Shear modulus of an elastic solid under external pressure as a function of temperature: The case of helium

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(Received 23 January 2012; published 7 February 2012)

The energy of a dislocation loop in a continuum elastic solid under pressure is considered within the framework of classical mechanics. For a circular loop, this is a function with a maximum at pressures that are well within reach of experimental conditions for solid helium, suggesting, in this case, that dislocation loops can be generated by a pressure-assisted thermally activated process. It is also pointed out that pinned dislocation segments can alter the shear response of solid helium by an amount consistent with current measurements, without any unpinning.

DOI: 10.1103/PhysRevB.85.064103 PACS number(s): 67.80.—s, 46.40.—f

I. INTRODUCTION

Dislocations in a solid, when present in sufficient number, change its elastic properties.1 This classic subject has been recently revisited2,3 with the aim of using acoustics as a nonintrusive probe of plasticity in metals.4 In the early days of dislocation theory, there was an interest in the pressure-assisted thermal generation of dislocation loops.5 Interest in this topic decayed because the needed pressures would be much too big for the usual engineering materials. Solid helium, however, is an extreme example and offers the possibility of laboratory measurements to test these ideas, since in this case experimental pressures are a significant fraction of the shear modulus and, as we point out below, have measurable effects in the experimental temperature range. Indeed, recent experimental results on the mechanical properties of solid helium have brought the influence of dislocations to the fore.

At temperatures on the order of 100 mK, torsional oscillator experiments suggest that solid helium may display superfluid properties,6–12 which was theoretically predicted more than 40 years ago.13–15 The mechanical properties of solid helium in that regime have also been probed: “almost static” strain stress,16 as well as acoustic17,18 and de rotation19 measurements, have shown that the shear modulus of solid helium presents an anomaly at low temperatures. Indeed, starting at about 70 mK, as the temperature increases, the shear modulus abruptly decreases to a constant value that is 4% to 10% smaller, at a temperature on the order of 200 mK. It has been suggested20,21 that the presence of dislocations may be responsible for this behavior. In this paper, we point out additional properties of dislocations, within a classical mechanics framework, that provide further insight into the observed shear modulus anomalies. One of them stems from the fact that solid helium exists only under pressure, at a level that is at least on the order of 15% of its shear modulus, and can go considerably over that value. The other is that even when strongly pinned, a dislocation network will alter the shear response of a solid.

An important aspect of the debate concerning the role of dislocations is to understand to what extent some of the available data can be understood on purely classical grounds. Although helium is a quantum solid, from a mechanical point of view the quantum character can be manifested computing a dimensionless analog of the de Boer parameter, in which the interaction energy is estimated through the shear modulus,

\[ \Lambda_\mu = \frac{\hbar^2}{m_{\text{He}} a^4 \mu}, \]

where \( \hbar \) is Planck’s constant, \( a \) is a typical microscopic length, say the lattice constant, \( m_{\text{He}} \) is the atomic mass, and \( \mu \) is the shear modulus at standard conditions.20 This gives \( \Lambda_\mu \approx 1.6 \times 10^{-2} \) for \(^4\text{He}\), to be compared with 3 × 10\(^{-3}\) for solid hydrogen, 3 × 10\(^{-5}\) for neon, and 3.5 × 10\(^{-7}\) for copper. The smallness of \( \Lambda_\mu \) indicates that a classical treatment of the mechanical properties of solid helium is a reasonable first approximation. In addition, continuum mechanics will be used because deformations occur at length scales of a few centimeters (see below).

II. SCATTERING OF ELASTIC WAVES BY DISLOCATION SEGMENTS

Maurel et al.,2 using multiple-scattering theory, have generalized the Granato-Lücke theory21 to study the coherent propagation of waves in an elastic medium that is filled with dislocation segments, pinned at their ends, and with random locations, orientations, equilibrium lengths, and Burgers vectors. These (vector) dislocation segments oscillate like strings when forced by an elastic wave (Fig. 1).

Consider a dislocation segment \( \vec{X}(s,t) \) of length \( L \) at equilibrium, moving at low velocities (i.e., small compared with the speeds of elastic waves), with pinned ends, in an isotropic, homogeneous, elastic continuum of density \( \rho \), (bare) Lamé parameters \( \lambda \) and \( \mu \), and corresponding longitudinal and transverse wave velocities

\[ c_L = \sqrt{(\lambda + 2\mu)/\rho} \quad \text{and} \quad c_T = \sqrt{\mu/\rho}. \]

Low accelerations are also assumed, so that the back reaction of the radiation on the dislocation dynamics can be neglected. Following Ref. 22 and under these hypotheses, the equation of motion of an edge dislocation takes the form of the equation of motion for a string endowed with mass and line tension, forced by the usual Peach-Koehler force23,24

\[ m \ddot{X}_L(s,t) - B \dot{X}_L(s,t) - \Gamma \dot{X}_T(s,t) = F_k, \quad (1) \]
and the associated boundary conditions at pinned ends, $X_i(\pm L/2, t) = 0$ (see Fig. 1). In Eq. (1),
\[ m = \frac{\rho b^2}{4\pi} (1 + \gamma^{-1}) \ln(\Lambda/\Lambda_0) \sim \rho b^2 \]
defines a mass per unit length (with $\Lambda, \Lambda_0$ the long- and short-distance cutoff lengths, respectively) in which
\[ \Gamma = \frac{\rho b^2}{2\pi} (1 - \gamma^{-1}) c_T \ln(\Lambda/\Lambda_0) \sim \mu b^2 \]
is the line tension, and
\[ \gamma = c_L/c_T = (2(1 - \nu)/(1 - 2\nu))^{1/2}, \]
with $\nu$ as the Poisson’s ratio, and $b = |\vec{b}|$ where $\vec{b}$ is the Burgers vector. $B$ is the viscous drag coefficient, and
\[ F_k = \epsilon_{ijk} l_n b_i \sigma_{ij} \]
is the Peach-Koehler force, where $l_n$ is the unit tangent along the dislocation segment ($\epsilon_{ijk}$ denotes the usual completely antisymmetric tensor). A similar expression is valid for screw dislocations.

In the following, the mass term will be ignored, since only overdamped dislocation motion will be considered, which is an approximation valid for frequencies $\omega$ that are small compared to the lowest resonant frequency of the dislocation segment,
\[ \omega \ll \omega_1 \equiv (\Gamma/m)^{1/2} \pi/L, \]
where $\omega_1/(2\pi)$ is of the order of GHz for helium. Equivalently, this is valid for wavelengths $\lambda$ that are very large compared to the dislocation distance between the pinning points: $\lambda \gg L$.

**III. EFFECTIVE ELASTIC CONSTANTS**

In the case where many of these dislocations are present, with probability $p(L)dL$ of having a length between $L$ and $L + dL$, Maurel et al.\(^2\) used multiple-scattering theory to compute an effective, complex index of refraction whose real part gives a renormalized velocity of propagation for both longitudinal and transverse waves, and whose imaginary part provides an attenuation, also for both longitudinal and transverse waves.

This is done in the following way: An homogeneous, isotropic, elastic medium is described by $u_i(\vec{x}, t)$, with the displacement of a particle at time $t$ from its equilibrium position $\vec{x}$, whose time derivative $v_i \equiv \partial u_i/\partial t$ obeys, in the presence of many dislocation segments, the inhomogeneous wave equation
\[ \frac{\rho}{\partial t^2} - c_{ijkl} \frac{\partial^2 v_k}{\partial x_j \partial x_l} = S_i(\vec{x}, t), \quad (5) \]
where
\[ c_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \]
and the source term is given by
\[ S_i(\vec{x}, t) = c_{ijkl} \epsilon_{mnk} \sum K \int d\bar{x}^K \sum n K(x^K, t) n K b^n l \frac{\partial}{\partial x_j} \delta(\vec{x} - \vec{x}^K). \]

Here, $K$ labels the dislocation segments, $\mathcal{L}_K$. Each segment has an arbitrary equilibrium position $\vec{x}_0^K$, length $L^K$, orientation $t_K$ and Burgers vector $b^n_K$.

Equation (1) can be solved, for a given external stress, in terms of the normal modes of the pinned dislocation segment and the external forcing $F_k$. The expression of the stress in the Peach-Koehler force (4) in terms of the particle displacement $u_i$ and the substitution of the solution into Eqs. (5) and (6) leads to
\[ \frac{\rho}{\partial t^2} - c_{ijkl} \frac{\partial^2 v_k}{\partial x_j \partial x_l} = V_{ik} v_k, \quad (7) \]
where $V_{ik}$ is an operator (a “potential term”) acting on $v_k$ that carries the information about the interaction of the elastic wave with the ensemble of dislocation segments. Its exact form can be found in Eq. (2.11) of Maurel et al.\(^2\).

The next step is to look for coherent waves propagating in the medium described by (7). This is achieved, in multiple-scattering theory, by finding the poles of (G), where $G$ is the Green function (also known as the response function) of (7), and the brackets $\langle \rangle$ denote an ensemble average over all possible realizations of the dislocations. The function $G(\varepsilon)$ can be found in perturbation theory around $G_0$, the “bare” Green function, alias the response function for (7) when $V_{ik}$ is set equal to zero, which is known. In order to proceed, the probability of the values for the various dislocation parameters must be specified. Here we take dislocations uniformly distributed in space, with orientations also uniformly distributed within the solid angle. The geometry that is considered is shown in Fig. 2. We take edge dislocations, all with a Burgers vector of the same magnitude, so the Burgers vector is perpendicular to the dislocation, but with a uniform orientation. As already mentioned, the probability of having a length between $L$ and $L + dL$ is $p(L)dL$ with, as yet, arbitrary $p(L)$.

Finally, it is possible to find, to leading order in perturbation theory, the poles of (G). They provide a dispersion relation, that is, a relation between the frequency and wave number, from which it is possible to read an (“effective”) complex index of refraction. Its real part provides an effective (“renormalized”) speed of propagation for longitudinal and transverse waves.
waves, and its imaginary part provides an attenuation for the coherent waves.

With the above considerations, the effective speed of propagation comes out to be

$$c_T^{\text{eff}} = c_T \int \left[ 1 - \frac{\delta}{1 + (\omega t)^2} \right] p(L) dL,$$

where

$$\delta = \frac{4}{5\pi^4} \frac{\mu b^2}{\Gamma} n L^3 \sim nL^3,$$

is the relaxation time related to the parameters determining the dislocation dynamics. The attenuation of transverse wave comes out, being the imaginary part of a wave vector, in units of inverse distance, from which a quality factor can be extracted. It is

$$Q_T^{-1} = \int \frac{2\delta}{1 + (\omega t)^2} \left[ (\omega t) + \mathcal{O} \left( \frac{L}{x} \right)^3 \right] p(L) dL.$$

Similar expressions can be obtained for longitudinal waves. Expressions such as (9) and (12) have been considered by Beamish et al., with relaxation times corresponding to thermally activated relaxation processes with a log-normal distribution of excitation energies.

The reasoning above suggests that the shear modulus behavior studied by Beamish et al. could, at least in part, be attributed to the dynamical response of dislocation segments. But, where would the dislocations come from? They could be an artifact of preparation. On the other hand, as we show below, they could also be generated by a thermally activated process, with an activation energy that depends on the external pressure.

### IV. THERMAL ACTIVATION OF A SINGLE DISLOCATION LOOP

Consider a circular dislocation loop of radius $R$, core radius $r$ (Fig. 3) in the presence of an external pressure $\Delta P$ above the liquid-solid transition pressure $P_{LS} \approx 25$ bar. For $R \gg r$, the energy of the loop is

$$U(R,\theta) = V \sin^2 \theta + W \cos^2 \theta + \mathcal{C} \cos \theta,$$

where $\theta$ is the angle between the Burgers vector and the normal to the plane that contains the loop,

$$V(R) = \frac{\mu \alpha (2 - \nu) b^2 R}{4(1 - \nu)} \left[ \ln \left( \frac{R}{r} \right) + C_1 \right],$$

$$W(R) = \frac{\mu_0 b^2 R}{2(1 - \nu)} \left[ \ln \left( \frac{R}{r} \right) + C_2 \right],$$

$$\mathcal{C}(R) = \frac{\pi R^2 b}{\Delta P},$$

and $C_1$, $C_2$ are constants of order one; they provide the energy it takes to create a loop of minimal radius $R = \tau$. These parameters, $C_1$, $C_2$, and $\tau$, are in practice very empirical. Indeed, one estimates them as a fit of the asymptotic energy behavior for large dislocation loops. Moreover, they are related together because there is an extra freedom: one may take $\tau = b$ and fit some values for $C_1$ and $C_2$; similarly we can consider $\tau = \alpha b$ and fit the corresponding values for $C_1 = C_1 - \log \alpha$ and $C_2 = C_2 - \log \alpha$. In practice, we set $\tau = b$ and both constants, $C_1$ and $C_2$, are typically of the order of unity. We shall discuss later the dependence of our results in terms of the precise values of these “core” parameters. In the same vein, we shall use this formula even for small radii, respecting $R \gg \tau$. Note that we take as $\Delta P$ the excess pressure above the minimum value needed to have a solid.

As shown in Fig. 4, the energy surface has a global minimum on the circle $R = \tau$, and a saddle point on the axis $\theta = \pi (\Delta P > 0)$. The location of this saddle point provides an energy barrier to be overcome by a thermal activation process. Moreover, we shall see next that the curvature at the saddle provides the prefactor of the activation time.
The position \( R_s \) of the saddle is easily found as the point where the potential energy has a local maximum for \( \theta = \pi \):

\[
\frac{dU(R, \theta = \pi)}{dR} \bigg|_{R=R_s} = 0,
\]

and it is given by the solution of

\[
R_s = \frac{b\mu}{4\pi(1-v)\Delta P} \left( \ln \left( \frac{R_s}{\tau} \right) + C_2 + 1 \right). \tag{17}
\]

The corresponding energy is

\[
U(R_s, \pi) = \frac{\mu^2 b^3}{16\pi(1-v)^2\Delta P} \left( \ln \left( \frac{R_s}{\tau} \right) + C_2 \right)^2 - 1.
\]

When \( \Delta P = 0 \), the critical radius \( R_s \) diverges because the energy barrier for nucleation grows without limit. And, when \( \Delta P > 0 \), there is a significant change in the physics of dislocation generation, compared to the \( \Delta P = 0 \) case: at any temperature, there will now be a finite rate of dislocation loop generation given by an Arrhenius-like expression. A similar physics was considered by Langer and Fisher when studying loops in superfluid helium.26

The barrier height \( \Delta U \equiv U(R_s, \pi) - U(\tau, \pi) \) is given by

\[
\Delta U = U(R_s, \pi) - \frac{\mu b^3 \tau}{2(1-v)} C_2 - \pi \Delta P b \tau^2, \tag{18}
\]

and, at temperature \( T \), there will be a generation of dislocation loops at a rate \( f \) given by

\[
f = f_0 e^{-\Delta U/k_B T}, \tag{19}
\]

where \( f_0 \) is a microscopic frequency which we take to be of the order of \( c_T/b \approx 10^{12} \text{ s}^{-1} \).

Let us look at the conditions for the barrier to disappear, that is, when the saddle and the minimum collide, \( R_s = \tau \). In this case, from (17), the critical pressure is

\[
\Delta P = \mu \frac{C_2 + 1}{4\pi(1-v)\tau} b \approx 0.21 \mu.
\]

This is an excess external pressure of the order of 20% of the shear modulus. If one considers \( C_2 \approx 0 \), then one gets \( \Delta P \approx 0.1\mu \), while if taking \( C_2 = 5 \), then one has \( \Delta P \approx 0.6\mu \). Note that at this level, we do not consider the possible dependence of elastic constants and lattice parameters on external pressure.

For a barrier of finite height, the Arrhenius formula (19) provides a relation between \( \Delta P, T \) and the rate of dislocation loop generation:

\[
\frac{\Delta U}{k_B T} = \ln \left( \frac{f_0}{T} \right) \equiv L_f. \tag{20}
\]

Hence, because \( \Delta U \) depends explicitly on \( \Delta P \), it is possible to trace a \( P - T \) curve separating the regions of the large and small dislocation-loop-generation rate. This family of curves is plotted in Fig. 5(a). It gives the nucleation pressure as a remarkably flat function of temperature, at around 50 bar.

**V. DERIVATION OF EXIT TIME**

Next, we infer from the frequency rate for dislocation nucleation a drag coefficient that controls dislocation growth. From Eq. (13), dislocation loops with Burgers vector parallel to the normal to the dislocation loop (\( \theta = \pi \)) have an energy \( U(R) = W(R) - C(R) \).

We assume that due to thermal excitations, \( R \) will satisfy a Langevin-type equation,

\[
\ddot{B} \dot{R} = -\frac{\partial U}{\partial R} + \xi(t), \tag{21}
\]

with \( \xi(t) \) as a white \( \delta \)-correlated thermal noise

\[
\langle \xi(t)\xi(t') \rangle = 2\tilde{B}k_B T \delta(t-t')
\]

and \( \tilde{B} \) as a drag coefficient. Note that in the configuration considered, the defect is a prismatic dislocation loop whose radius will increase by climb, so this drag will differ qualitatively from the \( B \) coefficient that appears in Eq. (1), which describes glide conservative motion. Also, both coefficients have different units: \( B \sim \text{kg}(\text{m/s}) \) and \( \tilde{B} \sim \text{kg/s} \).

The Fokker-Planck equation for the probability distribution of size dislocation loops, \( \mathcal{P} \), associated to the Langevin equation (21) reads

\[
\ddot{B}\dot{\mathcal{P}} = \frac{\partial}{\partial R} \left[ \frac{\partial U(R)}{\partial R} \mathcal{P}(R) \right] + k_B T \frac{\partial^2 \mathcal{P}}{\partial R^2}.
\]

This equation determines the mean first-passage time \( \tau(R_1, R_0) \) of a dislocation loop that has initially a radius \( R_0 \), and finally a radius \( R_1 \). The corresponding equation for the exit time, which follows from the previous Fokker-Planck equation, is

\[
\ddot{B} \frac{d\mathcal{P}}{dR_0} = \frac{d\tau(R_1, R_0)}{dR_0} + k_B T \frac{d^2 \tau(R_1, R_0)}{dR_0^2} = 0. \tag{22}
\]

This equation is complemented with the reflecting boundary condition \( \frac{d\tau(R_1, R_0)}{dR_0} = 0 \) at \( R_0 = \tau \) and the absorbing boundary condition \( \tau(R_1' , R_1) = 0 \). Equation (22) has as its solution

\[
\tau(R_1, R_0) = \frac{\ddot{B}}{k_B T} \int_{R_0}^{R_1} dy \int_0^{\tau} dy' e^{-\frac{y}{k_B T}}. \tag{23}
\]
where it is understood that \( R_e \) depends on \( \Delta P \) through (17). The plot of \( \Phi \) as a function of \( \Delta P \) is given in Fig. 5(b).

One may estimate \( B \) taking \( f_0 \sim c_T/b = 10^{12} \text{s}^{-1} \) and \( \Phi \approx 60 \text{s}^2/\text{kg} \) [see Fig. 5(b)] to get

\[
\frac{B}{\tau} \sim \frac{1}{c_T \Phi} \approx 5 \times 10^{-5} \text{Pa s},
\]

which coincides with typical values for dislocation drag in ordinary metals at room temperature.\(^{28}\)

**VI. DISCUSSION**

We have shown that the low shear modulus of solid helium makes it possible to achieve pressure-driven thermally activated generation of dislocation loops at pressures that appear to be achievable in the laboratory. Their presence, according to the multiple-scattering theory of elastic waves by dislocations, can give rise to a change in shear modulus and to a quality factor of the type that has been considered by Beamish and collaborators,\(^{17}\) and by recent interpretation in terms of a complex rheology.\(^{29,30}\) Note that dislocations remain in place after an acoustic excitation is turned off. An Arrhenius formula for the rate of dislocation generation is in agreement with available data. However, the corresponding calculation has been carried out for an isolated dislocation loop that in the absence of interactions with impurities, grain boundaries, or other dislocations, will grow without limit. Therefore, the model cannot, by itself, account for the saturation of the medium with dislocations. Something, at some point, must stop the dislocation generation. How does this happen?

The presence of \(^{3}\)He impurities may prevent an unlimited increase of dislocation loops because as a dislocation touches an impurity, it is pinned, and thus the extension energy required becomes higher. A thermodynamical equilibrium state dominated by dislocation is then possible. Let us assume that the mean distance between pinning points, \( L \), is given by the mean distance between \(^{3}\)He impurities, or \( L \sim 10^2 \tau - 10^3 \tau \), depending on whether their concentration is 1 ppM or 1 ppb, respectively. If the dislocation segments covered all bonds associated with a simple cubic lattice of \(^{3}\)He atoms, then we would have \( nL^3 \sim 3 \).

According to (9) and (10), and the discussion in Ref. 17, there is a change in shear modulus as a function of temperature given by\(^{20}\)

\[
\frac{\Delta \mu}{\mu} \approx 0.02 nL^3,
\]

which under the previous assumption gives a change of about 6%, in agreement with current experimental results. Different geometrical arrangements could explain easily observed variations of this ratio. Notice that according to second-order elasticity theory,\(^{31}\) dislocations will cause volume expansion. At the estimated densities, this effect would yield a relative volume change in the range \(10^{-4} - 10^{-6} \), which is too small to modify significantly the pressure-assisted thermal generation.

Finally, the drag coefficient \( B \) can be estimated via the relaxation time \( t_R \) (11), which is, according to Beamish and coworkers,\(^{17}\) of the order of 9 ns. Thus,

\[
B = \pi^2 \Gamma t_R / L^2 \approx 10^{-4} - 10^{-6} \text{Pa s},
\]

In the low-temperature regime, the mean first-passage time is computed by the saddle-point approximation for \( R_1 > R_e \), and it is identified with the so-called exit time from the barrier. This asymptotic approximation can be obtained with little modification of the case in which the potential has a barrier. This asymptotic approximation can be obtained with the following approximation:

\[
\frac{1}{f} = \frac{\hat{B} \Phi}{U(\tau)} \sqrt{\frac{2\pi k_B T}{U(\infty)(R_e)}} \times e^{\Delta U / k_B T},
\]

Evaluating the derivatives of the potential \( U \) and substituting into Eq. (24), we get the prefactor to the Arrhenius law \( f_0 \) defined in Eq. (19),

\[
f_0^{-1} = \frac{\hat{B} \Phi}{b} \text{with}
\]

\[
\Phi = \frac{1}{b \sqrt{\frac{(1+c_T) \mu b - 2\pi \hat{b} \Delta P}{2\pi \hat{b} + \frac{(1+c_T) \mu b}{(1+c_T) \mu b - 2\pi \hat{b} \Delta P}}}}.
\]

**FIG. 5.** (Color online) (a) Plot of the most likely-unlikely critical pressure \( P \) for dislocation loop generation vs temperature, after (20). The inset plots the most likely-unlikely critical pressure as a function of \( \log(f_0/f) \). (b) The value of \( \Phi \), which is the function appearing in the prefactor of the Arrenhius’ law given by Eq. (24) as a function of pressure \( P \) for the values of temperature \( T = 50, 100, 200 \text{ mK} \). Both figures plot the actual imposed pressure \( P = P_{1.5} + \Delta P \) with \( P_{1.5} = 25 \text{ bar} \), for ease of visualization. The curves are computed using numerical values of Ref. 20.
depending on the value of \( L \). This is not very different from the "climb" drag estimated in (26), and is consistent with the smaller value for "glide" drag compared to "climb" drag that one would expect on classical grounds. No quantum modeling of dislocation drag appears to be available.

To conclude, we have shown that pinned dislocation segments can significantly alter the shear response of solid helium even without their unpinning, and that external pressure may generate thermally excited dislocation loops at a significant rate under experimentally realistic conditions. This suggests that it could be interesting to perform systematic measurements of the shear response of solid helium as a function of pressure.

**ACKNOWLEDGMENTS**

This work was supported by Fondecyt Grants No. 1110144 (F.B.), No. 1100289 (S.R.), and No. 1100198 (F.L. and N.M.). We also acknowledge Anillo Grants No. ACT 127 and No. ANR 38 (F.B., F.L., and N.M.).