}_{i+1}$ are constants, the potential of F_R is given by $W_R = c\,x_i^2 - c\,(\bar{x}_{i-1} + \bar{x}_{i+1})\,x_i$.

Assuming linear springs, the applied force F causes a linear potential. If the springs are nonlinear according to equation (17), there appear additional quadratic and cubic terms in the potential. Further investigations with the data in Appendix C show that these terms are much more smaller than the linear term so that they can be neglected.

Since an array of springs is related to an interacting model, the above considerations cannot be entirely consistent with the non-interacting model. But they are useful to demonstrate that there approximatively occurs a linear potential due to a constant hydrostatic force.

Appendix C

The data used in the previous sections are itemized below. The data are taken from [17].

	Fe
distance of equilibrium r_0 [Å]:	2.5
coefficient of thermal expansion α $[10^6\,\frac{1}{K}]$:	12
Young's modulus E $[10^{10}\,\frac{N}{m^2}]$:	16.83
specific heat capacity c_V $[\frac{J}{kg\ K}]$:	460
Poisson's ratio ν:	0.28
density ρ $[10^3\,\frac{kg}{m^3}]$:	7.87
atomic mass m_A $[1.66 \times 10^{-27}$kg]:	55.85

	Al
distance of equilibrium r_0 [Å]:	2.88
coefficient of thermal expansion α $[10^6\,\frac{1}{K}]$:	23.8
Young's modulus E $[10^{10}\,\frac{N}{m^2}]$:	7.22
specific heat capacity c_V $[\frac{J}{kg\ K}]$:	945
Poisson's ratio ν:	0.34
density ρ $[10^3\,\frac{kg}{m^3}]$:	2.66
atomic mass m_A $[1.66 \times 10^{-27}$kg]:	26.98

	Au
distance of equilibrium r_0 [Å]:	2.88
coefficient of thermal expansion α $[10^6\,\frac{1}{K}]$:	14.2
Young's modulus E $[10^{10}\,\frac{N}{m^2}]$:	8
specific heat capacity c_V $[\frac{J}{kg\ K}]$:	130
Poisson's ratio ν:	0.424
density ρ $[10^3\,\frac{kg}{m^3}]$:	19.32
atomic mass m_A $[1.66 \times 10^{-27}$kg]:	196.97.

With these data, we get the following values for the constants W_0'' and W_0'''.

	iron	aluminium	gold
W_0'' $[\frac{N}{m}]$:	42.075	20.794	23.04
W_0''' $[10^{12}\,\frac{N}{m^2}]$:	0.5074	0.2694	0.2074.

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