

Derivation of Equations of State for Ideal Crystals of Simple Structure

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Abstract—We consider an approach to the derivation of thermodynamic equations of state by averaging the dynamic equations of particles of the crystal lattice. Microscopic analogs of macroscopic variables such as pressure, volume, and thermal energy are introduced. An analysis of the introduced variables together with the equations of motion permits obtaining the equation of state. Earlier, this approach was used to obtain the equation of state in the Mie–Grüneisen form for a one-dimensional lattice. The aim of this paper is to develop and generalize this approach to the three-dimensional case. As a result, we obtain the dependence of the Grüneisen function on the volume, which is compared with the computations performed according to well-known models with experimental data taken into account. It is proved that the Grüneisen coefficient substantially depends on the form of the strain state. Moreover, we refine the equation of state; namely, we show that the Grüneisen coefficient depends on the thermal energy, but this dependence in the three-dimensional case is much weaker than in the one-dimensional case. A refined equation of state containing a nonlinear dependence on the thermal energy is obtained.

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1. INTRODUCTION

The problem of deriving equations of state for condensed matter with admissible accuracy in a sufficiently wide range of thermal actions and mechanical loads is still a complicated and hard-to-solve problem of modern physics. The fundamental laws of nature such as the first and second laws of thermodynamics and the principle of material objectivity permit obtaining only some restrictions on the structure of the constitutive equations [1, 2], and the remaining ambiguity in the construction of equations of state is still rather large. As a result, the empirical equations of state used in practice in application software packages can often lead to instabilities of various kind and physically wrong results [3].

In such a situation, it is extremely useful to develop models in which the equations of state can be obtained analytically with some accuracy. In practice, the Mie–Grüneisen equation is often used, in which the dependence of the pressure p on the thermal energy E_T is assumed to be linear [4],

$$p = p(V, E_T) = p_0(V) + \frac{\Gamma(V)E_T}{V},$$

where V is the volume. As a rule, methods of statistical physics are used to obtain $\Gamma(V)$, which is called the Grüneisen function. Here the key role is played by the assumption that the interatomic interactions are linear. An expression for the Grüneisen function was obtained for a one-dimensional lattice in [5]. In the three-dimensional case, $\Gamma(V)$ can be expressed via the so-called “cold curve” (i.e., via the dependence $p_0(V)$) [6–8]. For the cold curve, there are many analytic expressions and experimental data [4, 9, 10]. In [11], the results obtained by using the models [6–8] are written in general form by introducing a parameter such that all above-listed models are obtained for different values of this

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parameter. Moreover, as shown in [4], the desired dependence $\Gamma(V)$ is significantly different for different models. In [12], it was noted that this dependence holds only for isotropic structures or structures with cubic symmetry. In the general case, it is necessary to take into account the tensor properties of the Grüneisen coefficient. Moreover, the use of these methods in the case of an anharmonic interaction potential is a very hard problem, which is not solved yet. A qualitative estimate of the influence of the anharmonic terms can be found in [4].

An alternative approach based on the assumption that a solid is a set of interacting particles moving according to the laws of classical mechanics has been intensively developed in the last years because of increasing interest in studying the mechanical behavior of nanostructure systems [13–16]. By averaging the equations of particle dynamics, one can derive the macroscopic equation of state; this was shown in [17–19] on the example of a one-dimensional crystal. In [17–19], the microscopic counterparts of pressure, thermal energy, and other macroscopic variables were introduced for discrete systems. Then these variables were averaged over time and expanded in series in a small parameter characterizing the thermal motion. Thus, the Mie–Grüneisen equation of state was derived for a one-dimensional lattice and the dependence of the Grüneisen coefficient on the specific volume was computed. It was also shown that the Mie–Grüneisen equation of state cannot be used in the case of strong tensile strains, and a refined equation of state was obtained for this case.

In the present paper, we generalize and develop the approaches in [17, 18]. We consider a set of particles forming an ideal crystal lattice in spaces of various dimension, which permits generalizing the equations earlier constructed in [17, 18] for one-dimensional crystals. We determine the dependence of the Grüneisen coefficient on the volume and show that the form of this dependence is determined by the strain state of the crystal. The Grüneisen function thus obtained is compared with the results of computations according to known models with experimental data taken into account. Moreover, the equation of state is also refined.

2. BASIC ASSUMPTIONS AND NOTATION

Consider an ideal infinite monocrystal in a space of dimension 1, 2, or 3. We only deal with crystals of simple structure (i.e., crystals that do not change under parallel translation by a vector connecting any two nodes of the crystal lattice). The interatomic interaction is described by a pairwise central potential; by way an example, we consider the Lennard–Jones, Mie, and Morse potentials.

We introduce the time averaging operator

$$\langle f(t) \rangle = \frac{1}{T} \int_0^T f(t) dt,$$

where T is a time interval much greater than the characteristic period of atomic vibrations in the lattice. In addition to time averaging, it is expedient to introduce averaging over the space (to increase the approximation accuracy), but here, for simplicity, we do not perform this averaging. Then any variable f can be represented as the sum of the averaged component $\langle f \rangle$ slowly varying in time and the oscillatory component \tilde{f} , $f = \langle f \rangle + \tilde{f}$, rapidly varying in time. We assume that the oscillatory component is small compared with the averaged component.

We also assume that the averaged variables obey the long-wave approximation [20] according to which the variations in these variables at distances of the order of the distance between neighboring particles are small. This allows us to assume that this distance is a small parameter in which the averaged equations can be expanded in a series.

Let us introduce the basic notation [19]. We choose some original particle and number all particles interacting with it by the index α . By \mathbf{a}_α we denote the vector connecting the original particle with particle α in the reference (undeformed) configuration. The same vector in the actual (deformed) configuration is represented as the sum of the time-averaged component \mathbf{A}_α and the oscillatory component $\tilde{\mathbf{A}}_\alpha$. We also introduce the specific volume V per particle in the actual configuration. In the case of bulk strain of a densely packed crystal lattice, it can be computed by the formula

$$V = \frac{\sqrt{5-d}}{2} A^d,$$

where A is the lattice spacing (the distance between nearest atoms) and d is the space dimension. The Cauchy stress tensor is determined by the formula in [19] generalized to the case of nonzero thermal motion,

$$\tau = \frac{1}{2V} \sum_{\alpha} \mathbf{A}_{\alpha} \langle \mathbf{F}_{\alpha}(\mathbf{A}_{\alpha} + \tilde{\mathbf{A}}_{\alpha}) \rangle, \quad (2.1)$$

where \mathbf{F}_{α} is the force exerted by the particle α on the particle under study. The expressions for the Cauchy and Piola stress tensors for discrete systems without thermal motion taken into account were obtained in [19]. Let us present a similar derivation with thermal motion taken into account.

We write out the averaged equation of motion for a particle (which will be called the original particle) and transform it as follows:

$$m\ddot{\mathbf{u}} = \sum_{\alpha} \langle \mathbf{F}_{\alpha} \rangle = \sum_{\alpha} \langle \mathbf{F}_{-\alpha} \rangle = \frac{1}{2} \sum_{\alpha} \langle \mathbf{F}_{\alpha} + \mathbf{F}_{-\alpha} \rangle, \quad (2.2)$$

where \mathbf{u} is the averaged displacement of the particle. Consider the particle with index $-\alpha$ in the numbering related to the original particle. For this particle, we construct a similar numbering, where the original particle has index α . Then, by denoting the position vector of the reference particle in the undeformed configuration by \mathbf{r} and by applying Newton's third law, we can write

$$\mathbf{F}_{\alpha}(\mathbf{r} - \mathbf{a}_{\alpha}) = -\mathbf{F}_{-\alpha}(\mathbf{r}). \quad (2.3)$$

By averaging this expression and by applying the long-wave approximation, we obtain

$$\langle \mathbf{F}_{-\alpha} \rangle(\mathbf{r}) \approx -\langle \mathbf{F}_{\alpha} \rangle(\mathbf{r}) + \mathbf{a}_{\alpha} \cdot \overset{\circ}{\nabla} \langle \mathbf{F}_{\alpha} \rangle(\mathbf{r}), \quad (2.4)$$

where $\overset{\circ}{\nabla}$ is the nabla operator in the reference configuration. By substituting formula (2.4) into Eq. (2.2) and by dividing both sides by the volume V_0 of the elementary cell in the reference configuration, we obtain

$$\rho_0 \ddot{\mathbf{u}} = \overset{\circ}{\nabla} \cdot \frac{1}{2V_0} \sum_{\alpha} \mathbf{a}_{\alpha} \langle \mathbf{F}_{\alpha} \rangle, \quad \rho_0 = \frac{m}{V_0}. \quad (2.5)$$

Let us compare this expression with the continuum dynamic equation in the Piola form [24]. One can readily see that the expression for the Piola stress tensor has the form

$$\mathbf{P} = \frac{1}{2V_0} \sum_{\alpha} \mathbf{a}_{\alpha} \langle \mathbf{F}_{\alpha} \rangle. \quad (2.6)$$

Now let us obtain the expression for the Cauchy stress tensor. Consider the vectors \mathbf{a}_{α} and \mathbf{A}_{α} . Let $\mathbf{R}(\mathbf{r})$ be the position vector of the reference particle in the actual configuration. Then, in the long-wave approximation, we have

$$\mathbf{A}_{\alpha} = \langle \mathbf{R}(\mathbf{r} + \mathbf{a}_{\alpha}) - \mathbf{R}(\mathbf{r}) \rangle \approx \mathbf{a}_{\alpha} \cdot \langle \overset{\circ}{\nabla} \mathbf{R} \rangle. \quad (2.7)$$

By applying the well-known relation [24]

$$\tau = \frac{V_0}{V} \langle \overset{\circ}{\nabla} \mathbf{R} \rangle^T \cdot \mathbf{P}$$

between the Cauchy and Piola tensors and formula (2.7), we obtain formula (2.1) for the Cauchy stress tensor.

For convenience, in what follows we represent \mathbf{F}_{α} in the form

$$\mathbf{F}(\mathbf{A}) = -\Phi(A^2)\mathbf{A}, \quad \Phi(A^2) = -\frac{\Pi'(A)}{A}, \quad (2.8)$$

where Π is the potential of interaction between these two particles and A is the modulus of the vector \mathbf{A} . We rewrite expression (2.1) using formula (2.8),

$$\tau = -\frac{1}{2V} \sum_{\sigma} \langle \Phi_{\sigma} \rangle \mathbf{A}_{\sigma} \mathbf{A}_{\sigma} - \frac{1}{2V} \sum_{\alpha} \mathbf{A}_{\alpha} \langle \tilde{\Phi}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \rangle. \quad (2.9)$$

For the obtained Cauchy stress tensor to be symmetric, it is necessary that both tensors on the right-hand side in (2.9) be symmetric. It is well known that the symmetry of the Cauchy tensor follows from the momentum balance equation for an elementary volume of the continuum. In the case under study, the role of elementary volume is played by an elementary cell of the crystal lattice. Let us write out the equilibrium condition for the elementary cell. Then we calculate the moments of forces with respect to the cell center determined by the vector $\langle \mathbf{R} \rangle$:

$$\left\langle \tilde{\mathbf{u}} \times \sum_{\alpha} \tilde{\mathbf{F}}_{\alpha} \right\rangle = 0. \quad (2.10)$$

Using the long-wave approximation, one can readily show that

$$\left\langle \tilde{\mathbf{u}} \times \sum_{\alpha} \tilde{\mathbf{F}}_{\alpha} \right\rangle \approx -\frac{1}{2} \sum_{\alpha} \langle \tilde{\mathbf{A}}_{\alpha} \times \tilde{\mathbf{F}}_{\alpha} \rangle = \sum_{\alpha} \mathbf{A}_{\alpha} \times \langle \tilde{\Phi}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \rangle = 0. \quad (2.11)$$

It follows from the last formula that the tensor $\sum_{\alpha} \mathbf{A}_{\alpha} \langle \tilde{\Phi}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \rangle$, as well as the Cauchy tensor determined by formula (2.1), is symmetric. Note that in the absence of the thermal motion formula (2.1) for the stress tensor coincides with the result obtained in [21].

Let us introduce the specific thermal energy E_T per particle. By the thermal energy we mean the part of internal energy corresponding to the chaotic motion of particles. The specific thermal energy can be represented as the sum of two components, the kinetic energy K_T and the potential energy U_T , determined by the formulas

$$K_T = \frac{1}{2} m \langle \dot{\tilde{\mathbf{u}}}^2 \rangle, \quad U_T = \frac{1}{2} \sum_{\alpha} \Pi \langle (|\mathbf{A}_{\alpha} + \tilde{\mathbf{A}}_{\alpha}|) - \Pi(A_{\alpha}) \rangle, \quad (2.12)$$

where A_{α} is the modulus of the vector \mathbf{A}_{α} .

3. SERIES EXPANSION. THE FIRST APPROXIMATION

Following the above approach to the derivation of the equations of state, we expand the expressions (2.1) and (2.12) in series in the small parameter \tilde{A}_{α} characterizing the thermal motion.

To expand the kinetic component of the thermal energy, we make transformations similar to those used in the proof of the virial theorem [22],

$$\langle \dot{\tilde{\mathbf{u}}}^2 \rangle = \frac{1}{T} \int_0^T \dot{\tilde{\mathbf{u}}}^2 dt = \frac{1}{T} (\dot{\tilde{\mathbf{u}}} \cdot \tilde{\mathbf{u}}) \Big|_0^T - \frac{1}{m} \sum_{\alpha} \langle \tilde{\mathbf{u}} \cdot \tilde{\mathbf{F}}_{\alpha} \rangle,$$

where we have used the equation of motion $m \ddot{\tilde{\mathbf{u}}} = \sum_{\alpha} \tilde{\mathbf{F}}_{\alpha}$. Assuming that the displacements and velocities of points are bounded, we neglect the first term on the right-hand side in the obtained formula because of its smallness for large T . Then we obtain

$$K_T = \frac{1}{2} m \langle \dot{\tilde{\mathbf{u}}}^2 \rangle = -\frac{1}{2} \sum_{\alpha} \langle \tilde{\mathbf{u}} \cdot \tilde{\mathbf{F}}_{\alpha} \rangle. \quad (3.1)$$

By expanding $\mathbf{F}_{\alpha} = \mathbf{F}(\mathbf{A}_{\alpha} + \tilde{\mathbf{A}}_{\alpha})$ in a series in the small oscillatory component $\tilde{\mathbf{A}}_{\alpha}$ and by preserving the terms up to the order of $\tilde{\mathbf{A}}_{\alpha}^2$ inclusively, we obtain

$$K_T = -\frac{1}{4} \sum_{\alpha} \left[\Phi(A_{\alpha}^2) \mathbf{E} + 2\Phi'(A_{\alpha}^2) \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \right] \cdot \langle \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \rangle. \quad (3.2)$$

When deriving formula (3.2), we have used the identity

$$\langle \tilde{\mathbf{u}} \tilde{\mathbf{A}}_{\alpha} \rangle^S = -\frac{1}{2} \langle \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \rangle. \quad (3.3)$$

To prove this identity, consider the tensor $\langle \tilde{\mathbf{A}}_\alpha \tilde{\mathbf{A}}_\alpha \rangle$. By \mathbf{u}_α we denote the oscillatory component of the displacement of the atom α . Obviously, we have

$$\tilde{\mathbf{A}}_\alpha = \tilde{\mathbf{u}}_\alpha - \tilde{\mathbf{u}}. \quad (3.4)$$

We express $\langle \tilde{\mathbf{A}}_\alpha \tilde{\mathbf{A}}_\alpha \rangle$ via $\tilde{\mathbf{u}}_\alpha$ and $\tilde{\mathbf{u}}$ and obtain

$$\langle \tilde{\mathbf{A}}_\alpha \tilde{\mathbf{A}}_\alpha \rangle = 2\langle \tilde{\mathbf{u}}\tilde{\mathbf{u}} \rangle - 2\langle \tilde{\mathbf{u}}\tilde{\mathbf{u}}_\alpha \rangle^S. \quad (3.5)$$

Here we have used the fact that $\langle \tilde{\mathbf{u}}\tilde{\mathbf{u}} \rangle \equiv \langle \tilde{\mathbf{u}}_\alpha \tilde{\mathbf{u}}_\alpha \rangle$, because the state of the crystal lattice under study is homogeneous. Identity (3.3) follows directly from (3.4) and (3.5).

Now consider $\langle \tilde{\mathbf{A}}_\alpha^2 \rangle$, i.e., the trace of the tensor $\langle \tilde{\mathbf{A}}_\alpha \tilde{\mathbf{A}}_\alpha \rangle$. Formula (3.5) implies that

$$\langle \tilde{\mathbf{A}}_\alpha^2 \rangle = 2\langle \tilde{\mathbf{u}}^2 \rangle - 2\langle \tilde{\mathbf{u}} \cdot \tilde{\mathbf{u}}_\alpha \rangle. \quad (3.6)$$

Let us show that, when deriving the equation of state, we can assume that $\langle \tilde{\mathbf{A}}_\alpha^2 \rangle$ is independent of α . The first term in formula (3.6), i.e., the displacement dispersion $\langle \tilde{\mathbf{u}}^2 \rangle$, is indeed independent of α . But the second term, i.e., the correlation $\langle \tilde{\mathbf{u}} \cdot \tilde{\mathbf{u}}_\alpha \rangle$, in general depends on α . This dependence can be insignificant for atoms belonging to the same coordination sphere, but for atoms belonging to different coordination spheres the correlations differ significantly; namely, their modulus must decrease with increasing radius of the sphere. But we can still neglect the dependence of $\langle \tilde{\mathbf{A}}_\alpha^2 \rangle$ on α because of the following considerations. First, the correlation modulus is less than the dispersion, $\langle \tilde{\mathbf{u}} \cdot \tilde{\mathbf{u}}_\alpha \rangle < \langle \tilde{\mathbf{u}}^2 \rangle$, and possibly significantly less. Second, the largest contribution to the equation of state comes from the terms corresponding to the first coordination sphere. The error in determining $\langle \tilde{\mathbf{A}}_\alpha^2 \rangle$ for the subsequent coordination spheres is multiplied by small factors corresponding to the rapid decay of the interatomic interaction and hence does not contribute significantly to the error in the equation of state.

The expansion of the potential component of the thermal energy defined by formula (2.12) gives the expression identical to (3.2), so that in our approximation we obtain

$$K_T = U_T = \frac{1}{2}E_T,$$

which, on the other hand, is a straightforward consequence of the virial theorem [22].

Let us introduce the thermal stress tensor τ_T as follows:

$$\tau_T = \tau - \tau_0, \quad \tau_0 = \tau|_{\tilde{\mathbf{A}}_\alpha=0} = -\frac{1}{2V} \sum_\alpha \Phi(A_\alpha^2) \mathbf{A}_\alpha \mathbf{A}_\alpha. \quad (3.7)$$

For the thermal stress tensor, we use an expansion similar to that considered above and obtain the system of equations

$$\begin{aligned} \tau_T &= -\frac{1}{2V} \sum_\alpha \left[2\Phi'_\alpha \mathbf{A}_\alpha \mathbf{E} \mathbf{A}_\alpha + \Phi'_\alpha \mathbf{A}_\alpha \mathbf{A}_\alpha \mathbf{E} + \Phi''_\alpha \mathbf{A}_\alpha \mathbf{A}_\alpha \mathbf{A}_\alpha \mathbf{A}_\alpha \right] \cdot \langle \tilde{\mathbf{A}}_\alpha \tilde{\mathbf{A}}_\alpha \rangle, \\ E_T &= -\frac{1}{2} \sum_\alpha \left[\Phi_\alpha \mathbf{E} + 2\Phi'_\alpha \mathbf{A}_\alpha \mathbf{A}_\alpha \right] \cdot \langle \tilde{\mathbf{A}}_\alpha \tilde{\mathbf{A}}_\alpha \rangle, \quad \Phi_\alpha^{(n)} = \Phi^{(n)}(A_\alpha^2). \end{aligned} \quad (3.8)$$

To obtain the constitutive equation in explicit form, one should make some assumption about the structure of the tensor $\langle \tilde{\mathbf{A}}_\alpha \tilde{\mathbf{A}}_\alpha \rangle$. We assume that this is a spherical tensor independent of α . Note that, strictly speaking, the second of these assumptions is not satisfied if one considers more than one coordination sphere. But, as was shown above, this does not lead to a significant error in the equations of state obtained below. Thus, under the cited assumptions, the tensor $\langle \tilde{\mathbf{A}}_\alpha \tilde{\mathbf{A}}_\alpha \rangle$ can be represented as

$$\langle \tilde{\mathbf{A}}_\alpha \tilde{\mathbf{A}}_\alpha \rangle = \frac{1}{d} \kappa^2 \mathbf{E}, \quad \kappa^2 = \langle \tilde{\mathbf{A}}_\alpha^2 \rangle. \quad (3.9)$$

This representation allows completely specifying the thermal state in an elementary volume by a single scalar parameter, which permits relating the obtained results to the classical thermodynamics, where the

role of this parameter is played by temperature (or thermal energy). Using (3.9), we rewrite Eqs. (3.8) as

$$\begin{aligned}\tau_T &= -\frac{\kappa^2}{2dV} \sum_{\alpha} [(d+2)\Phi'_{\alpha} + 3\Phi''_{\alpha}A_{\alpha}^2] \mathbf{A}_{\alpha} \mathbf{A}_{\alpha}, \\ E_T &= -\frac{\kappa^2}{2d} \sum_{\alpha} (d\Phi_{\alpha} + 2\Phi'_{\alpha}A_{\alpha}^2).\end{aligned}\quad (3.10)$$

4. MIE–GRÜNEISEN EQUATION OF STATE

Consider the classical Mie–Grüneisen equation of state

$$p = p_0(V) + p_T(V, E_T), \quad p_T(V, E_T) = \Gamma(V) \frac{E_T}{V}. \quad (4.1)$$

Here p_0 is the “cold pressure” and Γ is the dimensionless Grüneisen coefficient. According to (4.1), both variables are functions of the specific volume V alone. Let us find the relation between the pressure, the thermal energy, and the specific volume in our case. We define the total, cold, and thermal pressure by the formulas

$$p = -\frac{1}{d} \operatorname{tr} \tau, \quad p_0 = -\frac{1}{d} \operatorname{tr} \tau_0, \quad p_T = -\frac{1}{d} \operatorname{tr} \tau_T.$$

Then, by using (3.7) and by eliminating κ^2 from system (3.10), we readily obtain the relation between the pressure and the thermal energy in the form (4.1), where

$$p_0 = \frac{1}{2Vd} \sum_{\alpha} \Phi_{\alpha} A_{\alpha}^2, \quad \Gamma = -\frac{\sum_{\alpha} [(d+2)\Phi'_{\alpha} A_{\alpha}^2 + 2\Phi''_{\alpha} A_{\alpha}^4]}{d \sum_{\alpha} (d\Phi_{\alpha} + 2\Phi'_{\alpha} A_{\alpha}^2)}. \quad (4.2)$$

It follows from (4.2) that in general the cold pressure and the Grüneisen coefficient depend on the total strain (rather than on its bulk component, as is usually assumed). The dependence of the Grüneisen coefficient on the form of the strain state will be considered below.

Now consider the case of bulk strain. Then we have

$$\mathbf{A}_{\alpha} = \theta \mathbf{a}_{\alpha}, \quad \theta = \left(\frac{V}{V_0} \right)^{1/d},$$

where V_0 is the reference value of the specific volume. In what follows, it is convenient to pass from summation over atoms to summation over the coordination spheres. As a result, formulas (4.2) become

$$p_0 = \frac{1}{2V_0 d \theta^d} \sum_{k=1}^n N_k \Phi_k A_k^2, \quad \Gamma = -\frac{\sum_{k=1}^n N_k [(d+2)\Phi'_k A_k^2 + 2\Phi''_k A_k^4]}{d \sum_{k=1}^n N_k (d\Phi_k + 2\Phi'_k A_k^2)}, \quad (4.3)$$

where n is the number of coordination spheres, N_k is the number of atoms on the k th coordination sphere, $A_k = \rho_k R \theta$ is the radius of the k th coordination sphere, the numbers $\rho_k = A_k/A_1$ are dimensionless lattice constants, R is the radius of the first coordination sphere in the reference configuration, and $\Phi_k^{(n)} = \Phi^{(n)}(A_k^2)$. If only the nearest neighbor interaction in the crystal lattice is taken into account, then, using definition (2.8) of the functions $\Phi(A^2)$, we can rewrite formulas (4.3) in the form

$$p_0 = -\frac{M}{2V_0 d \theta^d} \Pi'(A) A, \quad \Gamma = -\frac{1}{2d} \frac{\Pi'''(A) A^2 + (d-1)[\Pi''(A) A - \Pi'(A)]}{\Pi''(A) A + (d-1)\Pi'(A)}, \quad (4.4)$$

where M is the coordination number¹⁾ and $A = R\theta$. If the reference state of the lattice is unstressed, then for formula (4.4) we obtain $R \equiv a$, where a is the bond distance (the equilibrium distance in a two-atom system). Note that, according to (4.4), the Grüneisen coefficient does not in any way depend on the structure of the crystal lattice (provided that the interaction is restricted to the first coordination sphere).

¹⁾The number of nearest neighbors of an atom in the lattice.

5. IMPORTANT SPECIAL CASES

In what follows, we present the formulas for three classical interaction potentials and the expressions for the cold pressure computed for them by the first formula in (4.4):

The Lennard–Jones potential

$$\Pi(r) = D \left[\left(\frac{a}{r} \right)^{12} - 2 \left(\frac{a}{r} \right)^6 \right] \Rightarrow p_0 = \frac{6MD}{dV_0\theta^d} (\theta^{-12} - \theta^{-6}).$$

The Mie potential

$$\Pi(r) = \frac{D}{n-m} \left[m \left(\frac{a}{r} \right)^n - n \left(\frac{a}{r} \right)^m \right] \Rightarrow p_0 = \frac{mnMD}{2d(n-m)V_0\theta^d} (\theta^{-n} - \theta^{-m}).$$

The Morse potential

$$\Pi(r) = D [e^{2\alpha(a-r)} - 2e^{\alpha(a-r)}] \Rightarrow p_0 = \frac{\alpha a MD}{dV_0\theta^{d-1}} [e^{2\alpha a(1-\theta)} - 2e^{\alpha a(1-\theta)}].$$

Here D is the binding energy, a is the bond distance, α is a parameter characterizing the potential well width, and m and n are parameters of the Mie potential. In what follows, we present formulas for the Grüneisen coefficient computed for the above potentials by the second formula in (4.4).

For the Lennard–Jones potential,

$$\Gamma = \frac{1}{d} \frac{4(8-d)\theta^6 - 7(14-d)}{(8-d)\theta^6 - (14-d)}.$$

For the Mie potential,

$$\Gamma = \frac{1}{2d} \frac{(n+2)(n-d+2)\theta^{m-n} - (m+2)(m-d+2)}{(n-d+2)\theta^{m-n} - (m-d+2)}. \tag{5.1}$$

For the Morse potential,

$$\Gamma = \frac{1}{2d} \frac{e^{\alpha a(1-\theta)}(4\alpha^2 a^2 \theta^2 - 2d_1 \alpha a \theta - d_1) - (\alpha^2 a^2 \theta^2 - d_1 \alpha a \theta - d_1)}{e^{\alpha a(1-\theta)}(2\alpha a \theta - d_1) - (\alpha a \theta - d_1)}, \tag{5.2}$$

$$d_1 = d - 1, \quad \theta = \left(\frac{V}{V_0} \right)^{1/d}.$$

The Grüneisen coefficient Γ_0 computed for $V = V_0$ ($\theta = 1$) is of great practical importance, because the dependence on the volume is often neglected in engineering computations. (For small volume variations, this simplification is often quite reasonable.)

For the Lennard–Jones potential,

$$\Gamma_0 = \frac{11}{d} - \frac{1}{2}, \quad d = 3 \Rightarrow \Gamma_0 = \frac{19}{6} \approx 3.17. \tag{5.3}$$

For the Mie potential,

$$\Gamma_0 = \frac{m+n+4}{2d} - \frac{1}{2}, \quad d = 3 \Rightarrow \Gamma_0 = \frac{n+m+1}{6}. \tag{5.4}$$

For the Morse potential,

$$\Gamma_0 = \frac{3\alpha a + 1}{2d} - \frac{1}{2}, \quad d = 3 \Rightarrow \Gamma_0 = \frac{3\alpha a - 2}{6}. \tag{5.5}$$

Note that the values of Γ_0 for the Lennard–Jones and Morse potentials coincide for $\alpha a = 7$ (regardless of the space dimension). According to the above formulas, the value of the Grüneisen coefficient rapidly decays with increasing space dimension. For example, for the Lennard–Jones potential we have $d = 1 \Rightarrow \Gamma_0 = 10.5$, $d = 2 \Rightarrow \Gamma_0 = 5$, and $d = 3 \Rightarrow \Gamma_0 \approx 3.17$.

Since the values of Γ_0 were experimentally obtained for many materials [9], formulas (5.2)–(5.4) for $d = 3$ can be used to choose the parameters of the potential from known experimental data.

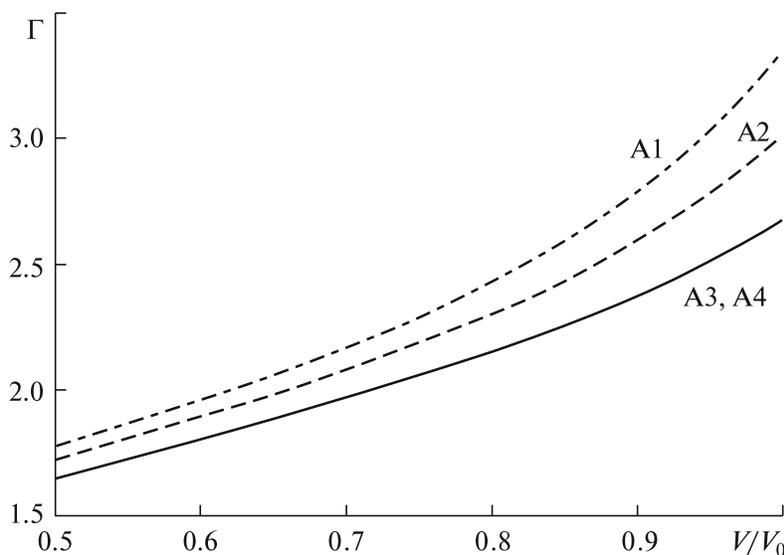


Fig. 1.

6. COMPARISON WITH CLASSICAL MODELS

There are many substantially different approaches to determining the Grüneisen coefficient. The models proposed in [6–8] are used most frequently. The comparison performed in [11] showed that all models proposed above can be reduced to the generalized form

$$\Gamma(V) = -\frac{4-3n}{6} - \frac{V}{2} \frac{d^2(p_0 V^n)/dV^2}{d(p_0 V^n)/dV}, \quad (6.1)$$

where p_0 is the “cold” pressure, V is the elementary cell volume, and n is the model parameter equal to 0, 2/3, and 4/3 for [6–8], respectively. Thus, the Grüneisen coefficient in these models is determined on the basis of the so-called “cold curve,” i.e., the dependence $p_0(V)$. This curve in a small range of volumes can relatively easily be obtained from experiments. However, as was shown in [4], the Grüneisen functions constructed on the basis of the above models differ significantly, and there is still no final answer to the question as to which of the models is preferable.

By substituting the expression (4.4) for the pressure into (6.1), we obtain $\Gamma(V/V_0)$. In Fig. 1, we present the dependencies $\Gamma(V/V_0)$ for $\alpha a = 6$ for various values of the parameter n . The curves corresponding to the models [6–8] and to the proposed model are denoted on the graph by A1–A4, respectively. The graphs corresponding to the proposed model and the model [8] are practically indistinguishable. In [8], the free volume theory was used to consider the vibrations of atoms in a spherically symmetric field of their neighbors. Such a model approximately corresponds to vibrations of an atom in an elementary cell of a crystal with fixed neighbors. By using the first formula in (4.4) for $p_0(V)$, one can show that formula (6.1) with $n = 4/3$ gives precisely the same dependence $\Gamma(V)$ as the second formula in (4.4). Thus, if only the nearest neighbor interaction is taken into account, then our model gives the same result as the model [8]. If the subsequent coordination spheres are taken into account, then the results will be different.

Let us compare our results with those obtained in [23] on the basis of classical models with experimental data taken into account. In Figs. 2 and 3, we present the graphs of the dependence $\Gamma(V/V_0)$, which are computed by formula (5.1) and illustrate the data given in [22] for several metals with a face-centered cubic lattice. Curves A1 (solid line) and A2 (dashed line) in Fig. 2 correspond to the dependence of the Grüneisen coefficient on the volume of aluminum and lead proposed in the present paper, while curves B1 (squares) and B2 (triangles) correspond to similar dependencies given in [23]. The same curves for nickel (C1 (dash-dotted line) and D1 (triangles)) and for copper (C2 (dashed line) and D2 (squares)) are shown in Fig. 3.

The values of the parameter αa were chosen so that the values of Γ_0 coincide with the values presented in [23].

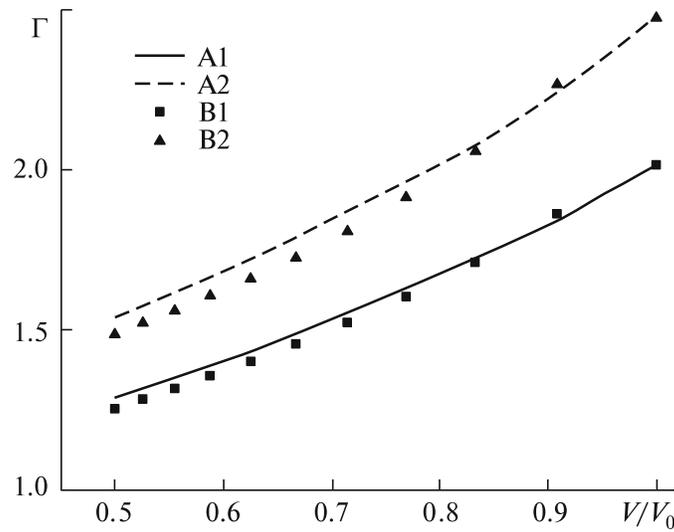


Fig. 2.

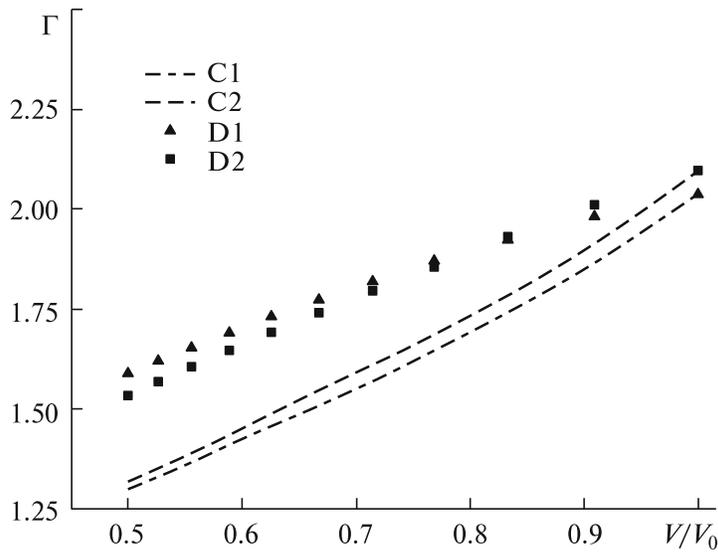


Fig. 3.

For aluminum and lead, the coincidence is rather good; the error does not exceed 4%. For nickel and copper, there are rather significant distinctions; the error does not exceed 18%.

7. SERIES EXPANSION. THE SECOND APPROXIMATION

An analysis of formula (4.4) shows that its denominator is zero for some value of the volume, and this means that the Grüneisen function has a singularity. This result was obtained in [17] for a one-dimensional model in which the singular point corresponds to the case of critical extension of the lattice. In [17], it was shown that by preserving the fourth-order terms in the expansions of the thermal pressure and the thermal energy one can obtain a new equation of state without any singularities. By using formula (4.4), one can show that in the two- and three-dimensional cases the strain at which the Grüneisen coefficient becomes infinite is somewhat greater than the critical strain; i.e., such a strain cannot be realized in practice. However, for large tensile strains and especially for near-critical strains, the Grüneisen equation can give a large error, and hence it is necessary to study the influence of the fourth-order terms in the expansions of the thermal pressure and the thermal energy.

Consider the tensors $\langle \tilde{A}_\alpha \tilde{A}_\alpha \rangle$, $\langle \tilde{A}_\alpha \tilde{A}_\alpha \tilde{A}_\alpha \rangle$, and $\langle \tilde{A}_\alpha \tilde{A}_\alpha \tilde{A}_\alpha \tilde{A}_\alpha \rangle$. By definition, they have the property

of absolute symmetry, i.e., are invariant under any permutation of the vectors occurring in them. We assume that these tensors are isotropic, because the thermal motion is chaotic. Then $\langle \tilde{\mathbf{A}}_\alpha \tilde{\mathbf{A}}_\alpha \tilde{\mathbf{A}}_\alpha \rangle \equiv 0$, just as for any isotropic absolutely symmetric tensor of odd rank [19]. By expanding the expressions for the tensors of thermal stress (2.1) and thermal energy (2.12), (3.1) into series and by preserving the fourth-order terms, we obtain

$$\tau_T = \tau_1 + \tau_2, \quad E_T = E_1 + E_2, \quad (7.1)$$

$$\begin{aligned} \tau_2 = & -\frac{1}{12V} \sum_{\alpha} (3\Phi''_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{E} \mathbf{E} + 12\Phi''_{\alpha} \mathbf{A}_{\alpha} \mathbf{E} \mathbf{A}_{\alpha} \mathbf{E} + 12\Phi'''_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{E} \\ & + 8\Phi'''_{\alpha} \mathbf{A}_{\alpha} \mathbf{E} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} + 4\Phi''''_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha}) \cdots \langle \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \rangle, \end{aligned} \quad (7.2)$$

$$E_2 = -\frac{3}{8} \sum_{\alpha} \left(\Phi'_{\alpha} \mathbf{E} \mathbf{E} + 4\Phi''_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{E} + \frac{4}{3} \Phi'''_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \mathbf{A}_{\alpha} \right) \cdots \langle \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \rangle, \quad (7.3)$$

$$\Phi_{\alpha}^{(n)} = \Phi^{(n)}(A_{\alpha}^2).$$

Here τ_1 and E_1 are determined by the first approximation formulas (3.7). Every isotropic absolutely symmetric tensor of rank four can be represented in the form [19]

$$\langle \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \tilde{\mathbf{A}}_{\alpha} \rangle = \frac{\lambda \kappa^4}{d(d+2)} (\mathbf{E} \mathbf{E} + \mathbf{e}_k \mathbf{E} \mathbf{e}_k + \mathbf{e}_k \mathbf{e}_n \mathbf{e}_k \mathbf{e}_n), \quad \lambda \kappa^4 = \langle \tilde{\mathbf{A}}_{\alpha}^4 \rangle, \quad (7.4)$$

where the \mathbf{e}_k are the unit vectors of some Cartesian basis, the summation is performed over the repeated indices k and n from 1 to d , κ^2 is determined by formula (3.9), and λ is a dimensionless coefficient. By using (7.4), we reduce Eqs. (7.2) and (7.3) to the form

$$\tau_2 = -\frac{\lambda \kappa^4}{4d(d+2)V} \sum_{\alpha} [(d+2)(d+4)\Phi''_{\alpha} + 4(d+4)\Phi'''_{\alpha} A_{\alpha}^2 + 4\Phi''''_{\alpha} A_{\alpha}^4] \mathbf{A}_{\alpha} \mathbf{A}_{\alpha}, \quad (7.5)$$

$$E_2 = -\frac{3\lambda \kappa^4}{8} \sum_{\alpha} \left[\Phi'_{\alpha} + \frac{4}{d} \Phi''_{\alpha} A_{\alpha}^2 + \frac{4}{d(d+2)} \Phi'''_{\alpha} A_{\alpha}^4 \right]. \quad (7.6)$$

As a result, relations (7.1) with the use of formulas (3.10) for τ_1 and E_1 and formulas (7.5) and (7.6) for τ_2 and E_2 lead to the system of equations

$$p_T = f_1 \kappa^2 + f_2 \lambda \kappa^4, \quad E_T = f_3 \kappa^2 + f_4 \lambda \kappa^4, \quad (7.7)$$

where the functions f_i can be obtained from relations (3.10), (7.5), and (7.6):

$$f_1 = \frac{1}{2d^2V} \sum_{\alpha} [(d+2)\Phi'_{\alpha} A_{\alpha}^2 + 2\Phi''_{\alpha} A_{\alpha}^4],$$

$$f_2 = \frac{1}{4d^2(d+2)V} \sum_{\alpha} [(d+2)(d+4)\Phi''_{\alpha} A_{\alpha}^2 + 4(d+4)\Phi'''_{\alpha} A_{\alpha}^4 + 4\Phi''''_{\alpha} A_{\alpha}^6],$$

$$f_3 = -\frac{1}{2d} \sum_{\alpha} (d\Phi_{\alpha} + 3\Phi'_{\alpha} A_{\alpha}^2),$$

$$f_4 = -\frac{3}{8} \sum_{\alpha} \left[\Phi'_{\alpha} + \frac{4}{d} \Phi''_{\alpha} A_{\alpha}^2 + \frac{4}{d(d+2)} \Phi'''_{\alpha} A_{\alpha}^4 \right].$$

Following the argument in the one-dimensional case [18, 19], we assume that the parameter λ can be approximately treated as a constant. This is confirmed by computations by the method of molecular dynamics, where it was shown that λ is practically independent of the thermal energy and volume. For the Lennard–Jones potential and $d = 3$, numerical computations give $\lambda \approx 1.7$. Now, by eliminating the variable κ from system (7.7), we obtain the following equation of state:

$$p_T = \frac{1}{2\lambda f_4^2} (f_2 f_3 - f_1 f_4) \left(f_3 - \sqrt{f_3^2 + 4\lambda f_4 E_T} \right) + \frac{f_2}{f_4} E_T. \quad (7.8)$$

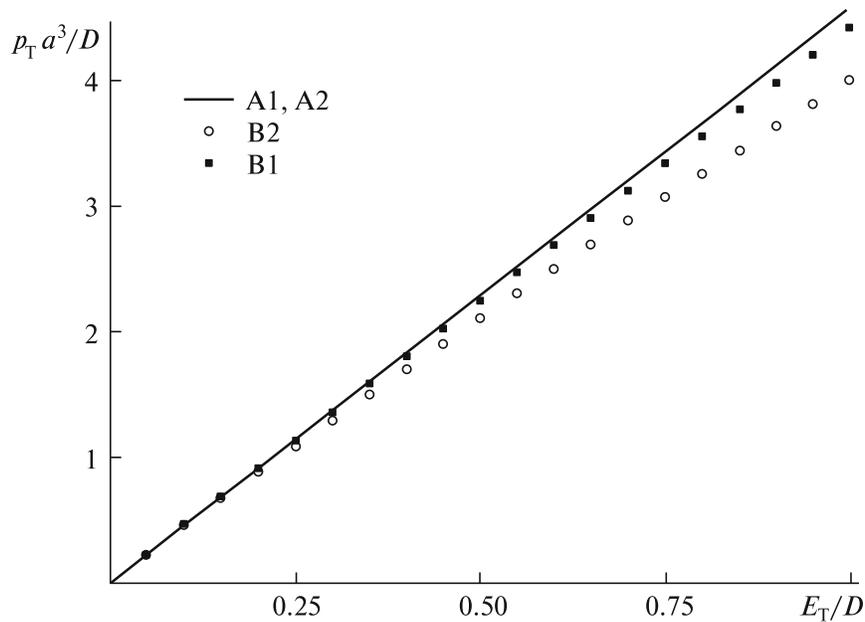


Fig. 4.

This equation is qualitatively different from the Mie–Grüneisen equation, where the linear dependence on the thermal energy is assumed.

By setting $\lambda = 1.7$, we construct the dependence $p_T(E_T)$ for the Lennard–Jones potential for various values of the bulk strain. Curves A1 and A2 (solid line) in Fig. 4 correspond to the Mie–Grüneisen equation of state for $V/V_0 = 0.9$ and $V/V_0 = 1.1$; curves B1 (squares) and B2 (circles) correspond to the specified equation of state (7.8) for $V/V_0 = 0.9$ and $V/V_0 = 1.1$. By Eq. (4.1), the Grüneisen function characterizes the slope of the dependence $p_T(E_T)$. Figure 4 shows that the function $p_T(E_T)$ is practically linear, and hence the Grüneisen coefficient in the proposed mode weakly depends on the thermal energy. The maximal error of the Mie–Grüneisen equation in the thermal energy range under study is approximately 10%.

8. DEPENDENCE OF THE GRÜNEISEN COEFFICIENT ON THE STRAIN STATE

Earlier, it was noted that the Grüneisen coefficient must generally depend on the total strain tensor rather than on its spherical part (the volume variation). Let us estimate the influence of the shear strain on the Grüneisen coefficient.

Consider the case of small strains. We expand Eq. (4.2) in a series in the small parameter $(2/a^2)\mathbf{a}_\alpha\mathbf{a}_\alpha \cdot \varepsilon$, where ε is the small strain tensor. In this case, we have the representation [19]

$$A_\alpha^2 = a_\alpha^2 + 2\mathbf{a}_\alpha\mathbf{a}_\alpha \cdot \varepsilon.$$

By expanding Eq. (4.2) in a series and by preserving the terms up to the second order of magnitude, we obtain

$$\Gamma(\varepsilon) = \Gamma(0) \left(1 + \eta_1 \sum_\alpha \mathbf{a}_\alpha\mathbf{a}_\alpha \cdot \varepsilon + \frac{1}{2} \eta_2 \sum_\alpha \mathbf{a}_\alpha\mathbf{a}_\alpha\mathbf{a}_\alpha\mathbf{a}_\alpha \cdots \varepsilon\varepsilon \right), \tag{8.1}$$

where the coefficients η_1 and η_2 are determined by the parameters of the interaction potential. For the most widely used simple lattices, the tensor $\mathbf{a}_\alpha\mathbf{a}_\alpha$ is spherical, and hence in the first approximation the Grüneisen coefficient determined by formula (8.1) depends only on the bulk strain. However, the second approximation already depends on the shape change strain. For simplicity, we illustrate this fact by a two-dimensional triangular lattice in the case of nearest neighbor interaction. In this case, the tensors contained in (8.1) are isotropic and have the form [19]

$$\sum_\alpha \mathbf{a}_\alpha\mathbf{a}_\alpha = 3a^2\mathbf{E}, \quad \sum_\alpha \mathbf{a}_\alpha\mathbf{a}_\alpha\mathbf{a}_\alpha\mathbf{a}_\alpha = \frac{3}{4}a^4(\mathbf{E}\mathbf{E} + \mathbf{e}_k\mathbf{E}\mathbf{e}_k + \mathbf{e}_k\mathbf{e}_n\mathbf{e}_k\mathbf{e}_n), \tag{8.2}$$

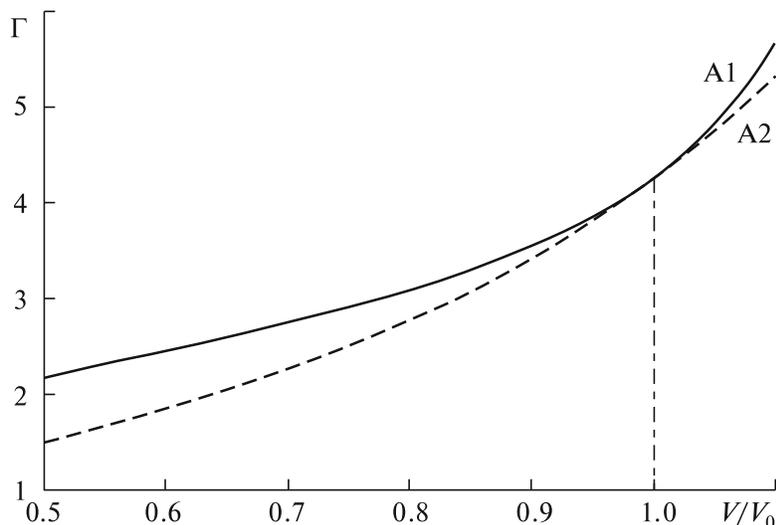


Fig. 5.

where $a = |\mathbf{a}_\alpha|$ and \mathbf{e}_k are the unit vectors of some Cartesian basis and the summation is performed over repeated Latin indices from 1 to 2. By substituting (8.1) into (8.2), we obtain

$$\Gamma(\varepsilon) = \Gamma(0)\left(1 + 3\eta_1 a \operatorname{tr} \varepsilon + \frac{3}{4}\eta_2 a^4 \operatorname{tr}^2 \varepsilon + \frac{3}{4}\eta_2 a^4 \operatorname{dev} \varepsilon \cdot \operatorname{dev} \varepsilon\right).$$

Here $\operatorname{tr} \varepsilon$ and $\operatorname{dev} \varepsilon$ are the strain tensor trace and deviator, respectively. In the first approximation, the trace describes the volume variation $\operatorname{tr} \varepsilon \approx V/V_0 - 1$, and the deviator characterizes the shape change under constant volume (shear strains). Therefore, the deviation from the bulk strain affects the value of the Grüneisen coefficient. We use an example to show that, in the case of large strains, these deviations can significantly change the Grüneisen coefficient.

Consider a two-dimensional crystal with a triangular lattice under a uniaxial strain along one of its crystallographic axes. Such a strain state is implemented, for example, in slabbing fracture problems. Denoting the relative strain by δ , we readily obtain the following expression for \mathbf{A}_α :

$$\mathbf{A}_1 = \mathbf{A}_{-1} = a\delta, \quad \mathbf{A}_2 = \mathbf{A}_{-2} = \mathbf{A}_3 = \mathbf{A}_{-3} = a\sqrt{3 + \frac{1}{2}(1 - \delta)^2}.$$

The graphs of $\Gamma(V)$ for two different strain modes, the bulk and uniaxial strains, is presented in Fig. 5 (curves A1 (solid line) and A2 (dashed line), respectively). These graphs show that for large strains the Grüneisen coefficient significantly depends on the strain mode. This fact must be taken into account in experiments.

9. CONCLUSION

In this paper, we generalize the approach to determining equations of state suggested in [17, 18]. We show that this approach permits obtaining not only equations in the Mie–Grüneisen form, but also more precise equations that are nonlinear in the thermal energy and take into account shear strains. In the first approximation, we obtain the Mie–Grüneisen equation and determine the dependence of the Grüneisen function on the volume. In the case where only the nearest neighbors are taken into account, the obtained results agree with the free volume theory [8]. We show that for large strains the Grüneisen function significantly depends on the form of the deformed state. One should take into account this fact in experiments. The following qualitative distinction from the one-dimensional case was discovered: the singular point of the Grüneisen function is displaced into the region of unrealizable strains. Therefore, in the two- and three-dimensional cases, the Mie–Grüneisen equation (4.1) need not be modified. In the thermal energy range under study, the maximum error in Eq. (4.1) is approximately 10%, which is quite admissible in a majority of applications. But it should be noted that, for large degrees of matter compression at which the Mie–Grüneisen equation is used as a rule, the thermal energy can vary in much wider ranges than those considered in the present paper. Therefore, the error in the Mie–Grüneisen equation can be significantly larger. This problem requires more detailed study and is beyond the framework of this paper.

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REFERENCES

1. V. A. Palmov, *Vibrations of Elasto-Plastic Bodies* (Nauka, Moscow, 1976; Springer, Berlin, 1998).
2. P. A. Zhilin, "Mathematical Theory of Inelastic Bodies," *Uspekhi Mekh.* **2** (4), 3–36 (2003).
3. S. B. Segletes, "Thermodynamic Stability of the Mie–Grüneisen Equation of State and Its Relevance to Hydrocode Computations," *J. Appl. Phys.* **70** (5), 2489–2499 (1991).
4. V. N. Zharkov and V. A. Kalinin, *Equations of State for Solids at High Pressures and Temperatures* (Nauka, Moscow, 1968; Consultants Bureau, New York, 1971).
5. A. I. Melker and A. V. Ivanov, "Dilatons of Two Types," *Fiz. Tverd. Tela* **28** (11), 3396–3402 (1986) [*Sov. Phys. Solid State (Engl. Transl.)* **28** (11), 1912–1914 (1986)].
6. J. C. Salter, *Introduction to Chemical Physics* (McGraw Hill, New York, 1939).
7. J. S. Dugdale and D. K. C. MacDonald, "The Thermal Expansion of Solids," *Phys. Rev.* **89** (4), 832–834 (1953).
8. V. Ya. Vashchenko and V. N. Zubarev, "Concerning the Grüneisen constant," *Fiz. Tverd. Tela* **5** (3), 886–890 (1963) [*Sov. Phys. Solid State (Engl. Transl.)* **5** (3), 653–655 (1963)].
9. I. S. Grigoriev and E. Z. Melikhov (Editors), *Handbook of Physical Quantities* (Energoatomizdat, Moscow, 1991; CRC Press, Boca Raton, 1997).
10. S. B. Segletes, "A Frequency-Based Equation of State for Metals," *Int. J. Impact Engng* **21** (9), 747–760 (1998).
11. L. V. Altshuller, "Use of Shock Waves in High-Pressure Physics," *Uspekhi Fiz. Nauk* **85** (2), 197–258 (1965) [*Sov. Phys. Uspekhi (Engl. Transl.)* **8** (1), 52–91 (1965)].
12. E. I. Kraus, "Small-Parameter Equation of State of a Solid," *Vestnik NGU. Ser. Fizika* **2** (2), 65–73 (2007).
13. R. V. Goldstein and A. V. Chentsov, "Discrete–Continuum Model of a Nanotube," *Izv. Akad. Nauk. Mekh. Tverd. Tela*, No. 4, 57–74 (2005) [*Mech. Solids (Engl. Transl.)* **40** (4), 45–59 (2005)].
14. O. S. Loboda and A. M. Krivtsov, "The Influence of the Scale Factor on the Elastic Moduli of a 3D Nanocrystal," *Izv. Akad. Nauk. Mekh. Tverd. Tela*, No. 4, 27–41 (2005) [*Mech. Solids (Engl. Transl.)* **40** (4), 20–32 (2005)].
15. I. E. Berinskii, E. A. Ivanova, A. M. Krivtsov, and N. F. Morozov, "Application of Moment Interaction to the Construction of a Stable Model of Graphite Crystal Lattice," *Izv. Akad. Nauk. Mekh. Tverd. Tela*, No. 5, 6–16 (2007) [*Mech. Solids (Engl. Transl.)* **42** (5), 663–671 (2007)].
16. E. A. Ivanova, A. M. Krivtsov, and N. F. Morozov, "Derivation of Macroscopic Relations of the Elasticity of Complex Crystal Lattices Taking into Account the Moment Interactions at the Microlevel," *Prikl. Mat. Mekh.* **71** (4), 595–615 (2007) [*J. Appl. Math. Mech. (Engl. Transl.)* **71** (4), 543–561 (2007)].
17. A. M. Krivtsov, "Thermoelasticity of One-Dimensional Chain of Interacting Particles," *Izv. Vyssh. Uchebn. Zaved. Sev.-Kavkaz. Region. Estestv. Nauki*, Special Issue. Nonlinear Problems of Continuum Mechanics, 231–243 (2003).
18. A. M. Krivtsov, "From Nonlinear Oscillations to Equation of State in Simple Discrete Systems," *Chaos, Solitons, and Fractals* **17** (1), 79–87 (2003).
19. A. M. Krivtsov, *Deformation and Failure of Solids with Microstructure* (Fizmatlit, Moscow, 2007) [in Russian].
20. M. Born and H. Kun, *Dynamical Theory of Crystal Lattices* (Clarendon Press, Oxford, 1954; Izd-vo Inostr. Liter., Moscow, 1958).
21. M. Zhou, "A New Look at the Atomic Level Virial Stress: On Continuum-Molecular System Equivalence," *Proc. Roy. Soc. London. Ser. A* **459** (2037), 2347–2392 (2003).
22. V. Ph. Zhuravlev, *Foundations of Theoretical Mechanics* (Fizmatlit, Moscow, 2008) [in Russian].
23. B. L. Glushak, V. F. Kuropatenko, and S. A. Novikov, *Studies of Material Strength under Dynamical Loads* (Nauka, Novosibirsk, 1992) [in Russian].
24. A. I. Lurie, *Nonlinear Theory of Elasticity* (Nauka, Moscow, 1980) [in Russian].